An Introduction to Information Retrieval

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Brief Contents

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Symbol	Page	Meaning
γ	p. 92	γ code
γ	p. 174	Weight of negative documents in Rocchio relevance feedback
γ	p. 240	Classification or clustering function: $\gamma(d)$ is d's class or cluster
Γ	p. 240	Supervised learning method in Chapters 13 and 14: $\Gamma(D)$ is the classification function γ learned from training set D
$\mu(.)$	p. 273	Centroid of a class (in Rocchio classification) or a cluster (in K-means and centroid clustering)
$\Theta(\cdot)$	p. 10	A tight bound on the complexity of an algorithm
ω_k	p. 316	Cluster in clustering
Ω	p. 316	Clustering or set of clusters $\{\omega_1, \ldots, \omega_K\}$
$\arg\max_x f(x)$	p. 173	The value of x for which f reaches its maximum
$\arg\min_x f(x)$	p. 173	The value of x for which f reaches its minimum
c, c_j	p. 239	Class or category in classification
cf_i	p. 83	The collection frequency of term i (the total number of times the term appears in the document collection)
$\mathbb{C}$	p. 239	Set $\{c_1, \ldots, c_j, \ldots, c_J\}$ of all classes
C	p. 251	A random variable that takes as values members of $\mathbb{C}$
d	p. 4	Index of the d^{th} document in the collection D
d	p. 65	A document

$\vec{d}, \vec{q}$	p. 173	Document vector, query vector
$\lvert\vec{d}\rvert$		Length (or Euclidean norm) of $\vec{d}$
D	p. 240	Set $\{d_1, \ldots, d_n, \ldots, d_N\}$ of all documents (or document vectors); set $\{\langle d_1, c_1\rangle, \ldots, \langle d_n, c_n\rangle, \ldots, \langle d_N, c_N\rangle\}$ of all labeled documents in Chapters 13–15
df_t	p. 111	The document frequency of term i (the total number of documents in the collection the term appears in)
H	p. 93	Entropy
H	p. 94	Harmonic number
J	p. 239	Number of classes
k	p. 270	Top k items from a set, e.g., k nearest neighbors in kNN, top k retrieved documents, top k selected features from the vocabulary V
K	p. 314	Number of clusters
L_d	p. 220	Length of document d (in tokens)
L_{ave}	p. 95	Average length of a document (in tokens)
M	p. 5	Size of the vocabulary ($\lvert V\rvert$)
M_{ave}	p. 72	Average size of the vocabulary in a document in the collection
M_d	p. 225	Language model for document d
N	p. 4	Number of documents in the retrieval or training collection
N_j	p. 243	Number of documents in class c_j
$N(\omega)$	p. 277	Number of times the event ω occurred
n		Number of attributes in the representation of d: $\langle x_1, x_2, \ldots, x_n\rangle$
n		Number of postings
$O(\cdot)$	p. 10	A bound on the complexity of an algorithm
q	p. 53	A query
T	p. 41	Total number of tokens in the document collection
T_j		Number of tokens in documents in class c_j
T_{ij}	p. 243	Number of occurrences of word i in class c_j
t	p. 4	Index of the t^{th} term in the vocabulary V
t	p. 55	An indexing term
t	p. 195	A structural term (word + context in XML retrieval)

$\text{tf}_{t,d}$	p. 110	The term frequency of term t in document d (the total number of occurrences of t in d)
U_w	p. 249	Random variable taking values 0 (w is present) and 1 (w is not present)
V	p. 196	Vocabulary of terms $\{t_1, \ldots, t_i, \ldots, t_M\}$ in a collection (a.k.a. the lexicon)
$\vec{v}(d)$	p. 118	Length-normalized document vector
$\vec{V}(d)$	p. 117	Vector or document d, not length-normalized
w_i	p. 227	Word i of the vocabulary
w	p. 105	A weight, for example for zones or terms
$\|\vec{w}\|$	p. 130	Length of a vector
$\vec{w}^{\mathrm{T}}\vec{x} = b$	p. 276	Hyperplane; $\vec{w}$ is the normal vector of the hyperplane and w_i component i of $\vec{w}$
$\vec{x}$	p. 210	Term incidence vector $\vec{x} = (x_1, \ldots, x_i, \ldots, x_M)$; more generally: document feature representation
X	p. 249	Random variable taking values in V, the vocabulary (e.g., at a given position k in a document)
$\mathbb{X}$	p. 239	Document space in text classification
$\|\vec{x} - \vec{y}\|$	p. 125	Euclidean distance of $\vec{x}$ and $\vec{y}$

Preface

As recently as the 1990s, studies showed that most people preferred getting information from other people rather than information retrieval systems. Of course, in that time period, most people also interacted with human travel agents to book their travel. While academic discussion of this process is unfortunately scant, in the last decade, relentless optimization of formal measures of information retrieval effectiveness has driven web search engines to new quality levels where most people are satisfied most of the time, and web search has become a standard and often preferred source of information finding. For example, the 2004 Pew Internet Survey (Fallows 2004) found that "92% of Internet users say the Internet is a good place to go for getting everyday information." To the surprise of many, the field of information retrieval has moved from being a sleepy backwater to being most people's preferred means of information access.

Notation

Worked examples in the text appear with a little pencil sign next to them in the margins. Advanced, difficult, or esoteric material appears in sections or subsection indicated with an X mark in the margin. Exercises at the end of sections or a chapter indicate whether they are easy (⋆), medium (⋆⋆), or difficult (⋆⋆⋆).

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Parts of the initial drafts of Chapters 13–15 were based on slides that were generously provided by Ray Mooney. While the material has gone through extensive revisions, we gratefully acknowledge Ray's contribution to the three chapters in general and to the description of the time complexities of text classification algorithms in particular.

The above is unfortunately an incomplete list: we are still in the process of incorporating feedback we have received. And, like all opinionated authors, we did not always heed the advice that was so freely given. The published versions of the chapters remain solely the responsiblity of the authors.

1 *Information retrieval using the Boolean model*

INFORMATION RETRIEVAL

The meaning of the term *information retrieval* can be very broad. Just getting a credit card out of your wallet so that you can type in the card number is a form of information retrieval. However, as an academic field of study, *information retrieval* might be defined thus:

> Information retrieval (IR) is finding material (usually documents) of an unstructured nature (usually text) that satisfy an information need from within large collections (usually stored on computers).

As defined in this way, information retrieval used to be an activity that only a few people engaged in: reference librarians, paralegals, and similar professional searchers. Now the world has changed, and hundreds of millions of people engage in information retrieval every day when they use a web search engine or search their email.[1] Information retrieval is fast becoming the dominant form of information access, overtaking traditional database-style searching (the sort that is going on when a clerk says to you: "I'm sorry, I can only look up your order if you can give me your Order ID").

IR can also cover other kinds of data and information problems beyond that specified in the core definition above. The term "unstructured data" refers to data which does not have clear, semantically overt, easy-for-a-computer structure. It is the opposite of structured data, the canonical example of which is a relational database, of the sort companies usually use to maintain product inventories and personnel records. In reality, almost no data are truly "unstructured". This is definitely true of all text data if you count the latent linguistic structure of human languages. But even accepting that the intended notion of structure is overt structure, most text has structure, such as headings and paragraphs and footnotes, which is commonly represented in documents by explicit markup (such as the coding underlying web

1. In modern parlance, the word "search" has tended to replace "(information) retrieval"; the term "search" is quite ambiguous, but in context we use the two synonymously.

pages). IR is also used to facilitate "semistructured" search such as finding a document where the title contains Java and the body contains threading.

The field of information retrieval also covers supporting users in browsing or filtering document collections or further processing a set of retrieved documents. Given a set of documents, clustering is the task of coming up with a good grouping of the documents based on their contents. It is similar to arranging books on a bookshelf according to their topic. Given a set of topics, standing information needs, or other categories (such as suitability of texts for different age groups), classification is the task of deciding which class(es), if any, each of a set of documents belongs to. It is often approached by first manually classifying some documents and then hoping to be able to classify new documents automatically.

Information retrieval systems can also be distinguished by the scale at which they operate, and it is useful to distinguish three prominent scales. In *web search*, the system has to provide search over billions of documents stored on millions of computers. Distinctive issues are needing to gather documents for indexing, being able to build systems that work efficiently at this enormous scale, and handling particular aspects of the web, such as the exploitation of hypertext and not being fooled by site providers manipulating page content in an attempt to boost their search engine rankings, given the commercial importance of web. We focus on all these issues in Chapters 19–21. At the other extreme is *personal information retrieval*. In the last few years, consumer operating systems have integrated information retrieval (such as Apple's Mac OS X Spotlight or Windows Vista's Instant Search). Email programs usually not only provide search but also text classification: they at least provide a spam (junk mail) filter, and commonly also provide either manual or automatic means for classifying mail so that it can be placed directly into particular folders. Distinctive issues here include handling the broad range of document types on a typical personal computer, and making the search system maintenance free and sufficiently lightweight in terms of startup, processing, and disk space usage that it can run on one machine without annoying its owner. In between is the space of *enterprise, institutional, and domain-specific search*, where retrieval might be provided for collections such as a corporation's internal documents, a database of patents, or research articles on biochemistry. In this case, the documents will typically be stored on centralized file systems and one or a handful of dedicated machines will provide search over the collection. While this book contains techniques of value over this whole spectrum, we concentrate on this middle case, both because it is the scenario underlying the vast bulk of the 6 decades of academic research on information retrieval, and because, outside of half-a-dozen companies, it is the scenario that a software developer is most likely to encounter.

In this chapter we begin with a very simple example of an information retrieval problem, and introduce the idea of a term-document matrix (Section 1.1) and the central inverted index data structure (Section 1.2). We will then examine the Boolean retrieval model and how Boolean queries are processed (Sections 1.3 and 1.4).

1.1 An example information retrieval problem

A fat book which many people own is Shakespeare's Collected Works. Suppose you wanted to determine which plays of Shakespeare contain the words Brutus AND Caesar AND NOT Calpurnia. One way to do that is to start at the beginning and to read through all the text, noting for each play whether it contains Brutus and Caesar and excluding it from consideration if it contains Calpurnia. The simplest form of document retrieval is for a computer to do this sort of linear scan through documents. This process is commonly
GREP referred to as *grepping* through text, after the Unix command `grep`, which performs this process. Grepping through text can be a very effective process, especially given the speed of modern computers, and often allows useful possibilities for wildcard pattern matching through the use of regular expressions. With modern computers, for simple querying of modest collections (the size of Shakespeare's Collected Works is a bit under one million words of text in total), you really need nothing more.

But for many purposes, you do need more:

1. To process large document collections quickly. The amount of online data has grown at least as quickly as the speed of computers, and we would now like to be able to search collections that total in the order of billions to trillions of words.
2. To allow more flexible matching operations. For example, it is impractical to perform the query Romans NEAR countrymen with `grep`, where NEAR might be defined as "within 5 words" or "within the same sentence".
3. To allow ranked retrieval: in many cases you want the best answer to an information need among many documents that contain certain words.

INDEX The way to avoid linearly scanning the texts for each query is to *index* the documents in advance. Let us stick with Shakespeare's Collected Works, and use it to introduce the basics of the Boolean retrieval model. Suppose we record for each document – here a play of Shakespeare's – whether it contains each word out of all the words Shakespeare used (Shakespeare used
INCIDENCE MATRIX about 32,000 different words). The result is a binary term-document *incidence*
TERM *matrix*, as in Figure 1.1. *Terms* are the indexed units (further discussed in Section 2.2); they are usually words, and for the moment you can think of

	Anthony and Cleopatra	Julius Caesar	The Tempest	Hamlet	Othello	Macbeth	...
Anthony	1	1	0	0	0	1	
Brutus	1	1	0	1	0	0	
Caesar	1	1	0	1	1	1	
Calpurnia	0	1	0	0	0	0	
Cleopatra	1	0	0	0	0	0	
mercy	1	0	1	1	1	1	
worser	1	0	1	1	1	0	
...							

► **Figure 1.1** A term-document incidence matrix. Matrix element (t, d) is 1 if the play in column d contains the word in row t, and is 0 otherwise.

them as words, but the information retrieval literature normally speaks of terms because some of them, such as perhaps I-9 or Hong Kong are not usually thought of as words. Now, depending on whether we look at the matrix rows or columns, we can have a vector for each term, which shows the documents it appears in, or a vector for each document, showing the terms that occur in it.[2]

To answer the query Brutus AND Caesar AND NOT Calpurnia, we take the vectors for Brutus, Caesar and Calpurnia, complement the last, and then do a bitwise AND:

110100 AND 110111 AND 101111 = 100100

The answers for this query are thus *Anthony and Cleopatra* and *Hamlet* (Figure 1.2).

BOOLEAN RETRIEVAL MODEL

The *Boolean retrieval model* is a model for information retrieval in which we can pose any query which is in the form of a Boolean expression of terms, that is, in which terms are combined with the operators AND, OR, and NOT. Such queries effectively view each document as a set of words.

DOCUMENT

Let us now consider a more realistic scenario, simultaneously using the opportunity to introduce some terminology and notation. Suppose we have $N = 1$ million documents. By *documents* we mean whatever units we have decided to build a retrieval system over. They might be individual memos or chapters of a book (see Section 2.1.2 (page 20) for further discussion). We will refer to the group of documents over which we perform retrieval as the (document) *collection*. It is sometimes also referred to as a *corpus* (a *body* of texts). Suppose each document is about 1000 words long (2–3 book pages). If

COLLECTION
CORPUS

2. Formally, we take the transpose of the matrix to be able to get the terms as column vectors.

Antony and Cleopatra, Act III, Scene ii
Agrippa [Aside to Domitius Enobarbus]: Why, Enobarbus,
When Antony found Julius Caesar dead,
He cried almost to roaring; and he wept
When at Philippi he found Brutus slain.

Hamlet, Act III, Scene ii
Lord Polonius: I did enact Julius Caesar: I was killed i' the
Capitol; Brutus killed me.

► **Figure 1.2** Results from Shakespeare for the query Brutus AND Caesar AND NOT Calpurnia.

we assume an average of 6 bytes per word including spaces and punctuation, then this is a document collection about 6 GB in size. Typically, there might be about $M = 500{,}000$ distinct terms in these documents. There is nothing special about the numbers we have chosen, and they might vary by an order of magnitude or more, but they give us some idea of the dimensions of the kinds of problems we need to handle. We will discuss and model these size assumptions in Section 5.1 (page 80).

AD HOC RETRIEVAL

Our goal is to develop a system to address the *ad hoc retrieval* task. This is the most standard IR task. In it, a system aims to provide documents from within the collection that are relevant to an arbitrary user information need, communicated to the system by means of a one-off, user-initiated query. An

INFORMATION NEED

information need is the topic about which the user desires to know more, and

QUERY

is differentiated from a *query*, which is what the user conveys to the computer in an attempt to communicate the information need. A document is

RELEVANCE

relevant if it is one that the user perceives as containing information of value with respect to their personal information need. Our example above was rather artificial in that the information need was defined in terms of particular words, whereas usually a user is interested in a topic like "pipeline leaks" and would like to find relevant documents regardless of whether they precisely use those words or express the concept with other words such as pipeline rupture. To assess the effectiveness of an IR system, a user will usually want to know two key statistics about the system's returned results for a query:

PRECISION

Precision: What fraction of the returned results are relevant to the information need?

RECALL

Recall: What fraction of the relevant documents in the collection were returned by the system?

Detailed discussion of relevance and evaluation measures including precision and recall is found in Chapter 8.

We now cannot build a term-document matrix in a naive way. A 500K $\times$ 1M matrix has half-a-trillion 0's and 1's – too many to fit in a computer's memory. But the crucial observation is that the matrix is extremely sparse, that is, it has few non-zero entries. Because each document is 1000 words long, the matrix has no more than one billion 1's, so a minimum of 99.8% of the cells are zero. A much better representation is to record only the things that do occur, that is, the 1 positions.

INVERTED INDEX

This idea is central to the first major concept in information retrieval, the *inverted index*. The name is actually redundant: an index always maps back from terms to the parts of a document where they occur. Nevertheless, *inverted index*, or sometimes *inverted file*, has become the standard term in information retrieval.[3] The basic idea of an inverted index is shown in Figure 1.3.

DICTIONARY
VOCABULARY
LEXICON

We keep a *dictionary* of terms (sometimes also referred to as a *vocabulary* or *lexicon*; in this book, we use *dictionary* for the data structure and *vocabulary* for the set of terms). Then for each term, we have a list that records which documents the term occurs in. Each item in the list – which records that a term appeared in a document (and, later, often, the positions in the document) – is conventionally called a *posting*. The list is then called a *postings list* (or inverted list), and all the postings lists taken together are referred to as the *postings*. The dictionary in Figure 1.3 has been sorted alphabetically and each postings list is sorted by document ID. We will see why this is useful in Section 1.3, below, but later we will also consider alternatives to doing this (Section 7.1.5).

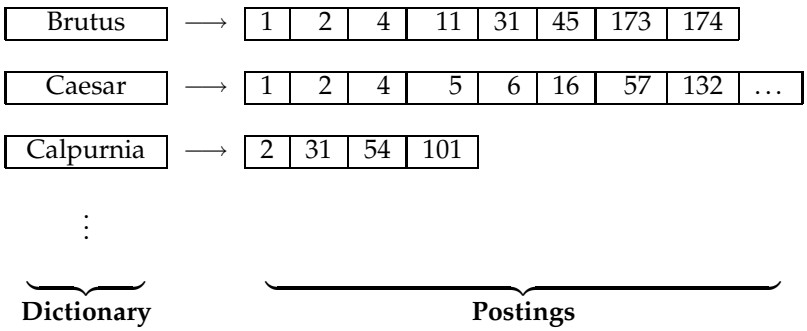
POSTING
POSTINGS LIST
POSTINGS

1.2 A first take at building an inverted index

To gain the speed benefits of indexing at retrieval time, we have to build the index in advance. The major steps in this are:

1. Collect the documents to be indexed:
   Friends, Romans, countrymen. | So let it be with Caesar | ...
2. Tokenize the text, turning each document into a list of tokens:
   Friends | Romans | countrymen | So | ...
3. Do linguistic preprocessing, producing a list of normalized tokens, which are the indexing terms: friend | roman | countryman | so | ...

3. Some information retrieval researchers prefer the term inverted file, but expressions like index construction and index compression are much more common than inverted file construction and inverted file compression. For consistency, we use (inverted) index throughout this book.



► **Figure 1.3** The two parts of an inverted index. The dictionary is commonly kept in memory, with pointers to each postings list, which is stored on disk.

4. Index the documents that each term occurs in by creating an inverted index, consisting of a dictionary and postings.

We will define and discuss the earlier stages of processing, that is, steps 1–3, in Section 2.2 (page 22), and until then you can think of *tokens* and *normalized tokens* as also loosely equivalent to *words*. Here, we assume that the first 3 steps have already been done, and we examine building a basic inverted index.

DOCID

Within a document collection, we assume that each document has a unique serial number, known as the document identifier (*docID*). During index construction, we can simply assign successive integers to each new document when it is first encountered. The input to indexing is a list of normalized tokens for each document, which we can equally think of as a list of pairs of term and docID, as in Figure 1.4. The core indexing step is *sorting* this list so that the terms are alphabetical, giving us the representation in the middle column of Figure 1.4. Multiple occurrences of the same term from the same document are then merged.[4] Instances of the same term are then grouped, and the result is split into a *dictionary* and *postings*, as shown in the right column of Figure 1.4. Since a term generally occurs in a number of documents, this data organization already reduces the storage requirements of the index. The dictionary also records some statistics, such as the number of documents which contain each term (the *document frequency*, which is here also the length of each postings list). This information is not vital for a basic Boolean search engine, but it allows us to improve the efficiency of the search engine at query time, and it is a statistic later used in many ranked retrieval models. The postings are secondarily sorted by docID. This provides the basis for efficient query processing. This inverted index structure is es-

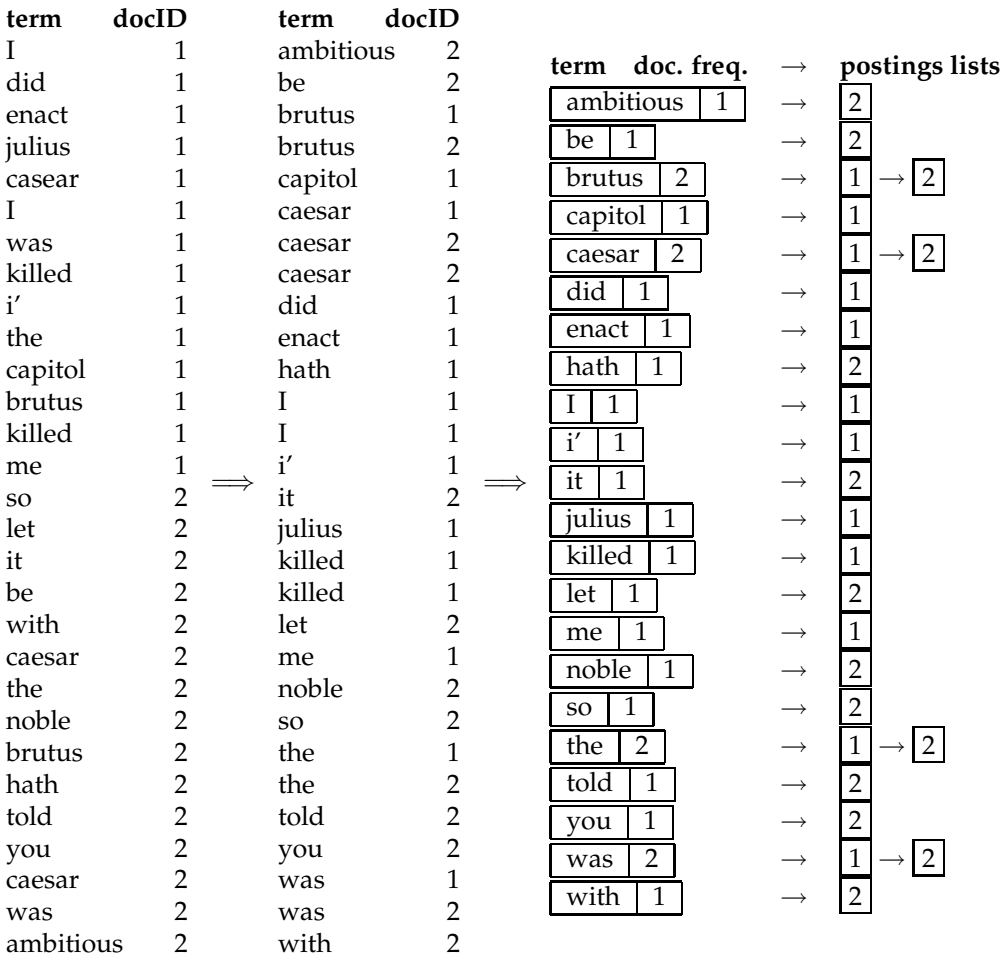
SORTING

DOCUMENT FREQUENCY

4. Unix users can note that these steps are similar to use of the `sort` and then `uniq` commands.

Doc 1
I did enact Julius Caesar: I was killed i' the Capitol; Brutus killed me.

Doc 2
So let it be with Caesar. The noble Brutus hath told you Caesar was ambitious:



► **Figure 1.4** Building an index by sorting and grouping. The sequence of terms in each document, tagged by their documentID (left) is sorted alphabetically (middle). Instances of the same term are then grouped by word and then by documentID. The terms and documentIDs are then separated out (right). The dictionary stores the terms, and has a pointer to the postings list for each term. It commonly also stores other summary information such as, here, the document frequency of each term. We use this information for improving query time efficiency and, later, for weighting in ranked retrieval models. Each postings list stores the list of documents in which a term occurs, and may store other information such as the term frequency (the frequency of each term in each document) or the position(s) of the term in each document.

sentially without rivals as the most efficient structure for supporting ad hoc text search.

In the resulting index, we pay for storage of both the dictionary and the postings lists. The latter are much larger, but the dictionary is commonly kept in memory, while postings lists are normally kept on disk, so the size of each is important, and in Chapter 5 we will examine how each can be optimized for storage and access efficiency. What data structure should be used for a postings list? A fixed length array would be wasteful as some words occur in many documents, and others in very few. For an in-memory postings list, two good alternatives are singly linked lists or variable length arrays. Singly linked lists allow cheap insertion of documents into postings lists (following updates, such as when recrawling the web for updated documents), and naturally extend to more advanced indexing strategies such as skip lists (Section 2.3.1), which require additional pointers. Variable length arrays win in space requirements by avoiding the overhead for pointers and in time requirements because their use of contiguous memory increases speed on modern processors with memory caches. Extra pointers can in practice be encoded into the lists as offsets. If updates are relatively infrequent, variable length arrays will be more compact and faster to traverse. We can also use a hybrid scheme with a linked list of fixed length arrays for each term. When postings lists are stored on disk, they are stored (perhaps compressed) as a contiguous run of postings without explicit pointers (as in Figure 1.3), so as to minimize the size of the postings list and the number of disk seeks to read a postings list into memory.

1.3 Processing Boolean queries

How do we process a query using an inverted index and the basic Boolean retrieval model? Consider processing the *simple conjunctive query*:

SIMPLE CONJUNCTIVE QUERIES

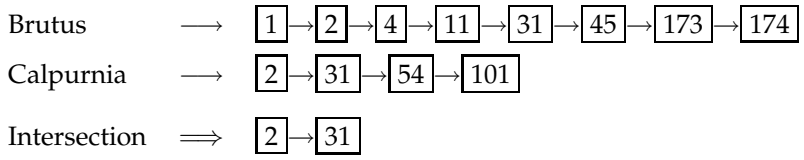
(1.1) Brutus AND Calpurnia

over the inverted index partially shown in Figure 1.3 (page 7). We:

1. Locate Brutus in the Dictionary
2. Retrieve its postings
3. Locate Calpurnia in the Dictionary
4. Retrieve its postings
5. Intersect the two postings lists, as shown in Figure 1.5.

POSTINGS LIST INTERSECTION

The *intersection* operation is the crucial one: we need to efficiently intersect



► **Figure 1.5** Intersecting the postings lists for Brutus and Calpurnia from Figure 1.3.

```
INTERSECT(p1, p2)
 1  answer ← ⟨ ⟩
 2  while p1 ≠ NIL and p2 ≠ NIL
 3  do if docID(p1) = docID(p2)
 4        then ADD(answer, docID(p1))
 5             p1 ← next(p1)
 6             p2 ← next(p2)
 7        else if docID(p1) < docID(p2)
 8                then p1 ← next(p1)
 9                else p2 ← next(p2)
10  return answer
```

► **Figure 1.6** Algorithm for the intersection of two postings lists p_1 and p_2.

POSTINGS MERGE

postings lists so as to be able to quickly find documents that contain both terms. (This operation is sometimes referred to as *merging* postings lists: this slightly counterintuitive name reflects using the term *merge algorithm* for a general family of algorithms that combine multiple sorted lists by interleaved advancing of pointers through each; here we are merging the lists with a logical AND operation.)

There is a simple and effective method of intersecting postings lists using the merge algorithm (see Figure 1.6): we maintain pointers into both lists and walk through the two postings lists simultaneously, in time linear in the total number of postings entries. At each step, we compare the docID pointed to by both pointers. If they are the same, we put that docID in the result list, and advance both pointers. Otherwise we advance the pointer pointing to the smaller docID. If the lengths of the postings lists are x and y, this merge takes $O(x+y)$ operations. Formally, the complexity of querying is $\Theta(N)$, where N is the number of documents in the collection.[5] Our indexing methods gain us just a constant, not a difference in Θ time complexity compared to a linear

5. The notation $\Theta(\cdot)$ is used to express an asymptotically tight bound on the complexity of an algorithm. Informally, this is often written as $O(\cdot)$, but this notation really expresses an asymptotic upper bound, which need not be tight (Cormen et al. 1990).

scan, but in practice the constant is huge. To use this algorithm, it is crucial that postings be sorted by a single global ordering. Using a numeric sort by docID is one simple way to achieve this.

We can extend the intersection operation to process more complicated queries like:

(1.2) (Brutus OR Caesar) AND NOT Calpurnia

QUERY OPTIMIZATION

Query optimization is the process of selecting how to organize the work of answering a query so that the least total amount of work needs to be done by the system. A major element of this for Boolean queries is the order in which postings lists are accessed. What is the best order for query processing? Consider a query that is an AND of t terms, for instance:

(1.3) Brutus AND Caesar AND Calpurnia

For each of the t terms, we need to get its postings, then AND them together. The standard heuristic is to process terms in order of increasing document frequency: if we start by intersecting the two smallest postings lists, then all intermediate results must be no bigger than the smallest postings list, and we are therefore likely to do the least amount of total work. So, for the postings lists in Figure 1.3 (page 7), we execute the above query as:

(1.4) (Calpurnia AND Brutus) AND Caesar

This is a first justification for keeping the frequency of terms in the dictionary: it allows us to make this ordering decision based on in-memory data before accessing any postings list.

Consider now the optimization of more general queries, such as:

(1.5) (madding OR crowd) AND (ignoble OR strife) AND (killed OR slain)

As before, we will get the frequencies for all terms, and we can then (conservatively) estimate the size of each OR by the sum of the frequencies of its disjuncts. We can then process the query in increasing order of the size of each disjunctive term.

For arbitrary Boolean queries, we have to evaluate and temporarily store the answers for intermediate expressions in a complex expression. However, in many circumstances, either because of the nature of the query language, or just because this is the most common type of query that users submit, a query is purely conjunctive. In this case, rather than viewing merging postings lists as a function with two inputs and a distinct output, it is more efficient to intersect each retrieved postings list with the current intermediate result in memory, where we initialize the intermediate result by loading the postings list of the least frequent term. This algorithm is shown in Figure 1.7. The intersection operation is then asymmetric: the intermediate result list

```
INTERSECT(⟨t_1, ..., t_n⟩)
1  terms ← SORTBYINCREASINGFREQUENCY(⟨t_1, ..., t_n⟩)
2  result ← POSTINGS(FIRST(terms))
3  terms ← REST(terms)
4  while terms ≠ NIL and result ≠ NIL
5  do result ← INTERSECT(result, POSTINGS(FIRST(terms)))
6     terms ← REST(terms)
7  return result
```

► **Figure 1.7** Algorithm for conjunctive queries that returns the set of documents containing each term in the input list of terms.

is in memory while the list it is being intersected with is being read from disk. Moreover the intermediate result list is always at least as short as the other list, and in many cases it is orders of magnitude shorter. The postings intersection can still be done by the algorithm in Figure 1.6, but when the difference between the list lengths is very large, opportunities to use alternative techniques open up. The intersection can be calculated in place by destructively modifying or marking invalid items in the intermediate result list. Or the intersection can be done as a sequence of binary searches in the long postings lists for each term in the intermediate result list. Another possibility is to store the long postings list as a hashtable, so that membership of an intermediate result item can be calculated in constant rather than linear or log time. However, such alternative techniques are difficult to combine with postings list compression of the sort discussed in Chapter 5. Moreover, standard postings list intersection operations remain necessary when both terms of a query are very common.

1.4 Boolean querying, extended Boolean querying, and ranked retrieval

RANKED RETRIEVAL MODELS
FREE-TEXT QUERIES

The Boolean retrieval model contrasts with *ranked retrieval models* such as the vector space model (Chapter 7), in which users largely use *free-text queries*, that is, just typing one or more words rather than using a precise language with operators for building up query expressions, and the system decides which documents best satisfy the query. Despite decades of academic research on the advantages of ranked retrieval, systems implementing the Boolean retrieval model were the main or only search option provided by large commercial information providers for three decades until the early 1990s (approximately the date of arrival of the World Wide Web). However, these

systems did not have just the basic Boolean operations (AND, OR, and NOT) which we have presented so far. A strict Boolean expression over terms with an unordered results set is too limited for many of the information needs that people have, and these systems implemented extended Boolean retrieval models by incorporating additional operators such as term proximity operators. A *proximity operator* is a way of specifying that two terms in a query must occur in a document close to each other, where closeness may be measured by limiting the allowed number of intervening words or by reference to a structural unit such as a sentence or paragraph.

PROXIMITY OPERATOR

✎ **Example 1.1: Commercial Boolean searching: Westlaw.** Westlaw (http://www.westlaw.com/) is the largest commercial legal search service (in terms of the number of paying subscribers), with over half a million subscribers performing millions of searches a day over tens of terabytes of text data. The service was started in 1975. In 2005, Boolean search (called "Terms and Connectors" by Westlaw) was still the default, and used by a large percentage of users, although ranked free-text querying (called "Natural Language" by Westlaw) was added in 1992. Here are some example Boolean queries on Westlaw:

Information need: Information on the legal theories involved in preventing the disclosure of trade secrets by employees formerly employed by a competing company. *Query:* "trade secret" /s disclos! /s prevent /s employe!

Information need: Requirements for disabled people to be able to access a workplace.
Query: disab! /p access! /s work-site work-place (employment /3 place)

Information need: Cases about a host's responsibility for drunk guests.
Query: host! /p (responsib! liab!) /p (intoxicat! drunk!) /p guest

Note the long, precise queries and the use of proximity operators, both uncommon in web search. Submitted queries average about ten words in length. Unlike web search conventions, a space between words represents disjunction (the tightest binding operator), & is AND and /s, /p, and /*k* ask for matches in the same sentence, same paragraph or within *k* words respectively. Double quotes give a *phrase search* (consecutive words); see Section 2.3.2 (page 37). The exclamation mark (!) gives a trailing wildcard query (see Section 3.1 (page 47)); thus liab! matches all words starting with liab. Additionally work-site matches any of *worksite*, *work-site* or *work site*; see Section 2.2.1 (page 22). Typical expert queries are usually carefully defined and incrementally developed until they obtain what look to be good results to the user.

Many users, particularly professionals, prefer Boolean query models. Boolean queries are precise: a document either matches the query or it does not. This offers the user greater control and transparency over what is retrieved. And some domains, such as legal materials, allow an effective means of document ranking within a Boolean model: Westlaw returns documents in reverse chronological order, which is in practice quite effective. In 2007, the majority of law librarians still seem to recommend terms and connectors for high recall searches. This does not mean though that Boolean queries are more effective for professional searchers. Indeed, experimenting on a Westlaw subcollection, Turtle (1994) found that free-text queries produced better results than Boolean queries prepared by Westlaw's own reference librarians for the

majority of the information needs in his experiments. A general problem with Boolean search is that using AND operators tends to produce high precision but low recall searches, while using OR operators gives low precision but high recall searches, and it is difficult or impossible to find a satisfactory middle ground.

In this chapter, we have looked at the structure and construction of a basic inverted index, comprising a dictionary and postings list. We introduced the Boolean retrieval model, and examined how to do efficient retrieval via linear time merges and simple query optimization. In Chapters 2–7 we will consider in detail richer query models and the sort of augmented index structures that are needed to handle them efficiently. Here we just mention a few of the main additional things we would like to be able to do:

1. We would like to better determine the set of terms in the dictionary and to provide retrieval that is tolerant to spelling mistakes and inconsistent choice of words.

2. It is often useful to search for compounds or phrases that denote a concept such as "operating system". As the Westlaw examples show, we might also wish to do proximity queries such as Gates NEAR Microsoft. To answer such queries, the index has to be augmented to capture the proximities of terms in documents.

3. A Boolean model only records term presence or absence, but often we would like to accumulate evidence, giving more weight to documents that have a term several times as opposed to ones that contain it only once. To be able to do this we need the *term frequency* information (the number of times a term occurs in a document) in postings lists.

TERM FREQUENCY

4. Boolean queries just retrieve a set of matching documents, but commonly we wish to have an effective method to order (or "rank") the returned results. This requires having a mechanism for determining a document score which encapsulates how good a match a document is for a query.

With these additional ideas, we will have seen most of the basic technology that supports ad hoc searching over unstructured information. Ad hoc searching over documents has recently conquered the world, powering not only web search engines but the kind of unstructured search that lies behind the large eCommerce websites. Although the main web search engines differ by emphasizing free-text querying, most of the basic issues and technologies of indexing and querying remain the same, as we will see in later chapters. Moreover, over time, web search engines have added at least partial implementations of some of the most popular operators from extended Boolean models: phrase search is especially popular and most have a very partial implementation of Boolean operators. Nevertheless, while these options are

liked by expert searchers, they are little used by most people and are not the main focus in work on trying to improve web search engine performance.

1.5 References and further reading

The practical pursuit of computerized information retrieval began in the late 1940s (Cleverdon 1991, Liddy 2005). A great increase in the production of scientific literature, much in the form of less formal technical reports rather than traditional journal articles, coupled with the availability of computers, led to interest in automatic document retrieval. However, in those days, document retrieval was always based on author, title, and keywords; full-text search came much later.

The article of Bush (1945) provided lasting inspiration for the new field:

> "Consider a future device for individual use, which is a sort of mechanized private file and library. It needs a name, and, to coin one at random, 'memex' will do. A memex is a device in which an individual stores all his books, records, and communications, and which is mechanized so that it may be consulted with exceeding speed and flexibility. It is an enlarged intimate supplement to his memory."

The term *Information Retrieval* was coined by Calvin Mooers in 1948/1950.

In 1958, much newspaper attention was paid to demonstrations at a conference (see Taube and Wooster 1958) of IBM "auto-indexing" machines, based primarily on the work of H. P. Luhn. Commercial interest quickly gravitated towards Boolean retrieval systems, but the early years saw a heady debate over various disparate technologies for retrieval systems. For example Mooers (1961) dissented:

> "It is a common fallacy, underwritten at this date by the investment of several million dollars in a variety of retrieval hardware, that the algebra of George Boole (1847) is the appropriate formalism for retrieval system design. This view is as widely and uncritically accepted as it is wrong."

The observation of AND vs. OR giving you opposite extremes in a precision/recall tradeoff, but not the middle ground comes from (Lee and Fox 1988).

Witten et al. (1999) is the standard reference for an in-depth comparison of the space and time efficiency of the inverted index versus other possible data structures; a more succinct and up-to-date presentation appears in Zobel and Moffat (2006). We further discuss several approaches in Chapter 5.

REGULAR EXPRESSIONS

Friedl (2006) covers the practical usage of *regular expressions* for searching. The underlying computer science appears in (Hopcroft et al. 2000).

1.6 Exercises

Exercise 1.1 [⋆]

Draw the inverted index that would be built for the following document collection. (See Figure 1.3 for an example.)

Doc 1 new home sales top forecasts
Doc 2 home sales rise in july
Doc 3 increase in home sales in july
Doc 4 july new home sales rise

Exercise 1.2 [⋆]

Consider these documents:

Doc 1 breakthrough drug for schizophrenia
Doc 2 new schizophrenia drug
Doc 3 new approach for treatment of schizophrenia
Doc 4 new hopes for schizophrenia patients

a. Draw the term-document incidence matrix for this document collection.
b. Draw the inverted index representation for this collection, as in Figure 1.3 (page 7).

Exercise 1.3 [⋆]

For the document collection shown in Exercise 1.2, what are the returned results for these queries:

a. schizophrenia AND drug
b. for AND NOT(drug OR approach)

Exercise 1.4 [⋆]

For the queries below, can we still run through the intersection in time $O(x + y)$, where x and y are the lengths of the postings lists for Brutus and Caesar? If not, what can we achieve?

a. Brutus AND NOT Caesar
b. Brutus OR NOT Caesar

Exercise 1.5 [⋆]

Exend the postings merge algorithm to arbitrary Boolean query formulas. What is its time complexity? For instance, consider:

c. (Brutus OR Caesar) AND NOT (Anthony OR Cleopatra)

Can we always merge in linear time? Linear in what? Can we do better than this?

Exercise 1.6 [⋆⋆]

We can use distributive laws for AND and OR to rewrite queries.

a. Show how to rewrite the above query into disjunctive normal form using the distributive laws.

b. Would the resulting query be more or less efficiently evaluated than the original form of this query?

c. Is this result true in general or does it depend on the words and the contents of the document collection?

Exercise 1.7 [⋆]

Recommend a query processing order for

d. (tangerine OR trees) AND (marmalade OR skies) AND (kaleidoscope OR eyes)

given the following postings list sizes:

Term	Postings size
eyes	213312
kaleidoscope	87009
marmalade	107913
skies	271658
tangerine	46653
trees	316812

Exercise 1.8 [⋆]

If the query is:

e. friends AND romans AND (NOT countrymen)

how could we use the frequency of countrymen in evaluating the best query evaluation order? In particular, propose a way of handling negation in determining the order of query processing.

Exercise 1.9 [⋆⋆]

For a conjunctive query, is processing postings lists in order of size guaranteed to be optimal? Explain why it is, or give an example where it isn't.

Exercise 1.10 [⋆⋆]

Write out a postings merge algorithm, in the style of Figure 1.6 (page 10), for an x OR y query.

Exercise 1.11 [⋆⋆]

How should the Boolean query x AND NOT y be handled? Why is naive evaluation of this query normally very expensive? Write out a postings merge algorithm that evaluates this query efficiently.

Exercise 1.12 [⋆]

Write a query using Westlaw syntax which would find any of the words professor, teacher, or lecturer in the same sentence as a form of the verb explain.

Exercise 1.13 [⋆]

Try using the Boolean search features on a couple of major web search engines. For instance, choose a word, such as burglar, and submit the queries (i) burglar, (ii) burglar AND burglar, and (iii) burglar OR burglar. Look at the estimated number of results and top hits. Do they make sense in terms of Boolean logic? Often they haven't for major

search engines. Can you make sense of what is going on? What about if you try different words? For example,query for (i) knight, (ii) conquer, and then (iii) knight OR conquer. What bound should the number of results from the first two queries place on the third query? Is this bound observed?

2 *The dictionary and postings lists*

Recall the major steps in inverted index construction:

1. Collect the documents to be indexed.
2. Tokenize the text.
3. Do linguistic preprocessing of tokens.
4. Index the documents that each term occurs in.

In this chapter we first briefly mention how the basic unit of a document can be defined and how the character sequence that it comprises is determined (Section 2.1). We then examine in detail some of the substantive linguistic issues of tokenization and linguistic preprocessing, which determine which terms are indexed in the dictionary (Section 2.2). Tokenization is the process of chopping character streams into tokens, while linguistic preprocessing then deals with building equivalence classes of tokens which are the set of terms that are indexed. Indexing itself is covered in Chapters 1 and 4. In Section 2.3, we examine extended postings list data structures that support faster querying and extended Boolean models, such as handling phrase and proximity queries.

2.1 Document delineation and character sequence decoding

2.1.1 Obtaining the character sequence in a document

Digital documents that are the input to an indexing process are typically bytes in a file or on a web server. The first step of processing is to convert this byte sequence into a linear sequence of characters. For the case of plain English text in ASCII encoding, this is trivial. But often things get much more complex. The sequence of characters may be encoded by one of various single byte or multibyte encoding schemes, such as Unicode UTF-8, or various national or vendor-specific standards. The correct encoding has to be

determined. This can be regarded as a machine learning classification problem, as discussed in Chapter 13,[1] but is often handled by heuristic methods, user selection, or by using provided document metadata. Once the encoding is determined, decoding to a character sequence has to be performed. The choice of encoding might be saved as it gives some evidence about what language the document is written in.

The characters may have to be decoded out of some binary representation like Microsoft Word DOC files and/or a compressed format such as zip files. Again, the document format has to be determined, and then an appropriate decoder has to be used. Even for plain text documents, additional decoding may need to be done. In XML documents (Section 10.1, page 188), character entities, such as `&`, need to be decoded to give the correct character, namely & for `&`. Finally, the textual part of the document may need to be extracted out of other material that will not be processed. You might want to do this with XML files if the markup is going to be ignored; you would almost certainly want to do this with postscript or PDF files. We will not deal further with these issues in this book, and will assume henceforth that our documents are a list of characters. Commercial products usually need to support a broad range of document types and encodings, since users want things to just work with their data as is. Often, they just think of documents as text inside applications and are not even aware of how it is encoded on disk. This problem is usually solved by licensing a software library that handles decoding document formats and character encodings.

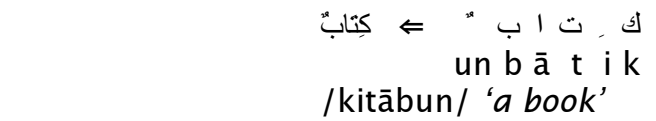
The idea that text is a linear sequence of characters is also called into question by some writing systems, such as Arabic, where text takes on some two dimensional and mixed order characteristics, as shown in Figures 2.1 and 2.2. But, despite some complicated writing system conventions, there is an underlying sequence of sounds being represented and hence an essentially linear structure remains, and this is what is represented in the digital representation of Arabic, as shown in Figure 2.1.

2.1.2 Choosing a document unit

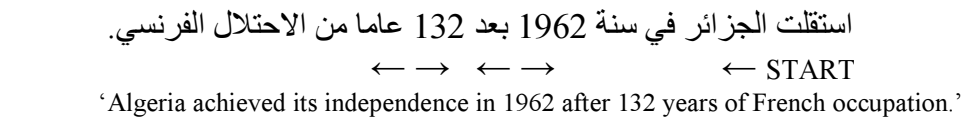
DOCUMENT UNIT

The next phase is to determine what the *document unit* for indexing is. Thus far we have assumed that documents are fixed units for the purposes of indexing. For example, we take each file in a folder as a document. But there are many cases in which you might want to do something different. A traditional Unix (mbox-format) email file stores a sequence of email messages (an email folder) in one file, but you might wish to regard each email mes-

1. A classifier is a function that takes objects of some sort and assigns them to one of a number of distinct classes. Usually classification is done by machine learning methods such as probabilistic models, but it can also be done by hand-written rules.



► **Figure 2.1** An example of a vocalized Modern Standard Arabic word. The writing is from right to left and letters undergo complex mutations as they are combined. The representation of short vowels (here, /i/ and /u/) and the final /n/ (nunation) departs from strict linearity by being represented as diacritics above and below letters. Nevertheless, the represented text is still clearly a linear ordering of characters representing sounds. Full vocalization, as here, normally appears only in the Koran and children's books. Day-to-day text is unvocalized (short vowels are not represented but the letter for ā would still appear) or partially vocalized, with short vowels inserted in places where the writer perceives ambiguities. These choices add further complexities to indexing.



► **Figure 2.2** The conceptual linear order of characters is not necessarily the order that you see on the page. In languages that are written right-to-left, such as Hebrew and Arabic, it is quite common to also have left-to-right text interspersed, such as numbers and dollar amounts. With modern Unicode representation concepts, the order of characters in files matches the conceptual order, and the reversal of displayed characters is handled by the rendering system, but this may not be true for documents in older encodings.

sage as a separate document. Many email messages now contain attached documents, and you might then want to regard the email message and each contained attachment as separate documents. If an email message has an attached zip file, you might want to decode the zip file and regard each file it contains as a separate document. Going in the opposite direction, various pieces of web software take things that you might regard as a single document (e.g., a Powerpoint file or a LaTeX document) and split them into separate HTML pages for each slide or subsection, stored as separate files. In these cases, you might want to combine multiple files into a single document.

INDEXING GRANULARITY

More generally, for very long documents, the issue of indexing *granularity* arises. For a collection of books, it would usually be a bad idea to index an entire book as a document. A search for Chinese toys might bring up a book that mentions China in the first chapter and toys in the last chapter, but this does not make it relevant to the query. Instead, we may well wish to index each chapter or paragraph as a mini-document. Matches are then more likely

to be relevant, and since the documents are smaller it will be much easier for the user to find the relevant passages in the document. But why stop there? We could treat individual sentences as mini-documents. It becomes clear that there is a precision/recall tradeoff here. If the units get too small, we are likely to miss important passages because terms were distributed over several mini-documents, while if units are too large we tend to get spurious matches and the relevant information is hard for the user to find.

The problems with large document units can be alleviated by use of explicit or implicit proximity search (Sections 2.3.2 and 7.2.2), and the tradeoffs in resulting system performance that we are hinting at are discussed in Chapter 8. The issue of index granularity, and in particular a need to simultaneously index documents at multiple levels of granularity, appears prominently in XML retrieval, and is taken up again in Chapter 10. An IR system should be designed to offer choices of granularity. For this choice to be made well, the person who is deploying the system must have a good understanding of the document collection, the users, and their likely information needs and usage patterns. For now, we will henceforth assume that a suitable size document unit has been chosen, together with an appropriate way of dividing or aggregating files, if needed.

2.2 Determining dictionary terms

2.2.1 Tokenization

Given a character sequence and a defined document unit, tokenization is the task of chopping it up into pieces, called *tokens*, perhaps at the same time throwing away certain characters, such as punctuation. Here is an example of tokenization:

Input: Friends, Romans, Countrymen, lend me your ears;
Output: | Friends | | Romans | | Countrymen | | lend | | me | | your | | ears |

These tokens are often loosely referred to as terms or words, but it is sometimes important to make a type/token distinction. A *token* is an instance of a sequence of characters in some particular document, which are grouped together as a useful semantic unit for processing. A *type* is the class of all tokens containing the same character sequence. A *term* is a (perhaps normalized) type that is indexed in the IR system's dictionary. The set of indexing terms could be entirely distinct from the tokens, for instance they could be semantic identifiers in a taxonomy, but in practice in modern IR systems they are strongly related to the tokens in the document. However, rather than being exactly the tokens that appear in the document, they may be derived

TOKEN
TYPE
TERM

from them by various normalization processes which are discussed in Section 2.2.3.[2]

The major question of the tokenization phase is what are the correct tokens to emit? For the example above, this looks fairly trivial: you chop on white-space and throw away punctuation characters. This is a starting point, but even for English there are a number of tricky cases. For example, what do you do about the various uses of the apostrophe for possession and contractions?

> Mr. O'Neill thinks that the boys' stories about Chile's capital aren't amusing.

For *O'Neill*, which of the following is the desired tokenization?

neill
oneill
o'neill
o' neill
o neill ?

And for *aren't*, is it:

aren't
arent
are n't
aren t ?

A simple strategy is to just split on all non-alphanumeric characters, but while o neill looks okay, aren t looks intuitively bad. For all of them, the choices determine which Boolean queries will match. A query of neill AND capital will match in three cases but not the other two. In how many cases would a query of o'neill AND capital match? If no preprocessing of a query is done, then it would match in only one of the five cases. For either Boolean or free-text queries, you always want to do the exact same tokenization of document and query words, generally by processing queries with the same tokenizer. This guarantees that a sequence of characters in a text will always match the same sequence typed in a query.[3]

2. That is, tokens that are not indexed (stop words) are not terms, and if multiple tokens are collapsed together via normalization, they are indexed as one term, under the normalized form.
3. For the free-text case, this is straightforward. The Boolean case is more complex: this tokenization may produce multiple terms from one query word. This can be handled by combining the terms with an AND or as a phrase query (see Section 2.3.2, page 37). It is harder for a system to handle the opposite case where the user entered as two terms something that was tokenized together in the document processing.

LANGUAGE IDENTIFICATION

These issues of tokenization are language-specific. It thus requires the language of the document to be known. *Language identification* based on classifiers that use short character subsequences as features is highly effective; most languages have distinctive signature patterns (see page 42 for references).

For most languages and particular domains within them there are unusual specific tokens that we wish to recognize as terms, such as the programming languages C++ and C#, aircraft names like B-52, or a T.V. show name such as M*A*S*H – which is sufficiently integrated into popular culture that you find usages such as *M*A*S*H-style hospitals*. Computer technology has introduced new types of character sequences that a tokenizer should probably tokenize as a single token, including email addresses (jblack@mail.yahoo.com), web URLs (http://stuff.big.com/new/specials.html), numeric IP addresses (142.32.48.231), package tracking numbers (1Z9999W99845399981), and more. One possible solution is to omit from indexing tokens such as monetary amounts, numbers, and URLs, since their presence greatly expands the size of the dictionary. However, this comes at a large cost in restricting what people can search for. For instance, people might want to search in a bug database for the line number where an error occurs. Items such as the date of an email, which have a clear semantic type, are often indexed separately as document metadata (see Section 6.1, page 103).

HYPHENS

In English, *hyphenation* is used for various purposes ranging from splitting up vowels in words (*co-education*) to joining nouns as names (*Hewlett-Packard*) to a copyediting device to show word grouping (*the hold-him-back-and-drag-him-away maneuver*). It is easy to feel that the first example should be regarded as one token (and is indeed more commonly written as just *coeducation*), the last should be separated into words, and that the middle case is unclear. Handling hyphens automatically can thus be complex: it can either be done as a classification problem, or more commonly by some heuristic rules, such as allowing short hyphenated prefixes on words, but not longer hyphenated forms.

Conceptually, splitting on white space can also split what should be regarded as a single token. This occurs most commonly with names (*San Francisco, Los Angeles*) but also with borrowed foreign phrases (*au fait*) and compounds that are sometimes written as a single word and sometimes space separated (such as *white space* vs. *whitespace*). Other cases with internal spaces that we might wish to regard as a single token include phone numbers ((800) 234-2333) and dates (Mar 11, 1983). Splitting tokens on spaces can cause bad retrieval results, for example, if a search for York University mainly returns documents containing *New York University*. The problems of hyphens and non-separating whitespace can even interact. Advertisements for air fares frequently contain items like *San Francisco-Los Angeles*, where simply doing whitespace splitting would give unfortunate results. In such cases issues of

tokenization interact with handling phrase queries (which we discuss in Section 2.3.2 (page 37)), particularly if we would like queries for all of *lowercase*, *lower-case* and *lower case* to return the same results. The last two can be handled by splitting on hyphens and using a phrase index. Getting the first case right would depend on knowing that it is sometimes written as two words and also indexing it in this way. One effective strategy in practice, which is used by some Boolean retrieval systems such as Westlaw and Lexis-Nexis (Example 1.1), is to encourage users to enter hyphens wherever they may be possible, and whenever there is a hyphenated form, the system will generalize the query to cover all three of the one word, hyphenated, and two word forms, so that a query for over-eager will search for over-eager OR "over eager" OR overeager. However, this strategy depends on user training, since if you query using either of the other two forms, you get no generalization.

Each new language presents some new issues. For instance, French has a variant use of the apostrophe for a reduced definite article 'the' before a word beginning with a vowel (e.g., *l'ensemble*) and has some uses of the hyphen with postposed clitic pronouns in imperatives and questions (e.g., *donne-moi* 'give me'). Getting the first case correct will affect the correct indexing of a fair percentage of nouns and adjectives: you would want documents mentioning both *l'ensemble* and *un ensemble* to be indexed under *ensemble*. Other languages make the problem harder in new ways. German writes

COMPOUNDS

compound nouns without spaces (e.g., *Computerlinguistik* 'computational linguistics'; *Lebensversicherungsgesellschaftsangestellter* 'life insurance company employee'). Retrieval systems for German greatly benefit from the use of a

COMPOUND-SPLITTER

compound-splitter module, which is usually implemented by seeing if a word can be subdivided into multiple words that appear in a dictionary. This phenomenon reaches its limit case with major East Asian Languages (e.g., Chinese, Japanese, Korean, and Thai), where text is written without any spaces between words. An example is shown in Figure 2.3. One approach here is

WORD SEGMENTATION

to perform *word segmentation* as prior linguistic processing. Methods of word segmentation vary from having a large dictionary and taking the longest dictionary match with some heuristics for unknown words to the use of machine learning sequence models, such as hidden Markov models or conditional random fields, trained over hand-segmented words (see the references in Section 2.4). Since there are multiple possible segmentations of character sequences (see Figure 2.4), all such methods make mistakes sometimes, and so you are never guaranteed a consistent unique tokenization. The other approach is to abandon word-based indexing and to do all indexing via just short subsequences of characters (character *k*-grams), regardless of whether particular sequences cross word boundaries or not. Three reasons why this approach is appealing are that an individual Chinese character is more like a syllable than a letter and usually has some semantic content, that most words are short (the commonest length is 2 characters), and that, given the lack of

莎拉波娃现在居住在美国东南部的佛罗里达。今年 4 月 9 日，莎拉波娃在美国第一大城市纽约度过了 18 岁生日。生日派对上，莎拉波娃露出了甜美的微笑。

► **Figure 2.3** The standard unsegmented form of Chinese text using the simplified characters of mainland China. There is no whitespace between words, nor even between sentences – the apparent space after the Chinese period (。) is just a typographical illusion caused by placing the character on the left side of its square box. The first sentence is just words in Chinese characters with no spaces between them. The second and third sentences include arabic numerals and punctuation breaking up the Chinese characters.

和尚

► **Figure 2.4** Ambiguities in Chinese word segmentation. The two characters can be treated as one word meaning 'monk' or as a sequence of two words meaning 'and' and 'still'.

a	an	and	are	as	at	be	by	for	from
has	he	in	is	it	its	of	on	that	the
to	was	were	will	with					

► **Figure 2.5** A stop list of 25 semantically non-selective words which are common in Reuters-RCV1.

standardization of word breaking in the writing system, it is not always clear where word boundaries should be placed anyway. Even in English, some cases of where to put word boundaries are just orthographic conventions – think of *notwithstanding* vs. *not to mention* or *into* vs. *on to* – but people are educated to write the words with consistent use of spaces.

2.2.2 Dropping common terms: stop words

STOP WORDS
COLLECTION FREQUENCY
STOP LIST

Sometimes, some extremely common words which would appear to be of little value in helping select documents matching a user need are excluded from the dictionary entirely. These words are called *stop words*. The general strategy for determining a stop list is to sort the terms by *collection frequency* (the total number of times each term appears in the document collection), and then to take the most frequent terms, often hand-filtered for their semantic content relative to the domain of the documents being indexed, as a *stop list*, the members of which are then discarded during indexing. An example of a stop list is shown in Figure 2.5. Using a stop list significantly

reduces the number of postings that a system has to store; we will present some statistics on this in Chapter 5 (see Table 5.1, page 80). And a lot of the time not indexing stop words does little harm: keyword searches with terms like the and by don't seem very useful. However, this is not true for phrase searches. The phrase query "President of the United States", which contains two stop words, is more precise than President AND "United States". The meaning of flights to London is likely to be lost if the word to is stopped out. A search for Vannevar Bush's article *As we may think* will be difficult if the first three words are stopped out, and the system searches simply for documents containing the word think. Some special query types are disproportionately affected. Some song titles and well known pieces of verse consist entirely of words that are commonly on stop lists (*To be or not to be*, *Let It Be*, *I don't want to be*, ...).

The general trend in IR systems over time has been from standard use of quite large stop lists (200–300 terms) to very small stop lists (7–12 terms) to no stop list whatsoever. Web search engines generally do not use stop lists. Some of the design of modern IR systems has focused precisely on how we can exploit the statistics of language so as to be able to cope with common words in better ways. We will show in Section 5.3 (page 89) how good compression techniques greatly reduce the cost of storing the postings for common words. Section 6.2.1 (page 111) then discusses how standard term weighting leads to very common words have little impact on document rankings and Section 7.1.5 (page 132) shows how an IR system with impact-sorted indexes can terminate scanning a postings list early when weights get small, and hence it does not incur a large additional cost on the average query even though postings lists for stop words are very long. So for most modern IR systems, the additional cost of including stop words is not that big – neither in terms of index size nor in terms of query processing time.

2.2.3 Normalization (equivalence classing of terms)

Having broken up our documents (and also our query) into tokens, the easy case is if tokens in the query just match tokens in the token list of the document. However, there are many cases when two character sequences are not quite the same but you would like a match to occur. For instance, if you search for *USA*, you might hope to also match documents containing *U.S.A.*

TOKEN NORMALIZATION
EQUIVALENCE CLASSES

Token normalization is the process of canonicalizing tokens so that matches occur despite superficial differences in the character sequences of the tokens.[4] The most standard way to normalize is to implicitly create *equivalence classes*, which are normally named after one member of the set. For instance,

4. It is also often referred to as *term normalization*, but we prefer to reserve the name *term* for the output of the normalization process.

Query term	Terms in documents that should be matched
Windows	Windows
windows	Windows, windows, window
window	window, windows

► **Figure 2.6** An example of how asymmetric expansion of query terms can usefully model users' expectations.

if the tokens *anti-discriminatory* and *antidiscriminatory* are both mapped onto the latter, in both the document text and queries, then searches for one term will retrieve documents that contain either.

The advantage of just using mapping rules that remove characters like hyphens is that the equivalence classing to be done is implicit, rather than being fully calculated in advance: the terms that happen to become identical as the result of these rules are the equivalence classes. It is only easy to write rules of this sort that remove characters. Since the equivalence classes are implicit, it is not obvious when you might want to add characters. For instance, it would be hard to know to turn *antidiscriminatory* into *anti-discriminatory*.

An alternative to creating equivalence classes is to maintain relations between unnormalized tokens. This method can be extended to hand-constructed lists of synonyms such as *car* and *automobile*, a topic we discuss further in Chapter 9. These term relationships can be achieved in two ways. The usual way is to index unnormalized tokens and to maintain a query expansion list of multiple dictionary entries to consider for a certain query term. A query term is then effectively a disjunction of several postings lists. The alternative is to perform the expansion during index construction. When the document contains automobile, we index it under car as well (and, usually, also vice-versa). Use of either of these methods is considerably less efficient than equivalence classing, as there are more postings to store and merge. The first method adds a query expansion dictionary and requires more processing at query time, while the second method requires more space for storing postings. Traditionally, expanding the space required for the postings lists was seen as more disadvantageous, but with modern storage costs, the increased flexibility that comes from distinct postings lists is appealing.

These approaches are more flexible than equivalence classes because the expansion lists can overlap while not being identical. This means there can be an asymmetry in expansion. An example of how such an asymmetry can be exploited is shown in Figure 2.6: if the user enters windows, we wish to allow matches with the capitalized *Windows* operating system, but this is not plausible if the user enters window, even though it is plausible for this query to also match lowercase *windows*.

The best amount of equivalence classing or query expansion to do is a

fairly open question. Doing some definitely seems a good idea. But doing a lot can easily have unexpected consequences of broadening queries in unintended ways. For instance, equivalence-classing *U.S.A.* and *USA* to the latter by deleting periods from tokens might at first seem very reasonable, given the prevalent pattern of optional use of periods in acronyms. However, if I put in as my query term *C.A.T.*, I might be rather upset if it matches every appearance of the word *cat* in documents.[5]

Below we present some of the forms of normalization that are commonly employed and how they are implemented. In many cases they seem helpful, but they can also do harm. In fact, you can worry about many details of equivalence classing, but it often turns out that providing processing is done consistently to the query and to documents, the fine details may not have much aggregate effect on performance.

Accents and diacritics. Diacritics on characters in English have a fairly marginal status, and we might well want *cliché* and *cliche* to match, or *naive* and *naïve*. This can be done by normalizing tokens to remove diacritics. In many other languages, diacritics are a regular part of the writing system and distinguish different sounds. Occasionally words are distinguished only by their accents. For instance, in Spanish, *peña* is 'a cliff', while *pena* is 'sorrow'. Nevertheless, the important question is usually not prescriptive or linguistic but is a question of how users are likely to write queries for these words. In many cases, users will enter queries for words without diacritics, whether for reasons of speed, laziness, limited software, or habits born of the days when it was hard to use non-ASCII text on many computer systems. In these cases, it might be best to equate all words to a form without diacritics.

CASE-FOLDING **Capitalization/case-folding.** A common strategy is to do *case-folding* by reducing all letters to lower case. Often this is a good idea: it will allow instances of *Automobile* at the beginning of a sentence to match with a query of *automobile*. It will also help on a web search engine when most of your users type in *ferrari* when they are interested in a *Ferrari* car. On the other hand, such case folding can equate words that might better be kept apart. Many proper nouns are derived from common nouns and so are distinguished only by case, including companies (*General Motors*, *The Associated Press*), government organizations (*the Fed* vs. *fed*) and person names (*Bush*, *Black*). We already mentioned an example of unintended query expansion with acronyms, which involved not only acronym normalization (*C.A.T.* → *CAT*) but also case-folding (*CAT* → *cat*).

5. At the time we wrote this chapter (Aug. 2005), this was actually the case on Google: the top result for the query *C.A.T.* was a site about cats, the Cat Fanciers Web Site http://www.fanciers.com/.

For English, an alternative to making every token lowercase is to just make some tokens lowercase. The simplest heuristic is to convert to lowercase words at the beginning of a sentence and all words occurring in a title that is all uppercase or in which most or all words are capitalized. These words are usually ordinary words that have been capitalized. Mid-sentence capitalized words are left as capitalized (which is usually correct). This will mostly avoid case-folding in cases where distinctions should be kept apart. The same task can be done more accurately by a machine learning sequence model which uses more features to make the decision of when to case-fold. This is known as *truecasing*. However, trying to get capitalization right in this way probably doesn't help if your users usually use lowercase regardless of the correct case of words. Thus, lowercasing everything often remains the most practical solution.

TRUECASING

Other issues in English. Other possible normalizations are quite idiosyncratic and particular to English. For instance, you might wish to equate *ne'er* and *never* or the British spelling *colour* and the American spelling *color*. Dates, times and similar items come in multiple formats, presenting additional challenges. You might wish to collapse together *3/12/91* and *Mar. 12, 1991*. However, correct processing here is complicated by the fact that in the U.S., *3/12/91* is *Mar. 12, 1991*, whereas in Europe it is *3 Dec 1991*.

Other languages. English has maintained a dominant position on the WWW; approximately 60% of web pages are in English (Gerrand 2007). But that still leaves 40% of the web, and the non-English portion might be expected to grow over time, since less than one third of Internet users and less than 10% of the world's population primarily speak English. And there are signs of change: Sifry (2007) reports that only about one third of blog posts are in English.

Other languages again present distinctive issues in equivalence classing. The French word for *the* has distinctive forms based not only on the gender (masculine or feminine) and number of the following noun, but also depending on whether the following word begins with a vowel: *le*, *la*, *l'*, *les*. We may well wish to equivalence class these various forms of *the*. German has a convention whereby vowels with an umlaut can be rendered instead as a two vowel digraph. We would want to treat *Schütze* and *Schuetze* as equivalent.

Japanese is a well-known difficult writing system, as illustrated in Figure 2.7. Modern Japanese is standardly an intermingling of multiple alphabets, principally Chinese characters, two syllabaries (hiragana and katakana) and western characters (Latin letters, Arabic numerals, and various symbols). While there are strong conventions and standardization through the education system over the choice of writing system, in many cases the same

ノーベル平和賞を受賞したワンガリ・マータイさんが名誉会長を務めるＭＯＴＴＡＩＮＡＩキャンペーンの一環として、毎日新聞社とマガジンハウスは「私 の、もったいない」を募集します。皆様が日ごろ「もったいない」と感じて実践していることや、それにまつわるエピソードを８００字以内の文章にまとめ、簡 単な写真、イラスト、図などを添えて１０月２０日までにお送りください。大賞受賞者には、５０万円相当の旅行券とエコ製品２点の副賞が贈られます。

► **Figure 2.7** Japanese makes use of multiple intermingled writing systems and, like Chinese, does not segment words. The text is mainly Chinese characters with the hiragana syllabary for inflectional endings and function words. The part in latin letters is actually a Japanese expression, but has been taken up as the name of an environmental campaign by 2004 Nobel Peace Prize winner Wangari Maathai. His name is written using the katakana syllabary in the middle of the first line. The first four characters of the final line shows a monetary amount that we would want to match with ¥500,000 (500,000 Japanese yen).

word can be written with multiple writing systems. For example, a word may be written in katakana for emphasis (somewhat like italics). Or a word may sometimes be written in hiragana and sometimes in Chinese characters. Successful retrieval thus requires complex equivalence classing across the writing systems. In particular, an end user might commonly present a query entirely in hiragana, because it is easier to type, just as Western end users commonly use all lowercase.

Document collections being indexed can include documents from many different languages. Or a single document can easily contain text from multiple languages. For instance, a French email might quote clauses from a contract document written in English. Most commonly, the language is detected and language-particular tokenization and normalization rules are applied at a predetermined granularity, such as whole documents or individual paragraphs, but this still will not correctly deal with cases where language changes occur for brief quotations. When document collections contain multiple languages, a single index may have to contain terms of several languages. One option is to run a language identification classifier on documents and then to tag terms in the dictionary for their language. Or this tagging can simply be omitted, since it is relatively rare for the exact same character sequence to be a word in different languages.

When dealing with foreign or complex words, particularly foreign names, the spelling may be unclear or there may be variant transliteration standards giving different spellings (for example, *Chebyshev* and *Tchebycheff* or *Beijing*

and *Peking*). One way of dealing with this is to use heuristics to equivalence class or expand terms with phonetic equivalents. The traditional and best known such algorithm is the Soundex algorithm, which we cover in Section 3.3 (page 57).

2.2.4 Stemming and lemmatization

For grammatical reasons, documents are going to use different forms of a word, such as *organize*, *organizes*, and *organizing*. Additionally, there are families of derivationally related words with similar meanings, such as *democracy*, *democratic*, and *democratization*. In many situations, it seems as if it would be useful for a search for one of these words to return documents that contain another word in the set.

The goal of both stemming and lemmatization is to reduce inflectional forms and sometimes derivationally related forms of a word to a common base form. For instance:

am, are, is ⇒ be
car, cars, car's, cars' ⇒ car

The result of this mapping of text will be something like:

the boy's cars are different colors ⇒
the boy car be differ color

STEMMING

LEMMATIZATION

LEMMA

However, the two words differ in their flavor. *Stemming* usually refers to a crude heuristic process that chops off the ends of words in the hope of achieving this goal correctly most of the time, and often includes the removal of derivational affixes. *Lemmatization* usually refers to doing things properly with the use of a dictionary and morphological analysis of words, normally aiming to remove inflectional endings only and to return the base or dictionary form of a word, which is known as the *lemma*. If confronted with the token *saw*, stemming might return just *s*, whereas lemmatization would attempt to return either *see* or *saw* depending on whether the use of the token was as a verb or a noun. The two may also differ in that stemming most commonly collapses derivationally related words, whereas lemmatization commonly only collapses the different inflectional forms of a lemma. Linguistic processing for stemming or lemmatization is often done by an additional plug-in component to the indexing process, and a number of such components exist, both commercial and open-source.

PORTER STEMMER

The most common algorithm for stemming English, and one that has repeatedly been shown to be empirically very effective, is *Porter's algorithm* (Porter 1980). The entire algorithm is too long and intricate to present here, but we will indicate its general nature. Porter's algorithm consists of 5 phases

Sample text: Such an analysis can reveal features that are not easily visible from the variations in the individual genes and can lead to a picture of expression that is more biologically transparent and accessible to interpretation

Lovins stemmer: such an analys can reve featur that ar not eas vis from th vari in th individu gen and can lead to a pictur of expres that is mor biolog transpar and acces to interpres

Porter stemmer: such an analysi can reveal featur that ar not easili visibl from the variat in the individu gene and can lead to a pictur of express that is more biolog transpar and access to interpret

Paice stemmer: such an analys can rev feat that are not easy vis from the vary in the individ gen and can lead to a pict of express that is mor biolog transp and access to interpret

► **Figure 2.8** A comparison of three stemming algorithms on a sample text.

of word reductions, applied sequentially. Within each phase there are various conventions to select rules, such as selecting the rule from each rule group that applies to the longest suffix. In the first phase, this convention is used with the following rule group:

(2.1)

Rule			**Example**		
SSES	→	SS	caresses	→	caress
IES	→	I	ponies	→	poni
SS	→	SS	caress	→	caress
S	→		cats	→	cat

Many of the later rules use a concept of the *measure* of a word, which loosely checks the number of syllables to see whether a word is long enough that it is reasonable to regard the matching portion of a rule as a suffix rather than as part of the stem of a word. For example, the rule:

$(m > 1)$ EMENT →

would map *replacement* to *replac*, but not *cement* to *c*. The official site for the Porter Stemmer is:

http://www.tartarus.org/~martin/PorterStemmer/

Other stemmers exist, including the older, one-pass Lovins stemmer (Lovins 1968), and newer entrants like the Paice/Husk stemmer (Paice 1990); see:

http://www.cs.waikato.ac.nz/~eibe/stemmers/
http://www.comp.lancs.ac.uk/computing/research/stemming/

Figure 2.8 presents an informal comparison of the different behavior of these stemmers. Stemmers use language-specific rules, but they require less knowledge than a lemmatizer, which needs a complete dictionary and morphological analysis to correctly lemmatize words. Particular domains may also require special stemming rules. However, the exact stemmed form does not matter, only the equivalence classes it forms.

LEMMATIZER

Rather than using a stemmer, you can use a *lemmatizer*, a tool from Natural Language Processing which does full morphological analysis to accurately identify the lemma for each word. Doing full morphological analysis produces at most very modest benefits for retrieval. It is hard to say more, because either form of normalization tends not to improve English information retrieval performance in aggregate – at least not by very much. While it helps a lot for some queries, it equally hurts performance a lot for others. Stemming increases recall while harming precision. As an example of what can go wrong, note that the Porter stemmer stems all of the following words:

operate operating operates operation operative operatives operational

to oper. However, since *operate* in its various forms is a common verb, we would expect to lose considerable precision on queries such as the following with Porter stemming:

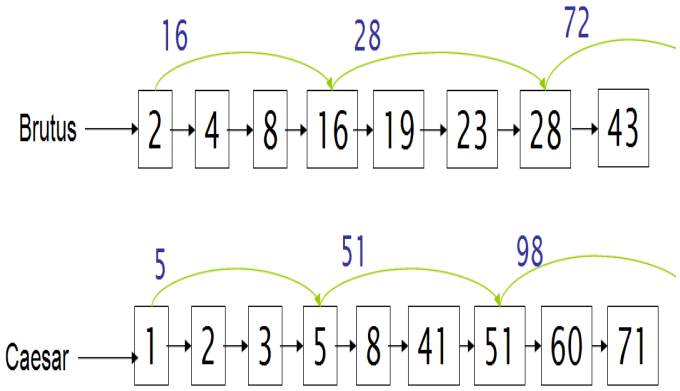
operational AND research
operating AND system
operative AND dentistry

For a case like this, moving to using a lemmatizer would not completely fix the problem because particular inflectional forms are used in particular collocations: a sentence with the words *operate* and *system* is not a good match for the query operating AND system.

The situation is different for languages with much more morphology (such as Spanish, German, and Finnish). Results in the European CLEF evaluations have repeatedly shown quite large gains from the use of stemmers (and compound splitting for languages like German); see the references in Section 2.4.

2.3 Postings lists, revisited

In the remainder of this chapter, we will discuss extensions to postings list data structures and ways to increase the efficiency of using postings lists.



► **Figure 2.9** Postings lists with skip pointers. The postings intersection can use a skip pointer when the end point is still less than the item on the other list.

2.3.1 Faster postings list intersection: Skip pointers

Recall the basic postings list intersection operation from Section 1.3 (page 9): we walk through the two postings lists simultaneously, in time linear in the total number of postings entries. If the list lengths are m and n, the intersection takes $O(m + n)$ operations. Can we do better than this? That is, empirically, can we usually process postings list intersection in sublinear time? We can, if the index isn't changing too fast.

SKIP LIST

One way to do this is to use a *skip list* by augmenting postings lists with skip pointers (at indexing time), as shown in Figure 2.9. Skip pointers are effectively shortcuts that allow us to avoid processing parts of the postings list that will not figure in the search results. The two questions are then where to place skip pointers and how to do efficient merging using skip pointers.

Consider first efficient merging, with Figure 2.9 as an example. Suppose we've stepped through the lists in the figure until we have matched 8 on each list and moved it to the results list. We advance both pointers, giving us 16 on the upper list and 41 on the lower list. The smallest item is then the element 16 on the top list. Rather than simply advancing the upper pointer, we first check the skip list pointer and note that 28 is also less than 41. Hence we can follow the skip list pointer, and then we advance the upper pointer to the item after 28, that is 43. We thus avoid stepping to 19 and 23 on the upper list. A number of variant versions of postings list intersection with skip pointers is possible depending on when exactly you check the skip pointer. One version is shown in Figure 2.10. Skip pointers will only be available for the original postings lists. For an intermediate result in a complex query, the

```
INTERSECTWITHSKIPS(p1, p2)
 1  answer ← ⟨ ⟩
 2  while p1 ≠ NIL and p2 ≠ NIL
 3  do if docID(p1) = docID(p2)
 4        then ADD(answer, docID(p1))
 5             p1 ← next(p1)
 6             p2 ← next(p2)
 7        else if docID(p1) < docID(p2)
 8                then while hasSkip(p1) and (docID(skip(p1) < docID(p2)))
 9                     do p1 ← skip(p1)
10                     p1 ← next(p1)
11                else while hasSkip(p2) and (docID(skip(p2) < docID(p1)))
12                     do p2 ← skip(p2)
13                     p2 ← next(p2)
14  return answer
```

► **Figure 2.10** Postings lists intersection with skip pointers.

call *hasSkip*(p) will always return false. Finally, note that the presence of skip pointers only helps for AND queries, not for OR queries.

Where do we place skips? There is a tradeoff. More skips means shorter skip spans, and that we are more likely to skip. But it also means lots of comparisons to skip pointers, and lots of space storing skip pointers. Fewer skips means few pointer comparisons, but then long skip spans which means that there will be fewer opportunities to skip. A simple heuristic for placing skips, which has been found to work well in practice is that for a postings list of length P, use $\sqrt{P}$ evenly-spaced skip pointers. This heuristic can be improved upon; it ignores any details of the distribution of query terms.

Building effective skip pointers is easy if an index is relatively static; it is harder if a postings list keeps changing because of updates. A malicious deletion strategy can render skip lists ineffective.

Choosing the optimal encoding for an inverted index is an ever-changing game for the system builder, because it is strongly dependent on underlying computer technologies and their relative speeds and sizes. Traditionally, CPUs were slow, and so highly compressed techniques were not optimal. Now CPUs are fast and disk is slow, so reducing disk postings list size dominates. However, if you're running a search engine with everything in memory then the equation changes again. We discuss the impact of hardware parameters on index construction time in Section 4.1 (page 61) and the role of index size on system speed in Chapter 5.

2.3.2 Phrase queries

Many complex or technical concepts and many organization and product names are multiword compounds or phrases. We would like to be able to pose a query such as Stanford University by treating it as a phrase so that a sentence in a document like *The inventor Stanford Ovshinsky never went to university.* is not a match. Most recent search engines support a double quotes syntax ("stanford university") for *phrase queries*, which has proven to be very easily understood and successfully used by users. As many as 10% of web queries are phrase queries, and many more are implicit phrase queries (such as person names), entered without use of double quotes. To be able to support such queries, it is no longer sufficient for postings lists to be simply lists of documents that contain individual terms. In this section we consider two approaches to supporting phrase queries and their combination. A search engine should not only support phrase queries, but implement them efficiently. A related but distinct concept is term proximity weighting, where a document is preferred to the extent that the query terms appear close to each other in the text. This technique is covered in Section 7.2.2 (page 134) in the context of ranked retrieval.

PHRASE QUERIES

Biword indexes

One approach to handling phrases is to consider every pair of consecutive terms in a document as a phrase. For example the text *Friends, Romans, Countrymen* would generate the *biwords*:

BIWORD INDEX

friends romans
romans countrymen

In this model, we treat each of these biwords as a dictionary term. Being able to process two-word phrase queries is immediate. Longer phrases can be processed by breaking them down. The query stanford university palo alto can be broken into the Boolean query on biwords:

"stanford university" AND "university palo" AND "palo alto"

This query could be expected to work fairly well in practice, but there can and will be occasional false positives. Without examining the documents, we cannot verify that the documents matching the above Boolean query do actually contain the original 4 word phrase.

Among possible queries, nouns and noun phrases have a special status in describing the concepts people are interested in searching for. But related nouns can often be divided from each other by various function words, in phrases such as *the abolition of slavery* or *renegotiation of the constitution*. These needs can be incorporated into the biword indexing model in the following

way. First, we tokenize the text and perform part-of-speech-tagging.[6] We can then group terms into nouns, including proper nouns, (N) and function words, including articles and prepositions, (X), among other classes. Now deem any string of terms of the form NX*N to be an extended biword. Each such extended biword is made a term in the dictionary. For example:

renegotiation	of	the	constitution
N	X	X	N

To process a query using such an extended biword index, we need to also parse it into N's and X's, and then segment the query into extended biwords, which can be looked up in the index.

This algorithm does not always work in an intuitively optimal manner when parsing longer queries into Boolean queries. Using the above algorithm, the query

cost overruns on a power plant

is parsed into

"cost overruns" AND "overruns power" AND "power plant"

whereas it might seem a better query to omit the middle biword. Better results can be obtained by using more precise part-of-speech patterns that define which extended biwords should be indexed.

PHRASE INDEX

The concept of a biword index can be extended to longer sequences of words, and if the index includes variable length word sequences, it is generally referred to as a *phrase index*. Indeed, searches for a single term are not naturally handled in a biword index (you would need to scan the dictionary for all biwords containing the term), and so we also need to have an index of single-word terms. While there is always a chance of false positive matches, the chance of a false positive match on indexed phrases of length 3 or more becomes very small indeed. But on the other hand, storing longer phrases has the potential to greatly expand the dictionary size. Maintaining exhaustive phrase indexes for phrases of length greater than two is a daunting prospect, and even use of an exhaustive biword dictionary greatly expands the size of the dictionary. However, towards the end of this section we discuss the utility of the strategy of using a partial phrase index in a compound indexing scheme.

6. Part of speech taggers classify words as nouns, verbs, etc. – or, in practice, often as finer-grained classes like "plural proper noun". Many fairly accurate (c. 96% per-tag accuracy) part-of-speech taggers now exist, usually trained by machine learning methods on hand-tagged text. See, for instance, Manning and Schütze (1999, ch. 10).

to, 993427:
⟨ 1, 6: ⟨7, 18, 33, 72, 86, 231⟩;
2, 5: ⟨1, 17, 74, 222, 55⟩;
4, 5: ⟨8, 16, 190, 429, 433⟩;
5, 2: ⟨363, 367⟩;
7, 3: ⟨13, 23, 191⟩; . . . ⟩

be, 178239:
⟨ 1, 2: ⟨17, 25⟩;
4, 5: ⟨17, 191, 291, 430, 434⟩;
5, 3: ⟨14, 19, 101⟩; . . . ⟩

► **Figure 2.11** Positional index example. to has a document frequency 993,477, and occurs 6 times in document 1 at positions 7, 18, 33, etc.

Positional indexes

POSITIONAL INDEX

For the reasons given, a biword index is not the standard solution. Rather, a *positional index* is most commonly employed. Here, for each term in the dictionary, we store postings of the form docID: ⟨position1, position2, . . . ⟩, as shown in Figure 2.11, where each position is a token index in the document. Each posting will also usually record the term frequency, for reasons discussed in Chapter 6.

To process a phrase query, you still need to access the inverted index entries for each distinct term. As before, you would start with the least frequent term and then work to further restrict the list of possible candidates. In the merge operation, the same general technique is used as before, but rather than simply checking that both documents are on a postings list, you also need to check that their positions of appearance in the document are compatible with the phrase query being evaluated. This requires working out offsets between the words.

✎ **Example 2.1: Satisfying phrase queries.** Suppose the postings lists for to and be are as in Figure 2.11, and the query is "to be or not to be". The postings lists to access are: to, be, or, not. We will examine intersecting the postings lists for to and be. We first look for documents that contain both terms. Then, we look for places in the lists where there is an occurrence of *be* with a token index one higher than a position of *to*, and then we look for another occurrence of each word with token index 4 higher than the first occurrence. In the above lists, the pattern of occurrences that is a possible match is:

to: ⟨. . . ; 4:⟨. . . ,429,433⟩; . . . ⟩
be: ⟨. . . ; 4:⟨. . . ,430,434⟩; . . . ⟩

```
POSITIONALINTERSECT(p1, p2, k)
 1  answer ← ⟨ ⟩
 2  while p1 ≠ NIL and p2 ≠ NIL
 3  do if docID(p1) = docID(p2)
 4        then l ← ⟨ ⟩
 5             pp1 ← positions(p1)
 6             pp2 ← positions(p2)
 7             while pp1 ≠ NIL
 8             do while pp2 ≠ NIL
 9                do if |pos(pp1) − pos(pp2)| > k
10                      then break
11                      else ADD(l, pos(pp2))
12                           pp2 ← next(pp2)
13                while l ≠ ⟨ ⟩ and |l[0] − pos(pp1)| > k
14                do DELETE(l[0])
15                for each ps ∈ l
16                do ADD(answer, ⟨docID(p1), pos(pp1), ps⟩)
17                pp1 ← next(pp1)
18             p1 ← next(p1)
19             p2 ← next(p2)
20        else if docID(p1) < docID(p2)
21                then p1 ← next(p1)
22                else p2 ← next(p2)
23  return answer
```

► **Figure 2.12** An algorithm for proximity intersection of postings lists p_1 and p_2. The algorithm finds places where the two terms appear within k words of each other and returns a list of triples giving docID and the term position in p_1 and p_2.

The same general method is applied for within k word proximity searches, of the sort we saw in Example 1.1 (page 13):

employment /3 place

Here, $/k$ means "within k words of (on either side)". Clearly, positional indexes can be used for such queries; biword indexes cannot. We show in Figure 2.12 an algorithm for satisfying within k word proximity searches; it is further discussed in Exercise 2.11.

Positional index size. Adopting a positional index expands required postings storage significantly, even if we compress position values/offsets as we will discuss in Section 5.3 (page 89). Indeed, moving to a positional index

also changes the asymptotic complexity of a postings intersection operation, because the number of items to check is now bounded not by the number of documents but by the total number of tokens in the document collection T. That is, the complexity of a boolean query is $\Theta(T)$ rather than $\Theta(N)$. However, most applications have little choice but to accept this, since most users now expect to have the functionality of phrase and proximity searches.

Let's examine the space implications of having a positional index. A posting now needs an entry for each occurrence of a term. The index size thus depends on the average document size. The average web page has less than 1000 terms, but documents like SEC stock filings, books, and even some epic poems easily reach 100,000 terms. Consider a term with frequency 1 in 1000 terms on average. The result is that large documents cause a two orders of magnitude increase in the space required to store the postings list:

Document size	Expected postings	Expected entries in positional posting
1000	1	1
100,000	1	100

While the exact numbers depend on the type of documents and the language being indexed, some rough rules of thumb are to expect a positional index to be 2 to 4 times as large as a non-positional index, and to expect a compressed positional index to be about one third to one half the size of the raw text (after removal of markup, etc.) of the original uncompressed documents. Specific numbers for an example collection are given in Table 5.1 (page 80) and Table 5.6 (page 97).

Combination schemes

The strategies of biword indexes and positional indexes can be fruitfully combined. If users commonly query on particular phrases, such as Michael Jackson, it is quite inefficient to keep merging positional postings lists. A combination strategy uses a phrase index, or just a biword index, for certain queries and uses a positional index for other phrase queries. Good queries to include in the phrase index are ones known to be common based on recent querying behavior. But this is not the only criterion: the most expensive phrase queries to evaluate are ones where the individual words are common but the desired phrase is comparatively rare. Adding *Britney Spears* as a phrase index entry may only give a speedup factor to that query of about 3, since most documents that mention either word are valid results, whereas adding *The Who* as a phrase index entry may speed up that query by a factor of 1000. Hence, having the latter is more desirable, even if it is a relatively less common query.

NEXT WORD INDEX

Williams et al. (2004) evaluate an even more sophisticated scheme which employs indexes of both these sorts and additionally a partial next word index as a halfway house between the first two strategies. For each term, a *next word index* records terms that follow it in a document. They conclude that such a strategy allows a typical mixture of web phrase queries to be completed in one quarter of the time taken by use of a positional index alone, while taking up 26% more space than use of a positional index alone.

2.4 References and further reading

EAST ASIAN LANGUAGES

Exhaustive discussion of the character-level processing of East Asian languages can be found in Lunde (1998). Character bigram indices are perhaps the most standard approach to indexing Chinese, although some systems use word segmentation, while due to differences in the language and writing system, word segmentation is most usual for Japanese (Luk and Kwok 2002, Kishida et al. 2005). The structure of a character k-gram index over unsegmented text differs from that in Section 3.1.2 (page 50): there the k-gram dictionary points to postings lists of entries in the regular dictionary, whereas here it points directly to document postings lists. For further discussion of Chinese word segmentation, see Sproat et al. (1996), Sproat and Emerson (2003), Tseng et al. (2005), and Gao et al. (2005).

Lita et al. (2003) present a method for truecasing. Natural language processing work on computational morphology is presented in (Sproat 1992, Beesley and Karttunen 2003).

Language identification was perhaps first explored in cryptography; for example, Konheim (1981) presents a character-level k-gram language identification algorithm. While other methods such as looking for particular distinctive function words and letter combinations have been used, with the advent of widespread digital text, many people have explored the character n-gram technique, and found it to be highly successful (Beesley 1998, Dunning 1994, Cavnar and Trenkle 1994). Written language identification is regarded as a fairly easy problem, while spoken language identification remains more difficult; see Hughes et al. (2006) for a recent survey.

Experiments on and discussion of the positive and negative impact of stemming in English can be found in the following works: Salton (1989), Harman (1991), Krovetz (1995), Hull (1996). Hollink et al. (2004) provide detailed results for the effectiveness of language-specific methods on 8 European languages: in terms of percent change in mean average precision (see page 152) over a baseline system, diacritic removal gains up to 23% (being especially helpful for Finnish, French, and Swedish), stemming helped markedly for Finnish (30% improvement) and Spanish (10% improvement), but for most langauges, including English, the gain from stemming was

in the range 0–5%, and results from a lemmatizer were poorer still. Compound splitting gained 25% for Swedish and 15% for German, but only 4% for Dutch. Rather than language-particular methods, indexing character k-grams (as we suggested for Chinese) could often give as good or better results: using within-word character 4-grams rather than words gave gains of 37% in Finnish, 27% in Swedish, and 20% in German, while even being slightly positive for other languages like Dutch, Spanish, and English. Tomlinson (2003) presents broadly similar results. Bar-Ilan and Gutman (2005) suggest that, at the time of their study (2003), the major commercial web search engines suffered from lacking decent language-particular processing; for example, a query on www.google.fr for l'électricité did not separate off the article *l'* but only matched pages with precisely this string of article+noun.

SKIP LIST

The classic presentation of skip pointers for IR can be found in Moffat and Zobel (1996). Extended techniques are discussed in Boldi and Vigna (2005). The main paper in the algorithms literature is Pugh (1990), which uses multilevel skip pointers to give expected $O(\log P)$ list access (the same expected efficiency as using a tree data structure) with less implementational complexity. In practice, the effectiveness of using skip pointers depends on various system parameters. Moffat and Zobel (1996) reported conjunctive queries running about five times faster with the use of skip pointers, but Bahle et al. (2002, p. 217) report that, with modern CPUs, using skip lists instead slows down search because it expands the size of the postings list (i.e., disk I/O dominates performance). In contrast, Strohman and Croft (2007) again show good performance gains from skipping, in a system architecture designed to optimize for the large memory spaces and multiple cores of recent CPUs.

Johnson et al. (2006) report that 11.7% of all queries in two 2002 web query logs contained phrase queries, though Kammenhuber et al. (2006) reports only 3% phrase queries for a different dataset. Silverstein et al. (1998) notes that many queries without explicit phrase operators are actually implicit phrase searches.

2.5 Exercises

Exercise 2.1

Are the following statements true or false?

a. In a Boolean retrieval system, stemming never lowers precision.
b. In a Boolean retrieval system, stemming never lowers recall.
c. Stemming increases the size of the vocabulary.
d. Stemming should be invoked at indexing time but not while processing a query.

Exercise 2.2

The following pairs of words are stemmed to the same form by the Porter stemmer. Which pairs would you argue shouldn't be conflated. Give your reasoning.

a. abandon/abandonment
b. absorbency/absorbent
c. marketing/markets
d. university/universe
e. volume/volumes

Exercise 2.3 [⋆]

For the Porter stemmer rule group shown in (2.1):

a. What is the purpose of including an identity rule such as SS → SS?
b. Applying just this rule group, what will the following words be stemmed to?
   circus *canaries* *boss*
c. What rule should be added to correctly stem *pony*?
d. The stemming for *ponies* and *pony* might seem strange. Does it have a deleterious effect on retrieval? Why or why not?

Exercise 2.4 [⋆]

Why are skip pointers not useful for queries of the form x OR y?

Exercise 2.5

We have a two-word query. For one term the postings list consists of the following 16 entries:

[4,6,10,12,14,16,18,20,22,32,47,81,120,122,157,180]

and for the other it is the one entry postings list:

[47].

Work out how many comparisons would be done to intersect the two postings lists with the following two strategies. Briefly justify your answers:

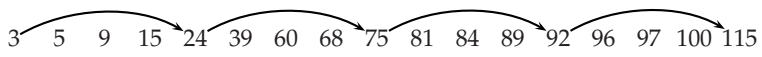
a. Using standard postings lists
b. Using postings lists stored with skip pointers, with a skip length of $\sqrt{P}$, as suggested in Section 2.3.1.

Exercise 2.6 [⋆]

Assume a biword index. Give an example of a document which will be returned for a query of New York University but is actually a false positive which should not be returned.

Exercise 2.7 [⋆]

Consider a postings intersection between this postings list, with skip pointers:



and the following intermediate result postings list (which hence has no skip pointers):

3 5 89 95 97 99 100 101

Trace through the postings intersection algorithm in Figure 2.10 (page 36).

a. How often is a skip pointer followed (i.e., p_1 is advanced to $skip(p_2)$)?
b. How many postings comparisons will be made by this algorithm while intersecting the two lists?
c. How many postings comparisons would be made if the postings lists are intersected without the use of skip pointers?

Exercise 2.8

Shown below is a portion of a positional index in the format: term: doc1: ⟨position1, position2, . . . ⟩; doc2: ⟨position1, position2, . . . ⟩; etc.

angels: 2: ⟨36,174,252,651⟩; 4: ⟨12,22,102,432⟩; 7: ⟨17⟩;
fools: 2: ⟨1,17,74,222⟩; 4: ⟨8,78,108,458⟩; 7: ⟨3,13,23,193⟩;
fear: 2: ⟨87,704,722,901⟩; 4: ⟨13,43,113,433⟩; 7: ⟨18,328,528⟩;
in: 2: ⟨3,37,76,444,851⟩; 4: ⟨10,20,110,470,500⟩; 7: ⟨5,15,25,195⟩;
rush: 2: ⟨2,66,194,321,702⟩; 4: ⟨9,69,149,429,569⟩; 7: ⟨4,14,404⟩;
to: 2: ⟨47,86,234,999⟩; 4: ⟨14,24,774,944⟩; 7: ⟨199,319,599,709⟩;
tread: 2: ⟨57,94,333⟩; 4: ⟨15,35,155⟩; 7: ⟨20,320⟩;
where: 2: ⟨67,124,393,1001⟩; 4: ⟨11,41,101,421,431⟩; 7: ⟨16,36,736⟩;

Which document(s) if any meet each of the following queries, where each expression within quotes is a phrase query?

a. "fools rush in"
b. "fools rush in" AND "angels fear to tread"

Exercise 2.9 [⋆]

Consider the following fragment of a positional index with the format:

word: document: ⟨position, position, . . .⟩; document: ⟩ position, . . .⟩
. . .

Gates: 1: ⟨3⟩; 2: ⟨6⟩; 3: ⟨2,17⟩; 4: ⟨1⟩;
IBM: 4: ⟨3⟩; 7: ⟨14⟩;
Microsoft: 1: ⟨1⟩; 2: ⟨1,21⟩; 3: ⟨3⟩; 5: ⟨16,22,51⟩;

The /k operator, word1 /k word2 finds occurrences of word1 within k words of word2 (on either side), where k is a positive integer argument. Thus $k = 1$ demands that word1 be adjacent to word2.

a. Describe the set of documents that satisfy the query Gates /2 Microsoft.
b. Describe each set of values for k for which the query Gates /k Microsoft returns a different set of documents as the answer.

Exercise 2.10 [⋆⋆]

Consider the general procedure for merging two positional postings lists for a given document, to determine the document positions where a document satisfies a /k

clause (in general there can be multiple positions at which each term occurs in a single document). We begin with a pointer to the position of occurrence of each term and move each pointer along the list of occurrences in the document, checking as we do so whether we have a hit for $/k$. Each move of either pointer counts as a step. Let L denote the total number of occurrences of the two terms in the document. What is the big-O complexity of the merge procedure, if we wish to have postings including positions in the result?

Exercise 2.11 [⋆⋆]

Consider the adaptation of the basic algorithm for intersection of two postings lists (Figure 1.6 (page 10)) to the one that handles proximity queries shown in Figure 2.12 (page 40). A naive algorithm for this operation could be $O(PL_{\max}{}^2)$, where P is the sum of the lengths of the postings lists (i.e., the sum of document frequencies) and $L_{\max}$ is the maximum length of a document (in tokens).

a. Go through this algorithm carefully and explain how it works.

b. What is the complexity of this algorithm? Justify your answer carefully.

c. For certain queries and data distributions, would another algorithm be more efficient? What complexity does it have?

Exercise 2.12 [⋆⋆]

Suppose we wish to use a postings intersection procedure to determine simply the list of documents that satisfy a $/k$ clause, rather than returning the list of positions, as in Figure 2.12 (page 40). For simplicity, assume $k \geq 2$. Let L denote the total number of occurrences of the two terms in the document collection (i.e., the sum of their collection frequencies). Which of the following is true? Justify your answer.

a. The merge can be accomplished in a number of steps linear in L and independent of k, and we can ensure that each pointer moves only to the right.

b. The merge can be accomplished in a number of steps linear in L and independent of k, but a pointer may be forced to move non-monotonically (i.e., to sometimes back up)

c. The merge can require kL steps in some cases.

Exercise 2.13 [⋆]

How could an engine combine use of a positional index and use of stop words? What is the potential problem, and how could it be handled?

3 *Tolerant retrieval*

In Chapters 1 and 2 we developed the ideas underlying inverted indexes for handling Boolean and proximity queries. Here, we study building an engine that is tolerant to typos, alternative spellings, and so on, and with minimum effort to the user tries to return the right results. We begin by studying *wildcard queries*: a query such as *a*e*i*o*u*, which seeks documents containing any term that includes all the five vowels in sequence. The * symbol indicates any (possibly empty) string of characters. We then turn to other forms of imprecisely posed queries, focusing on spelling errors. Users make spelling errors either by accident, or because the term they are searching for (e.g., Chebyshev) has no unambiguous spelling in the collection.

3.1 Wildcard queries

Wildcard queries are used in any of the following situations: (1) the user is uncertain of the spelling of a query term (e.g., Sydney vs. Sidney, which leads to the wildcard query S*dney); (2) the user is aware of multiple variants of rendering a term and seeks documents containing any of the variants (e.g., color vs. colour); (3) the user seeks documents containing variants of a term that would be caught by stemming, but is unsure whether the search engine performs stemming (e.g., judicial vs. judiciary, leading to the wildcard query judicia*); (4) the user is uncertain of the correct rendition of a foreign word (e.g., the query universit* Stuttgart).

WILDCARD QUERY

A query such as mon* is known as a *trailing wildcard query*, because the * symbol occurs only once, at the end of the search string. A search tree on the dictionary is a convenient way of handling trailing wildcard queries: we walk down the tree following the symbols m, o and n in turn, at which point we can enumerate the set W of terms in the dictionary with the prefix mon. Finally, we use the inverted index to retrieve all documents containing any term in W. Typically, the search tree data structure most suited for such applications is a *B-tree* – a search tree in which every internal node has a number of

B-TREE

children in the interval $[a, b]$, where a and b are appropriate positive integers. For instance when the index is partially disk-resident, the integers a and b are determined by the sizes of disk blocks. Section 3.4 contains pointers to further background on search trees and B-trees.

But what about wildcard queries in which the * symbol is not constrained to be at the end of the search string? Before handling the general case, we mention a slight generalization of trailing wildcard queries. First, consider *leading wildcard queries*, or queries of the form *mon. Consider a *reverse B-tree* on the dictionary – one in which each root-to-leaf path of the B-tree corresponds to a term in the dictionary written *backwards:* thus, the term lemon would, in the B-tree, be represented by the path root-n-o-m-e-l. A walk down the reverse B-tree then enumerates all terms R in the dictionary with a given suffix.

In fact, using a regular together with a reverse B-tree, we can handle an even more general case: wildcard queries in which there's a single * symbol, such as se*mon. To do this, we use the regular B-tree to enumerate the set W of dictionary terms beginning with the prefix se, then the reverse B-tree to enumerate the set R of dictionary terms ending with the suffix mon. Next, we take the intersection $W \cap R$ of these two sets, to arrive at the set of terms that begin with the prefix se and end with the suffix mon. Finally, we use the inverted index to retrieve all documents containing any terms in this intersection. We can thus handle wildcard queries that contain a single * symbol using two B-trees, the normal B-tree and a reverse B-tree.

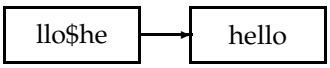
3.1.1 General wildcard queries

We now study two techniques for handling general wildcard queries. Both techniques share a common strategy: express the given wildcard query w as a Boolean query Q on a specially constructed index, such that the answer to Q is a superset of the set of dictionary terms matching w. Then, we check each term in the answer to Q against w, discarding those dictionary terms in the answer that do not match w. At this point we have the dictionary terms matching w and can resort to the standard inverted index.

Permuterm indexes

PERMUTERM INDEX

Our first special index for general wildcard queries is the *permuterm index*, a form of inverted index. First, we introduce a special symbol $ into our character set, to mark the end of a term; thus, the term hello is represented as hello$. Next, we construct a permuterm index, in which the dictionary consists of all rotations of each term (with the $ terminating symbol appended). The postings for each rotation consist of all dictionary terms containing that



► **Figure 3.1** Example of an entry in the permuterm index.

rotation. Figure 3.1 gives an example of such a permuterm index entry for a rotation of the term hello.

We refer to the set of rotated terms in the permuterm index as the *permuterm dictionary*.

How does this index help us with wildcard queries? Consider the wildcard query m*n. The key is to *rotate* such a wildcard query so that the * symbol appears at the end of the string – thus the rotated wildcard query becomes n$m*. Next, we look up this string in the permuterm index, where the entry n$m* points to the terms man and men. What of longer terms matching this wildcard query, such as moron? The permuterm index contains six rotations of moron, including n$moro. Now, n$m is a prefix of n$moro. Thus, when we traverse the B-tree into the permuterm dictionary seeking n$m, we find n$moro in the sub-tree, pointing into the original dictionary term moron.

Exercise 3.1

In the permuterm index, each permuterm dictionary term points to the original dictionary term(s) from which it was derived. How many original dictionary terms can there be in the postings list of a permuterm dictionary term?

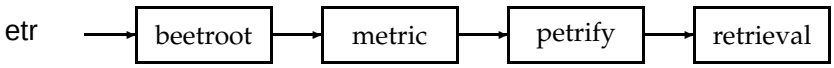
Exercise 3.2

Write down the entries in the permuterm index dictionary that are generated by the term mama.

Exercise 3.3

If you wanted to search for s*ng in a permuterm wildcard index, what key(s) would one do the lookup on?

Now that the permuterm index enables us to identify the original dictionary terms matching a wildcard query, we look up these terms in the standard inverted index to retrieve matching documents. We can thus handle any wildcard query with a single * symbol. But what about a query such as fi*mo*er? In this case we first enumerate the terms in the dictionary that are



► **Figure 3.2** Example of a postings list in a 3-gram index. Here the 3-gram etr is illustrated.

in the permuterm index of er$fi*. Not all such dictionary terms will have the string mo in the middle - we filter these out by exhaustive enumeration, checking each candidate to see if it contains mo. In this example, the term fishmonger would survive this filtering but filibuster would not. We then run the surviving terms through the regular inverted index for document retrieval. One disadvantage of the permuterm index is that its dictionary becomes quite large, including as it does all rotations of each term.

Notice the close interplay between the B-tree and the permuterm index above. Indeed, it suggests that the structure should perhaps be viewed as a permuterm B-tree. However, we follow traditional terminology here in describing the permuterm index as distinct from the B-tree that allows us to select the rotations with a given prefix.

3.1.2 *k*-gram indexes

We now present a second technique, known as the *k*-gram index, for processing wildcard queries. A *k-gram* is a sequence of *k* characters. Thus cas, ast and stl are all 3-grams occurring in the term castle. We use a special character $ to denote the beginning or end of a term, so the full set of 3-grams generated for castle is: $ca, cas, ast, stl, tle, le$.

k-GRAM INDEX

A *k-gram index* is an index in which the dictionary consists of all *k*-grams that occur in any term in the dictionary. Each postings list points from a *k*-gram to all dictioanry terms containing that *k*-gram. For instance, the 3-gram etr would point to dictionary terms such as metric and retrieval. An example is given in Figure 3.2.

How does such an index help us with wildcard queries? Consider the wildcard query re*ve. We are seeking documents containing any term that begins with re and ends with ve. Accordingly, we run the Boolean query $re AND ve$. This is looked up in the 3-gram index and yields a list of matching

terms such as relive, remove and retrieve. Each of these matching terms is then looked up in the inverted index to yield documents matching the query.

There is however a difficulty with the use of k-gram indexes, that demands one further step of processing. Consider using the 3-gram index described above for the query red*. Following the process described above, we first issue the Boolean query $re AND red to the 3-gram index. This leads to a match on terms such as retired, which contain the conjunction of the two 3-grams $re and red, yet do not match the original wildcard query red*.

To cope with this, we introduce a *post-filtering* step, in which the terms enumerated by the Boolean query on the 3-gram index are checked individually against the original query red*. This is a simple string-matching operation and weeds out terms such as retired that do not match the original query. Terms that survive are then run against the inverted index as usual.

Exercise 3.4

Consider again the query fi*mo*er from Section 3.1.1. What Boolean query on a bigram index would be generated for this query? Can you think of a term that meets this Boolean query but does not satisfy the permuterm query in Section 3.1.1?

Exercise 3.5

Give an example of a sentence that falsely matches the wildcard query mon*h if the search were to simply use a conjunction of bigrams.

We have seen that a wildcard query can result in multiple terms being enumerated, each of which becomes a single-term query on the inverted index. Search engines do allow the combination of wildcard queries using Boolean operators, for example, re*d AND fe*ri. What is the appropriate semantics for such a query? Since each wildcard query turns into a disjunction of single-term queries, the appropriate interpretation of this example is that we have a conjunction of disjunctions: we seek all documents that contain any term matching re*d *and* any term matching fe*ri.

Even without Boolean combinations of wildcard queries, the processing of a wildcard query can be quite expensive. A search engine may support such rich functionality, but most commonly, the capability is hidden behind an interface (say an "Advanced Query" interface) that most users never use. Surfacing such functionality often encourages users to invoke it, increasing the processing load on the engine.

3.2 Spelling correction

We next look at the problem of correcting spelling errors in queries. For instance, we may wish to retrieve documents containing the term carrot when the user types the query carot. Or, Google reports (http://www.google.com/jobs/britney.html)

that the following are all observed misspellings of the query britney spears: britian spears, britney's spears, brandy spears and prittany spears. We look at two approaches to this problem: the first based on *edit distance* and the second based on *k-gram overlap*. Before getting into the algorithmic details of these methods, we first review how search engines provide spell-correction as part of a user experience.

3.2.1 Implementing spelling correction

Search engines implement this feature in one of several ways:

1. On the query carot always retrieve documents containing carot as well as any "spell-corrected" version of carot, including carrot and tarot.
2. As in (1) above, but only when the query term carot is absent from the dictionary.
3. As in (1) above, but only when the original query (in this case carot) returned fewer than a preset number of documents (say fewer than five documents).
4. When the original query returns fewer than a preset number of documents, the search interface presents a *spell suggestion* to the end user: this suggestion consists of the spell-corrected query term(s).

3.2.2 Forms of spell correction

We focus on two specific forms of spell correction that we refer to as *isolated-term* correction and *context-sensitive* correction. In isolated-term correction, we attempt to correct a single query term at a time – even when we have a multiple-term query. The carot example demonstrates this type of correction. Such isolated-term correction would fail to detect, for instance, that the query flew form Heathrow contains a mis-spelling of the term from – because each term in the query is correctly spelled in isolation.

We begin by examining two methods for isolated-term correction: edit distance, and *k*-gram overlap. We then proceed to context-sensitive correction.

3.2.3 Edit distance

EDIT DISTANCE
LEVENSHTEIN DISTANCE

Given two character strings S_1 and S_2, the *edit distance* (also known as *Levenshtein distance*) between them is the minimum number of *edit operations* required to transform S_1 into S_2. Most commonly, the edit operations allowed for this purpose are: (i) insert a character into a string; (ii) delete a character from a string and (iii) replace a character of a string by another character. For example, the edit distance between cat and dog is 3. In fact, the notion of edit

```
m[i,j] = d(s1[1..i], s2[1..j])

m[0,0] = 0
m[i,0] = i, i=1..|s1|
m[0,j] = j, j=1..|s2|

m[i,j] = min(m[i-1,j-1]
             + if s1[i]=s2[j] then 0 else 1 fi,
             m[i-1, j] + 1,
             m[i, j-1] + 1 ), i=1..|s1|, j=1..|s2|
```

► **Figure 3.3** Dynamic programming algorithm for computing the edit distance between strings s1 and s2.

distance can be generalized to allowing varying weights for different kinds of edit operations, for instance a higher weight may be placed on replacing the character s by the character p, than on replacing it by the character a (the latter being closer to s on the keyboard). Setting weights in this way depending on the likelihood of letters substituting for each other is very effective in practice (see Section 3.3 for consideration of phonetic similarity). However, the remainder of our treatment here will focus on the case in which all edit operations have the same weight.

Exercise 3.6

If $|S|$ denotes the length of string S, show that the edit distance between S_1 and S_2 is never more than $\max\{|S_1|, |S_2|\}$.

It is well-known how to compute the (weighted) edit distance between two strings in time $O(|S_1| * |S_2|)$, where $|S|$ denotes the length of a string S. The idea is to use the dynamic programming algorithm in Figure 3.3.

The spell correction problem however is somewhat different from that of computing edit distance: given a set $\mathcal{S}$ of strings (corresponding to terms in the dictionary) and a query string q, we seek the string(s) in $\mathcal{S}$ of least edit distance from q. We may view this as a decoding problem, but one in which the codewords (the strings in $\mathcal{S}$) are prescribed in advance. The obvious way of doing this is to compute the edit distance from q to each string in $\mathcal{S}$, before selecting the string(s) of minimum edit distance. This exhaustive search is inordinately expensive. Accordingly, a number of heuristics are used in practice to efficiently retrieve dictionary terms likely to have low edit distance to the query q.

The simplest such heuristic is to restrict the search to dictionary terms beginning with the same letter as the query string; the hope would be that spelling errors do not occur in the first character of the query. A more sophisticated variant of this heuristic is to use the permuterm index, omitting

the end-of-word symbol. Consider the set of all rotations of the query string q. For each rotation r from this set, we traverse the B-tree into the permuterm index, thereby retrieving all dictionary terms that have a rotation beginning with r. For instance, if q is mase and we consider the rotation r=sema, we would retrieve dictionary terms such as semantic and semaphore. Unfortunately, we would miss more pertinent dictionary terms such as mare and mane. To address this, we refine this rotation scheme: for each rotation, we omit a suffix of ℓ characters before performing the B-tree traversal. This ensures that each term in the set R of dictionary terms retrieved includes a "long" substring in common with q. The value of ℓ could depend on the length of q. Alternatively, we may set it to a fixed constant such as 2.

Exercise 3.7

Compute the edit distance between paris and alice. Write down the 5×5 array of distances between all prefixes as computed by the algorithm in Figure 3.3.

Exercise 3.8

Show that if the query term q is edit distance 1 from a dictionary term t, then the set R includes t.

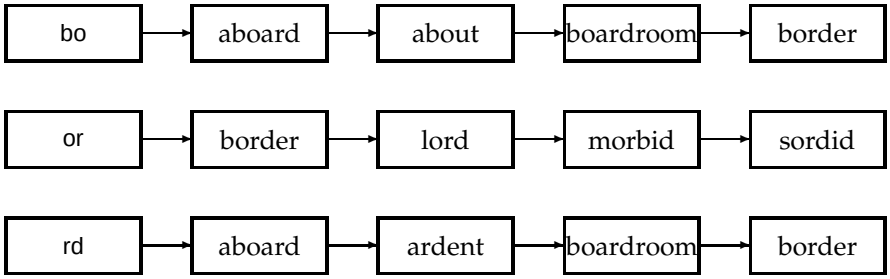
3.2.4 *k*-gram indexes

To further limit the set of dictionary terms for which we compute edit distances to the query term, we now show how to invoke the k-gram index of Section 3.1.2 (page 50) to assist with retrieving dictionary terms with low edit distance to the query q. Once we retrieve such terms, we can then find the ones of least edit distance from q.

In fact, we will use the k-gram index to retrieve dictionary terms that have many k-grams in common with the query. We will argue that for reasonable definitions of "many k-grams in common", the retrieval process is essentially that of a single scan through the postings for the k-grams in the query string q.

The 2-gram (or *bigram*) index in Figure 3.4 shows (a portion of) the postings for the three bigrams in the query bord. Suppose we wanted to retrieve dictionary terms that contained at least two of these three bigrams. A single scan of the postings (much as in Chapter 1) would let us enumerate all such terms; in the example of Figure 3.4 we would enumerate aboard, boardroom and border.

This straightforward application of the linear scan merge of postings immediately reveals the shortcoming of simply requiring matched dictionary terms to contain a fixed number of k-grams from the query q: terms like boardroom, an implausible "correction" of bord, get enumerated. Consequently, we require more nuanced measures of the overlap in k-grams between a dictionary term and q. The linear scan merge can be adapted when the measure



► **Figure 3.4** Matching at least two of the three 2-grams in the query bord.

JACCARD COEFFICIENT

of overlap is the *Jaccard coefficient* for measuring the overlap between two sets A and B, defined to be $|A \cap B|/|A \cup B|$. The two sets we consider are the set of k-grams in the query q, and the set of k-grams in a dictionary term. As the scan proceeds, we proceed from one dictionary term to the next, computing on the fly the Jaccard coefficient between the query q and a dictionary term t. If the coefficient exceeds a preset threshold, we add t to the output; if not, we move on to the next term in the postings. To compute the Jaccard coefficient, we need the set of k-grams in q and t.

Exercise 3.9

Compute the Jaccard coefficients between the query bord and each of the terms in Figure 3.4 that contain the bigram or.

Since we are scanning the postings for all k-grams in q, we immediately have these k-grams on hand. What about the k-grams of t? In principle, we could enumerate these on the fly from t; in practice this is not only slow but potentially infeasible since, in all likelihood, the postings entries themselves do not contain the complete string t but rather an integer encoding of t. The crucial observation is that we only need the length of the string t, to compute the Jaccard coefficient. To see this, recall the example of Figure 3.4 and consider the point when the postings scan for query $q =$ bord reaches term $t =$ boardroom. We know that two bigrams match. If the postings stored the (pre-computed) number of bigrams in boardroom (namely, 8), we have all the information we require. For the Jaccard coefficient is $2/(8 + 3 - 2)$; the numerator is obtained from the number of postings hits (2, from bo and rd) while the denominator is the sum of the number of bigrams in bord and boardroom, less the number of postings hits.

We could replace the Jaccard coefficient by other measures that allow efficient on the fly computation during postings scans. How do we use these for spell correction? One method that has some empirical support is to first use the k-gram index to enumerate a set of candidate dictionary terms that are potential corrections of q. We then compute the edit distance from q to each term in this set, selecting terms from the set with small edit distance to q.

3.2.5 Context sensitive spelling correction

Isolated-term correction would fail to correct typographical errors such as flew form Heathrow, where all three query terms are correctly spelled. When a phrase such as this retrieves few documents, a search engine may offer the corrected query flew from Heathrow. The simplest way to do this is to enumerate corrections of each of the three query terms (using the methods above) even though each query term is correctly spelled, then try substitutions of each correction in the phrase. For the example flew form Heathrow, we enumerate such phrases as fled form Heathrow and flew fore Heathrow. For each such substitute phrase, the engine runs the query and determines the number of matching results.

This enumeration can be expensive if we find many corrections of the individual terms, since we could encounter a large number of combinations of alternatives. Several heuristics are used to trim this space. In the example above, as we expand the alternatives for flew and form, we retain only the most frequent combinations in the collection. For instance, we would retain flew from as an alternative to try and extend to a three-term corrected query, but perhaps not fled fore or flea form. The choice of these alternatives is governed by the relative frequencies of biwords occurring in the collection: in this example, the biword fled fore is likely to be rare compared to the biword flew from. Then, we only attempt to extend the list of top biwords (such as flew from) in the first two terms, to corrections of Heathrow. As an alternative to using the biword statistics in the collection, we may use the logs of queries issued by users; these could of course include queries with spelling errors.

Exercise 3.10

Consider the four-term query catched in the rye and suppose that each of the query terms has five alternative terms suggested by isolated-term correction. How many possible corrected phrases must we consider if we do not trim the space of corrected phrases, but instead try all six variants for each of the terms?

Exercise 3.11

For each of the prefixes of the query — thus, catched, catched in and catched in the — we have a number of substitute prefixes arising from each term and its alternatives. Suppose that we were to retain only the top 10 of these substitute prefixes, as measured by its number of occurrences in the collection. We eliminate the rest from consideration for extension to longer prefixes: thus, if batched in is not one of the 10

most common 2-term queries in the collection, we do not consider any extension of batched in as possibly leading to a correction of catched in the rye. How many of the possible substitute prefixes are we eliminating at each phase?

Exercise 3.12

Are we guaranteed that retaining and extending only the 10 commonest substitute prefixes of catched in will lead to one of the 10 commonest substitute prefixes of catched in the?

3.3 Phonetic correction

Our final technique for tolerant retrieval has to do with *phonetic* correction: misspellings that arise because the user types a term that sounds like the target term. Such algorithms are especially applicable to searches on the names of people. The main idea here is to generate, for each term, a "phonetic hash" so that similar-sounding terms hash to the same value. The idea owes its origins to work in international police departments from the early 20th century, seeking to match names for wanted criminals despite the names being spelled differently in different countries. It is mainly used to correct phonetic misspellings in proper nouns.

SOUNDEX

Algorithms for such phonetic hashing are commonly collectively known as *soundex* algorithms. However, there is an original soundex algorithm, with various variants, built on the following scheme:

1. Turn every term to be indexed into a 4-character reduced form. Build an inverted index from these reduced forms to the original terms; call this the soundex index.
2. Do the same with query terms.
3. When the query calls for a soundex match, search this soundex index.

The variations in different soundex algorithms have to do with the conversion of terms to 4-character forms. A commonly used conversion results in a 4-character code, with the first character being a letter of the alphabet and the other three being digits between 0 and 9.

1. Retain the first letter of the term.
2. Change all occurrences of the following letters to '0' (zero): 'A', E', 'I', 'O', 'U', 'H', 'W', 'Y'.
3. Change letters to digits as follows:

   B, F, P, V to 1.

   C, G, J, K, Q, S, X, Z to 2.

D,T to 3.

L to 4.

M, N to 5.

R to 6.

4. Remove all pairs of consecutive digits.

5. Remove all zeros from the resulting string. Pad the resulting string with trailing zeros and return the first four positions, which will consist of a letter followed by three digits.

For an example of a soundex map, Hermann maps to H655. Given a query (say herman), we compute its soundex code and then retrieve all dictionary terms matching this soundex code from the soundex index, before running the resulting query on the standard term-document inverted index.

This algorithm rests on a few observations: (1) vowels are viewed as interchangeable, in transcribing names; (2) consonants with similar sounds (e.g., D and T) are put in equivalence classes. This leads to related names often having the same soundex codes. While these rules work for many cases, especially European languages, such rules tend to be writing system dependent. For example, Chinese names can be written in Wade-Giles or Pinyin transcription. While soundex works for some of the differences in the two transcriptions, for instance mapping both Wade-Giles hs and Pinyin x to 2, it fails in other cases, for example Wade-Giles j and Pinyin r are mapped differently.

3.4 References and further reading

Knuth (1997) is a comprehensive source for information on search trees, including B-trees.

Garfield (1976) gives one of the first complete descriptions of the permuterm index. Ferragina and Venturini (2007) gives an approach to addressing the space blowup in permuterm indexes.

One of the earliest formal treatments of spelling correction was due to Damerau (1964). The notion of edit distance is due to Levenshtein (1965). Peterson (1980) and Kukich (1992) developed variants of methods based on edit distances, culminating in a detailed empirical study of several methods by Zobel and Dart (1995), which shows that *k*-gram indexing is very effective for finding candidate mismatches, but should be combined with a more fine-grained technique such as edit distance to determine the most likely misspellings. Gusfield (1997) is a standard reference on non-probabilistic string algorithms such as edit distance.

Probabilistic models ("noisy channel" models) for spelling correction were pioneered by Kernighan et al. (1990) and further developed by Brill and Moore (2000) and Toutanova and Moore (2002). They have a similar mathematical basis to the language model methods presented in Chapter 12, and also provide ways of incorporating phonetic similarity, closeness on the keyboard, and data from the actual spelling mistakes of users. Many would regard them as the state-of-the-art approach. Cucerzan and Brill (2004) show how this work can be extended to learning spelling correction models based on query reformulations in search engine logs.

The soundex algorithm is attributed to Margaret K. Odell and Robert C. Russelli (from U.S. patents granted in 1918 and 1922); the version described here draws on Bourne and Ford (1961). Zobel and Dart (1996) evaluates various phonetic matching algorithms, and finds that a variant of the soundex algorithm performs poorly for general spell correction, but that other algorithms based on the phonetic similarity of term pronunciations perform well.

4 *Index construction*

INDEXING
INDEXER

In this chapter, we look at how to construct an inverted index. We will call this process *index construction* or *indexing* for short and the process or machine that performs it the *indexer*.

To build an index, we essentially have to perform a sort of the postings file. This is non-trivial for the large data sets that are typical in modern information retrieval. We will first introduce blocked sort-based indexing, an efficient single-machine algorithm designed for static collections (Section 4.2). For very large collections like the web, indexing has to be distributed over large computer clusters with hundreds or thousands of machines (Section 4.4). Collections with frequent changes require *dynamic indexing* so that changes in the collection are immediately reflected in the index (Section 4.5). Finally, we will cover some complicating issues that can arise in indexing – such as security and indexes for ranked retrieval – in Section 4.6.

Frequently, documents are not on a local file system, but have to be spidered or crawled, as we discuss in Chapter 20. Also, the indexer needs raw text, but documents are encoded in many ways, as we mentioned in Chapter 2. There are interactions between index compression (see Chapter 5) and construction because intermediate posting lists may have to be compressed and decompressed during construction. Finally documents are often encapsulated in varied content management systems, email applications and databases (we give some examples in Section 4.7). While most of these applications can be accessed via http, native APIs are usually more efficient. The reader should be aware that building the subsystem that feeds raw text to the indexing process can in itself be a challenging problem.

4.1 Hardware basics

Many decisions when building information retrieval systems are due to hardware constraints. We therefore begin this chapter with a brief review of aspects of computer hardware that are important for IR system design. Perfor-

symbol	statistic	value
s	disk seek	5 ms = 5×10^{-3} s
b	block transfer from disk (per byte)	0.1 μs = 10^{-7} s
	processor's clock cycle	10^{-9} s
p	other processor ops (e.g., compare&swap words)	0.1 μs = 10^{-7} s

► **Table 4.1** Tyical system parameters in 2007. A disk seek is the time needed to position the disk head in a new position. The block transfer rate is the rate of transfer when the head is in the right position.

mance characteristics typical of systems in 2007 are shown in Table 4.1. We now give a list of hardware basics that we will need in this book for system design.

- Access to data in memory is much faster than access to data on disk. It takes a few processor cycles (about 10^{-9} seconds) to access an integer in memory, but 100 times as long to transfer it from disk (about 10^{-7} seconds). Consequently, we want to keep as much data as possible in memory, especially those data that we need to access frequently.
- When doing a disk read or write, it takes a while for the disk head to move to the right track (5ms in Table 4.1). In order to maximize data transfer rates, chunks of data that will be read together should therefore be stored contiguously on disk. For example, using the numbers in Table 4.1 it will take as little as 100 seconds to transfer one GB from disk to memory if it is stored as one block, but up to $100 + 10{,}000 \times (5 \times 10^{-3}) = 150$ seconds if it is stored in 10,000 non-contiguous chunks because we need to move the disk head up to 10,000 times.
- Operating systems generally read and write entire blocks. So reading a single byte from a disk takes as much time as reading the entire block. Block sizes of 8 KB, 16 KB, 32 KB and 64 KB are common in 2007.
- Data transfers from disk to memory are handled by the system bus, not by the processor. This means that the processor is available to process data while it is being read. We can exploit this fact to speed up data transfers by storing compressed data on disk: the total time of reading and then decompressing compressed data is less than reading uncompressed data.

4.2 Blocked sort-based indexing

The basic steps in constructing a non-positional index are depicted in Figure 1.4 (page 8). We first make a pass through the collection assembling all

► **Figure 4.1** Document from the Reuters newswire.

postings (i.e., term-docID pairs). We then sort the entries with the term as the dominant key and docID as the secondary key. Finally, we organize the docIDs for each term into a posting list and compute statistics like term and document frequency. For small collections, all this can be done in memory. In this chapter, we describe methods for large collections that require the use of secondary storage.

To make index construction more efficient, we represent postings as termID-docID pairs (instead of term-docID pairs as we did in Figure 1.4). We can build the mapping from terms to termIDs on the fly while we are processing the collection; or, in a two-pass approach, we compile the vocabulary in the first pass and construct the inverted index in the second pass. The index construction algorithms described in this chapter use on-the-fly construction because it avoids the extra pass through the data and works well if the vocabulary is not too large. Section 4.7 gives references to algorithms that can handle very large vocabularies.

REUTERS-RCV1 We will work with the *Reuters-RCV1* collection as our model collection in this chapter, a collection with roughly one gigabyte of text. It consists of about 800,000 documents that were sent over the Reuters newswire during a one year period between August 20, 1996, and August 19, 1997. A typical document is shown in Figure 4.1, but note that we will ignore multimedia information like images in this book and only be concerned with text. Reuters-RCV1 covers a wide range of international topics, including politics, business, sports and (as in the example) science. Some key statistics of the collection are shown in Table 4.2.[1]

1. The numbers in this table correspond to the third line ("case folding") in Table 5.1, page 80. For the definitions of token and type, see Chapter 2, page 22.

symbol	statistic	value
N	documents	800,000
dlenave	avg. # tokens per document	200
M	term types	400,000
	avg. # bytes per token (incl. spaces/punct.)	6
	avg. # bytes per token (without spaces/punct.)	4.5
	avg. # bytes per term type	7.5
	non-positional postings	100,000,000

► **Table 4.2** Collection statistics for Reuters-RCV1. Values are rounded for the computations in this chapter. The unrounded values are: 806,791 documents, 222 tokens per document, 391,523 term types (or distinct terms), 6.04 bytes per token with spaces and punctuation, 4.5 bytes per token without spaces and punctuation, 7.5 bytes per term type and 96,969,056 non-positional postings.

BLOCKMERGEINDEXCONSTRUCTION()
1 $n \leftarrow 0$
2 **while** (all documents have not been processed)
3 **do** $n \leftarrow n + 1$
4 $block \leftarrow$ PARSENEXTBLOCK()
5 INVERT($block$)
6 WRITEBLOCKTODISK($block, f_n$)
7 MERGEBLOCKS($f_1, \ldots, f_n; f_{\text{merged}}$)

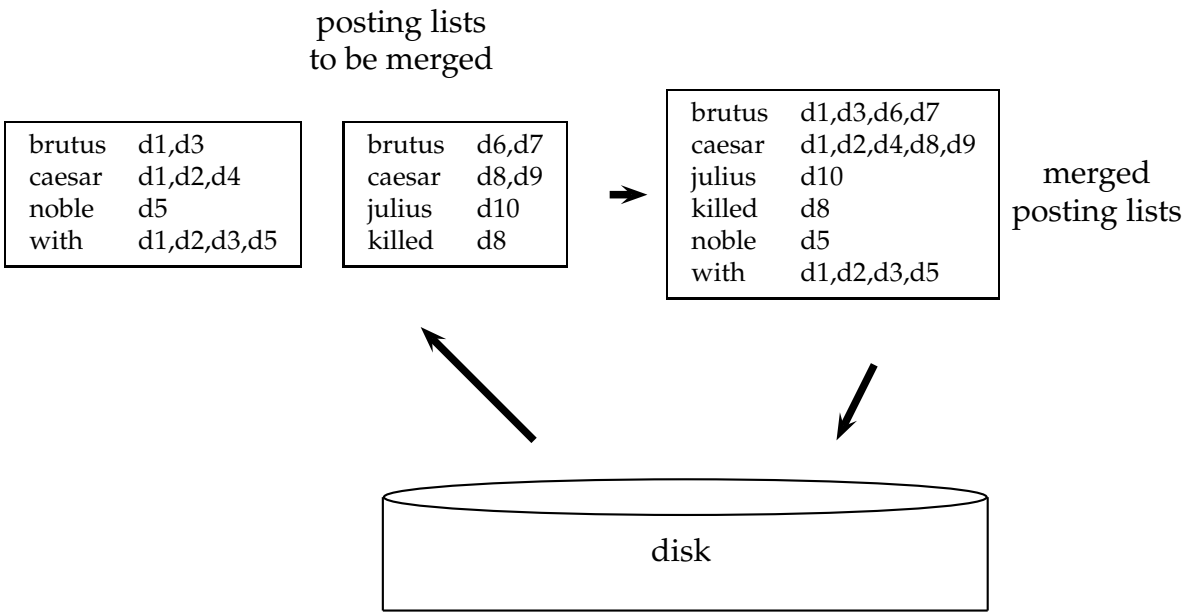
► **Figure 4.2** Blocked sort-based indexing. The algorithm stores inverted blocks in files $f_1, \ldots, f_n$ and the merged index in f_{merged}.

Reuters-RCV1 has 100 million postings. If we used 8 bytes per posting (4 bytes each for termID and docID), these 100 million postings will require 0.8 gigabyte of storage. Typical collections today are often one or two orders of magnitude larger than Reuters-RCV1. You can easily see how such collections will overwhelm even large computers if we tried to sort their postings files in memory. If the size of the postings file is within a small factor of available memory, then the compression techniques introduced in Chapter 5 can help; but the postings file of many large collections cannot fit into memory even after compression.

EXTERNAL SORTING

With main memory insufficient, we need to use an *external sorting* algorithm, i.e., one that uses disk. For acceptable speed, the central requirement of such an algorithm is that it minimize the number of random disk seeks during sorting (sequential disk reads are far faster than seeks as we explained above). One solution is the *blocked sort-based algorithm* in Figure 4.2, which

BLOCKED SORT-BASED ALGORITHM



► **Figure 4.3** Merging in blocked sort-based indexing. Two blocks ("posting lists to be merged") are loaded from disk into memory, merged in memory ("merged posting lists") and written back to disk. We show terms instead of termIDs for better readability.

sorts the postings of parts of the collection in memory, stores intermediate results on disk and then merges all intermediate results into the final index.

The first step of the algorithm is to parse documents into postings and accumulate the postings in memory until a block of a fixed size is full (PARSENEXTBLOCK). We choose the block size to fit comfortably into memory to permit a fast in-memory sort. The block is then inverted and written to disk. *Inversion* involves two steps. First we sort the postings. Next we collect all postings with the same termID into a posting list. The result, an inverted index for the block we have just read, is then written to disk. Applying this to Reuters-RCV1 and assuming we can fit 10 million postings into memory, we end up with 10 blocks, each an inverted index of part of the collection.

INVERSION

In the second step, the algorithm simultaneously merges the 10 blocks into one large merged index. An example with two blocks is shown in Figure 4.3 where we use d_i to denote the i^{th} document of the collection. To do this, we

open all block files simultaneously, and maintain small read buffers for the 10 blocks we are reading and a write buffer for the final merged index we are writing. In each iteration, we select the lowest termID that has not been processed yet using a priority queue or a similar data structure. All posting lists for this termID are read, merged and the merged list written back to disk. Each read buffer is refilled from its file when necessary.

How expensive is blocked sort-based indexing? Its time complexity is $\Theta(T \log T)$ because the step with the highest time complexity is sorting and T is an upper bound for the number of items we must sort (that is, the number of postings). But usually the actual indexing time is dominated by the time it takes to parse the documents (PARSENEXTBLOCK) and to do the final merge (MERGEBLOCKS). Exercise 4.2 asks you to compute the total index construction time for RCV1 that includes these steps as well as inverting the blocks and writing them to disk.

The reader will have noticed that Reuters-RCV1 is not particularly large in an age when one or more GB of memory are standard on personal computers. With appropriate compression (Chapter 5), we could have created an inverted index for RCV1 in memory on a not overly beefy server. The techniques we have described are needed, however, for collections that are several orders of magnitude larger.

4.3 Single-pass in-memory indexing

SINGLE-PASS IN-MEMORY INDEXING

Blocked sort-based indexing has excellent scaling properties, but it needs a data structure for mapping terms to termIDs. For very large collections, this data structure will not fit into memory. A more scalable alternative is *single-pass in-memory indexing* or *SPIMI* for short. SPIMI uses terms instead of termIDs, writes each block's dictionary to disk and then starts a new dictionary for the next block. SPIMI can index collections of any size as long as there is enough disk space available.

We show the SPIMI algorithm in Figure 4.4. We have omitted the part of the system that parses documents and turns them into a stream of postings. We call INVERT repeatedly on the postings stream until the entire collection has been processed.

Postings are processed one by one (line 3) during one call of INVERT. When a term occurs for the first time, it is added to the dictionary (best implemented as a hash), and a new posting list is created (line 5). The call in line 6 returns the posting list for subsequent occurrences of the term.

Another difference from blocked sort-based indexing is that SPIMI adds a posting directly to its posting list. Instead of first collecting all postings and then sorting them (as we did in blocked sort-based indexing), each posting list is dynamic (that is, its size is adjusted as it grows) and it is immediately

```
INVERT(postings_stream, output_file)
 1  dictionary = NEWHASH()
 2  while (free memory available)
 3  do posting ← next(postings_stream)
 4     if term(posting) ∉ dictionary
 5        then posting_list = ADDTODICTIONARY(dictionary, term(posting))
 6        else posting_list = GETPOSTINGLIST(dictionary, term(posting))
 7     if posting_list (full)
 8        then posting_list = DOUBLEPOSTINGLIST(dictionary, term(posting))
 9     ADDTOPOSTINGLIST(posting_list, posting)
10  sorted_terms ← SORTTERMS(dictionary)
11  WRITEBLOCKTODISK(sorted_terms, dictionary, output_file)
12  return output_file
```

► **Figure 4.4** Inversion of a block in single-pass in-memory indexing

available to collect postings. This has two advantages. It is faster as there is no sorting required. And it saves memory since we keep track of the term a posting list belongs to, so the termID need not be stored. As a result, the blocks that individual calls of INVERT can process are much larger and the index construction process as a whole is more efficient.

Since we do not know how large the posting list of a term will be when we first encounter it, we allocate space for a short posting list initially and double the space each time it is full (lines 7–8). This means that some memory will be wasted and counteracts the memory savings due to the omission of termIDs from postings. However, the overall memory requirements for the dynamically constructed index of a block in SPIMI are still lower than for blocked sort-based indexing.

When memory has been exhausted, we write the index of the block (which consists of the dictionary and the posting lists) to disk (line 11). We have to sort the terms (line 10) before doing this because we want to write posting lists in lexicographic order to facilitate the final merging step. If each block's posting lists were written in a different order, merging blocks could not be accomplished by a simple linear scan through each block index.

Each call of INVERT writes a block to disk, just as in blocked sort-based indexing. The last step of SPIMI (corresponding to line 7 in Figure 4.2, not shown in Figure 4.4) is then to merge the blocks into the final inverted index.

In addition to constructing a new dictionary structure for each block and eliminating the expensive sorting step, SPIMI has a third important component: compression. Both the docIDs in the posting lists and the dictionary terms on disk can be stored compactly if we employ compression. Compres-

sion increases the efficiency of the algorithm further because we can process even larger blocks; and because the individual block indexes require less space on disk. We refer readers to the literature for this aspect of the algorithm (Section 4.7).

4.4 Distributed indexing

Collections are often so large that we cannot perform index construction on a single machine. This is particularly true of the World Wide Web for which we need large computer clusters to construct any reasonably sized web index. Web search engines therefore use *distributed indexing* algorithms for index construction. The result of the construction process is an index that is partitioned across several machines – either according to term or according to document. In this section, we describe distributed indexing for a term-partitioned index. Most large search engines prefer a document-partitioned index (which can be easily generated from a term-partitioned index). We discuss this topic further in Section 20.3 (page 403).

MAPREDUCE

The distributed index construction method we describe in this section is an application of *MapReduce*, a general architecture for distributed computing. MapReduce is designed for large computer clusters. The point of a cluster is to solve large computing problems on cheap commodity machines or *nodes* that are built from standard parts (processor, memory, disk) as opposed to on a supercomputer with specialized hardware. While hundreds or thousands of machines are available in such clusters, individual machines can fail at any time. One requirement for robust distributed indexing is therefore that we divide the work up into chunks that we can easily assign and – in case of failure – reassign. A *master node* directs the process of assigning and reassigning tasks to individual worker nodes.

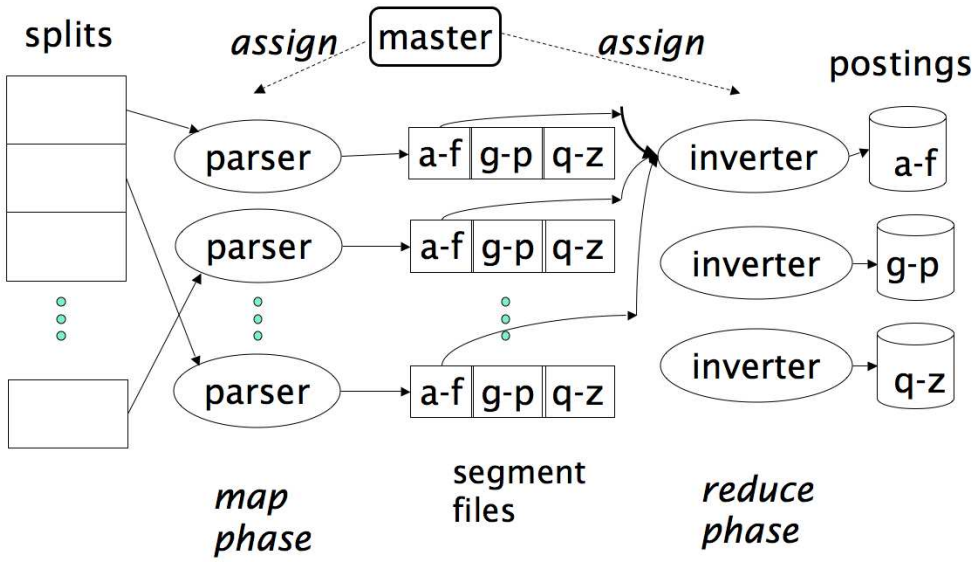
MASTER NODE

The *map* and *reduce* phases of MapReduce split up the computing job into chunks that standard machines can process in a short time. The various steps are shown in Figure 4.5 and an example for a collection with two documents is shown in Figure 4.6. First, the input data, in our case a collection of web pages, is split into *n splits* where the size of the split is chosen to ensure that the work can be distributed evenly (chunks shouldn't be too large) and efficiently (the total number of chunks we need to manage shouldn't be too large). 16 MB or 64 MB are good sizes in distributed indexing. Splits are not preassigned to machines, but are instead assigned by the master node on an ongoing basis: as a machine finishes processing one split, it is assigned the next one. If a machine dies or becomes a laggard due to hardware problems, the split it is working on is simply reassigned to another machine.

SPLITS

In general, MapReduce breaks a large computing problem into smaller parts by recasting it in terms of manipulation of *key-value pairs*. For indexing,

KEY-VALUE PAIRS



► **Figure 4.5** An example of distributed indexing with MapReduce. Adapted from Dean and Ghemawat (2004).

a key-value pair has the form (termID,docID) and, not surprisingly, is nothing other than a posting. In distributed indexing, the mapping from terms to termIDs is also distributed and therefore more complex than in single-machine indexing. A simple solution is to maintain a (perhaps precomputed) mapping for frequent terms that is copied to all nodes and to use terms directly (instead of termIDs) for infrequent terms. We will not address this problem here and assume that all nodes share a consistent term → termID mapping.

MAP PHASE

The *map phase* of MapReduce consists of mapping splits of the input data to postings or key-value pairs. This is the same parsing task we also encountered in blocked sort-based indexing, and we therefore call the machines that

PARSER

execute the map phase *parsers*. Each parser writes its output to three local

SEGMENT FILE

intermediate files, the *segment files* (shown as a-f | g-p | q-z in Figure 4.5).

REDUCE PHASE

For the *reduce phase*, we want all values for a given key to be stored close together, so that they can be read and processed quickly. This is achieved by partitioning the keys into j partitions and having the parsers write key-value pairs for each partition into a separate segment file. In Figure 4.5, the partitions are according to first letter: a–f, g–p, q–z, so $j = 3$. (We chose these key ranges for ease of exposition. In general, key ranges are not contiguous.)

The partitions are defined by the person who operates the indexing system (Exercise 4.8). The parsers then write corresponding segment files, one for each partition. Each partition thus corresponds to r segments files, where r is the number of parsers. For instance, Figure 4.5 shows three a–f segment files of the a–f partition, corresponding to the three parsers in the figure.

INVERTERS

Collecting all values (here: docIDs) for a given key (here: termID) into one list is the task of the *inverters* in the reduce phase. The master assigns each partition to a different inverter – and, as in the case of parsers, reassigns partitions in case of failing or slow inverters. Each partition (corresponding to k segment files, one on each parser) is processed by one inverter. Finally, the list of values is sorted for each key and written to the final sorted posting list ("postings" in the figure). Note that we assume that all posting lists are of a size that a single machine can handle (see Exercise 4.7). This data flow is shown for "a-f" in Figure 4.5. This completes the construction of the inverted index.

Parsers and inverters are not separate sets of machines. The master identifies idle machines and assigns tasks to them. The same machine can be a parser in the map phase and an inverter in the reduce phase. And there are often other jobs that run in parallel with index construction, so in between being a parser and an inverter a machine might do some crawling or another unrelated task.

To minimize write times before inverters reduce the data, each parser writes the segment files to its *local disk*. In the reduce phase, the master communicates to an inverter the locations of the relevant segment files (e.g., for the a-f partition). Each segment file only requires one sequential read since all data relevant to a particular inverter were written to a single segment file by the parser. This setup minimizes the amount of network traffic needed during indexing.

Figure 4.6 shows the general schema of the MapReduce functions. Input and output are often lists of key-value pairs themselves, so that several MapReduce jobs can be run in sequence. In fact, this was the design of the Google indexing system in 2004. What we have just covered in this section corresponds to only one of 5 to 10 MapReduce operations in that indexing system. Another MapReduce operation transform the term-partitioned index we just created into a document-partitioned one.

MapReduce offers a robust and conceptually simple framework for implementing index construction in a distributed environment. By providing a semi-automatic method for splitting index construction into smaller tasks, it can scale to almost arbitrarily large collections, given computer clusters of sufficient size.

Schema of map and reduce functions

map:	input	$\rightarrow$ list(k, v)
reduce:	$(k$,list$(v))$	$\rightarrow$ output

Instantiation of the schema for index construction

map:	web collection	$\rightarrow$ list$(\langle$termID, docID$\rangle)$
reduce:	$(\langle$termID$_1$, list(docID)$\rangle$, $\langle$termID$_2$, list(docID)$\rangle$, ...)	$\rightarrow$ (posting_list$_1$, posting_list$_2$, ...)

Example for index construction

map:	d_2 : C died. d_1 : C came, C c'ed.	$\rightarrow$ ($\langle$C, $d_2\rangle$, $\langle$died,$d_2\rangle$, $\langle$C,$d_1\rangle$, $\langle$came,$d_1\rangle$, $\langle$C,$d_1\rangle$, $\langle$c'ed,$d_1\rangle$)
reduce:	($\langle$C,(d_2,d_1,d_1)$\rangle$,$\langle$died,(d_2)$\rangle$,$\langle$came,(d_1)$\rangle$,$\langle$c'ed,(d_1)$\rangle$)	$\rightarrow$ ($\langle$C,(d_1:2,d_2:1)$\rangle$,$\langle$died,(d_2:1)$\rangle$,$\langle$came,(d_1:1)$\rangle$,$\langle$c'ed,(d_1:1)$\rangle$)

► **Figure 4.6** Map and reduce functions in MapReduce. In general, the map function produces a list of key-value pairs. All values for a key are collected into one list in the reduce phase. This list is then further processed. The instantiations of the two functions and an example are shown for index construction. Since the map phase processes documents in a distributed fashion, postings need not be ordered correctly initially as in this example. The example shows terms instead of termIDs for better readability. We abbreviate Caesar as C and conquered as c'ed.

4.5 Dynamic indexing

Thus far, we have assumed that the document collection is static. This is fine for collections that change infrequently or never (e.g., the Bible or Shakespeare). But most collections frequently change with documents being added, deleted and updated. This means that new terms need to be added to the dictionary; and posting lists need to be updated for existing terms.

The simplest way to achieve this is to periodically reconstruct the index from scratch. This is a good solution if the number of changes over time is small and a delay in making new documents searchable is acceptable – or if enough resources are available to construct a new index while the old one is still available for querying.

AUXILIARY INDEX

If there is a requirement that new documents be included quickly, one solution is to maintain two indexes: a large main index and a small *auxiliary index* that stores new documents. The auxiliary index is kept in memory. Searches are run across both indexes and results merged. Deletions are stored in an invalidation bit vector. We can then filter out deleted documents before returning the search result. Documents are updated by deleting and reinserting them.

Each time the auxiliary index becomes too large, we merge it into the main index. The cost of this merging operation depends on how we store the index in the file system. If we store each posting list as a separate file, then the merge simply consists of extending each posting list of the main index by

```
LMERGEPOSTING(indexes, Z_0, posting)
 1  Z_0 ← MERGE(Z_0, {posting})
 2  if |Z_0| = n
 3    then for i ← 0 to ∞
 4         do if I_i ∈ indexes
 5               then Z_{i+1} ← MERGE(I_i, Z_i)
 6                    (Z_{i+1} is a temporary index on disk.)
 7                    indexes ← indexes − {I_i}
 8               else I_i ← Z_i    (Z_i becomes the permanent index I_i.)
 9                    indexes ← indexes ∪ {I_i}
10                    BREAK
11         Z_0 ← ∅

LOGARITHMICMERGE()
1  Z_0 ← ∅    (Z_0 is the in-memory index.)
2  indexes ← ∅
3  while true
4  do LMERGEPOSTING(indexes, Z_0, GETNEXTPOSTING())
```

► **Figure 4.7** Logarithmic merging. Each posting (termID,docID) is initially added to in-memory index Z_0 by LMERGEPOSTING. LOGARITHMICMERGE initializes Z_0 and *indexes*.

the corresponding posting list of the auxiliary index. In this scheme, the reason for keeping the auxiliary index is to reduce the number of disk seeks required over time. Updating each document separately would require M_{ave} disk seeks, where M_{ave} is the average size of the vocabulary of documents in the collection. With an auxiliary index, we only put additional load on the disk when we merge auxiliary and main indexes.

Unfortunately, the one-file-per-posting-list scheme is inefficient because most file systems cannot efficiently handle very large numbers of files. The simplest alternative is to store the index as one large file, i.e., as a concatentation of all posting lists. In reality, we will often choose a compromise between the two extremes (Section 4.7). To simplify the discussion, we choose the simple option of storing the index as one large file here.

In this scheme, we process each posting $\lfloor T/n \rfloor$ times because we touch it during each of $\lfloor T/n \rfloor$ merges where n is the size of the auxiliary index and T the total number of postings. Thus, the overall time complexity is $\Theta(T^2/n)$. (We neglect the representation of terms here and consider only the docIDs. For the purpose of computing time complexity, a posting list is simply a list of docIDs.)

We can do better than $\Theta(T^2/n)$ by introducing $\Theta(\log_2 T)$ indexes I_0, I_1, I_2, ... of size $2^0 \times n$, $2^1 \times n$, $2^2 \times n$ .... Postings percolate up this sequence of indexes and are processed only once on each level. This scheme is called *logarithmic merging* (Figure 4.7). As before, up to n postings are accumulated in an in-memory index, which we call Z_0. When the limit n is reached, an index I_0 with $2^0 \times n$ postings is created on disk. The next time Z_0 is full, it is merged with I_0 to create an index Z_1 of size $2^1 \times n$. Then Z_1 is either stored as I_1 – if there isn't already an I_1 – or merged with I_1 into Z_2 if I_1 exists; and so on. We service search requests by querying in-memory Z_0 and all currently valid indexes I_i on disk and merging the results. Readers familiar with the binomial heap data structure[2] will recognize its similarity with the structure of the inverted indexes in logarithmic merging.

LOGARITHMIC MERGING

Overall index construction time is $\Theta(T \log(T/n))$. We trade this efficiency gain for a slow-down of query processing as we now need to merge results from $\log T$ indexes as opposed to just two (the main and auxiliary indexes). As in the auxiliary index scheme, we still need to merge very large indexes occasionally (which will slow down the search system during the merge), but this will happen less frequently and the indexes involved in a merge will on average be smaller.

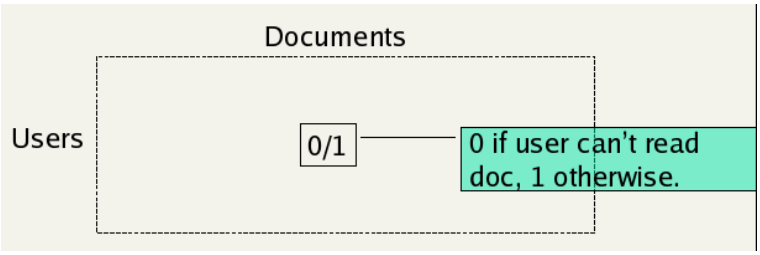
Having multiple indexes complicates the maintenance of collection-wide statistics. For example, it affects the spell correction algorithm in Section 3.2 (page 51) that selects the corrected alternative with the most hits. With multiple indexes and an invalidation bit vector, the correct number of hits for a term is no longer a simple lookup. And we will see that collection-wide statistics are also important in ranked retrieval (Section 1.4 (page 12), Chapter 6). In fact, all aspects of the system – index maintenance, query processing, distribution – are more complex in logarithmic merging.

Because of this complexity of dynamic indexing, some large search engines adopt a reconstruction-from-scratch strategy. They do not construct indexes dynamically. Instead, a new index is built from scratch periodically. Query processing is then switched from the new index and the old index is deleted.

4.6 Other types of indexes

This chapter only describes construction of non-positional indexes. Except for the much larger data volume we need to accommodate, the only difference for positional indexes is that (termID, docID, (position1, position2, ...)) triples instead of (termID, docID) pairs have to be sorted and posting lists contain position information in addition to docIDs. With this minor change, the algorithms discussed here can all be applied to positional indexes.

2. See, for example, (Cormen et al. 1990, ch. 19).



► **Figure 4.8** A user-document matrix for access control lists. Element (i, j) is 1 if user i has access to document j and 0 otherwise. During query processing, a user's access posting list is intersected with the result list returned by the text part of the index.

In the indexes we have considered so far, postings occur in document order. As we will see in the next chapter, this is advantageous for compression – instead of docIDs we can compress smaller *gaps* between IDs, thus reducing space requirements for the index. However, this structure for the index is not optimal when we build *ranked* (Chapters 6 and 7) – as opposed to Boolean – retrieval systems. In ranked retrieval, postings are often ordered according to weight or impact, with the highest-weighted postings occurring first. With this organization, scanning of long posting lists during query processing can usually be terminated early when weights have become so small that any further documents can be predicted to be of low similarity to the query (see Chapter 6). In a docID-sorted index, new documents are always inserted at the end of posting lists. In an impact-sorted index (Section 7.1.5, page 132), the insertion can occur anywhere, thus complicating the update of the inverted index.

RANKED RETRIEVAL

SECURITY

Security is an important consideration for retrieval systems in corporations. The average employee should not be able to find the salary roster of the corporation, but authorized managers need to be able to search for it. Users' result lists must not contain documents they are barred from opening since the very existence of a document can be sensitive information.

ACCESS CONTROL LISTS

User authorization is often mediated through *access control lists* or ACLs. ACLs can be dealt with in an inverted index data structure by representing each document as the set of users that can access them (Figure 4.8) and then inverting the resulting user-document matrix. The inverted ACL index has, for each user, a "posting list" of documents they can access – the user's access list. Search results are then intersected with this list. However, such an index is difficult to maintain when access permissions change – we discussed these difficulties in the context of incremental indexing for regular posting lists in the last section. It also requires the processing of very long posting lists for

users with access to large document subsets. User membership is therefore often verified by retrieving access lists directly from the file system at query time – even though this slows down retrieval.

4.7 References and further reading

Witten et al. (1999, ch. 5) contains an extensive treatment of the subject of index construction and present additional indexing algorithms with different tradeoffs of memory, disk space and time. In general, blocked sort-based indexing does well on all three counts. However, if conserving memory or disk space is the main criterion, then other algorithms may be a better choice See Witten et al. (1999), Tables 5.4 and 5.5; blocked sort-based indexing is closest to "sort-based multiway merge", but the two algorithsm differ in in dictionary structure and use of compression.

Moffat and Bell (1995) show how to construct an index "in-situ", that is, with disk space usage close to what is needed for the final index and with a minimum of additional temporary files (cf. also Harman and Candela (1990)). They give Lesk (1988) and Somogyi (1990) credit for being among the first to employ sorting for index construction.

Section 4.3 describes a simplified version of single-pass in-memory inversion in (Heinz and Zobel 2003). We recommend both Heinz and Zobel (2003) and Zobel and Moffat (2006) as up-do-date in-depth treatments of index construction.

The MapReduce architecture was introduced by Dean and Ghemawat (2004). An open source implementation of MapReduce is available at: http://lucene.apache.org/hadoop/. Ribeiro-Neto et al. (1999) and Melnik et al. (2001) describe other approaches to distributed indexing. Introductory chapters on distributed IR are (Baeza-Yates and Ribeiro-Neto 1999, ch. 9) and (Grossman and Frieder 2004, ch. 8).

Logarithmic index construction was first first used in Lucene (http://lucene.apache.org). Lester et al. (2005) and Büttcher and Clarke (2005) analyze its properties and compare it with other construction methods. Alternative dynamic indexing methods are discussed by Büttcher et al. (2006) and Lester et al. (2006). The latter paper also discusses the re-build strategy of replacing the old index by one built from scratch.

Heinz et al. (2002) compare data structures for accumulating text vocabularies in memory. Büttcher and Clarke (2005) discuss security models for a common inverted index for multiple users. A detailed characterization of the Reuters-RCV1 collection can be found in (Lewis et al. 2004). NIST distributes the corpus (see http://trec.nist.gov/data/reuters/reuters.html).

An effective enterprise search system needs to be able to communicate efficiently with a number of applications that hold text data in corporations, including Microsoft Outlook, IBM's Lotus software, databases like Oracle

	step	time
1	reading of collection (line 4)	
2	10 initial sorts of 10^7 records each (line 5)	
3	writing of 10 blocks (line 6)	
4	total disk transfer time for merging (line 7)	
5	time of actual merging (line 7)	
	total	

► **Table 4.3** The five steps in constructing an index for Reuters-RCV1 in blocked sort-based indexing. Line numbers refer to Figure 4.2.

symbol	statistic	value
N	# documents	1,000,000,000
dlenave	# tokens per document	1000
M	# distinct terms	44,000,000

► **Table 4.4** Collection statistics for a large collection.

and MySQL, content management systems like Open Text and enterprise resource planning software like SAP.

4.8 Exercises

Exercise 4.1

If we need $n \log_2 n$ comparisons (where n is the number of postings) and 2 disk seeks for each comparison, how much time would index construction for Reuters-RCV1 take if we used disk instead of memory for storage and an unoptimized sorting algorithm (i.e., not an external sorting algorithm)? Use the system parameters in Table 4.1.

Exercise 4.2

Total index construction time in blocked sort-based indexing is broken down in Table 4.3. Fill out the time column of the table for Reuters-RCV1 assuming a system with the parameters given in Table 4.1.

Exercise 4.3

Repeat Exercise 4.2 for the larger collection in Table 4.4. Choose a block size that is realistic for current technology (remember that a block should easily fit into main memory). How many blocks do you need?

Exercise 4.4

The dictionary has to be created on the fly in blocked sort-based indexing to avoid an extra pass for compiling the dictionary. How would you do this on-the-fly creation?

Exercise 4.5

Compare memory, disk and time requirements of the naive in-memory indexing algorithm (assuming the collection is small enough) and blocked sort-based indexing.

Exercise 4.6

For $n = 15$ splits, $k = 10$ segments and $j = 3$ key partitions, how long would distributed index creation take for Reuters-RCV1 in a MapReduce architecture? Base your assumptions about cluster machines on Table 4.1.

Exercise 4.7

How would you modify MapReduce for a posting list that is too large for a single machine?

Exercise 4.8

For optimal load balancing, the inverters in MapReduce must get segmented postings files of similar sizes. For a new collection, the distribution of key-value pairs may not be known in advance. How would you solve this problem?

Exercise 4.9

Apply MapReduce to the problem of counting how often each term occurs in a set of files. Specify map and reduce operations for this task. Write down an example along the lines of Figure 4.6.

Exercise 4.10

For $n = 2$ and $1 \leq T \leq 30$, perform a step-by-step simulation of the algorithm in Figure 4.7. Create a table that shows, for each point in time at which $T = 2 * k$ postings have been processed ($1 \leq k \leq 15$), which of the three indexes $I_0, \ldots, I_3$ are in use. The first three lines of the table are given below.

	I_3	I_2	I_1	I_0
2	0	0	0	0
4	0	0	0	1
6	0	0	1	0

Exercise 4.11

We claimed above (page 73) that an auxiliary index can impair the quality of collection statistics. An example is the term weighting method idf, which is defined as $\log(N/\mathrm{df}_i)$ where N is the total number of documents and df_i is the number of documents that term i occurs in Section 6.2.1 (page 111). Show that even a small auxiliary index can cause significant error in idf when it is computed on the main index only. Consider a rare term that suddenly occurs frequently (e.g., Flossie as in Tropical Storm Flossie).

Exercise 4.12

Can spell correction compromise document-level security? Consider the case where a spell correction is based on documents the user does not have access to.

5 *Index compression*

Chapter 1 introduced the dictionary and the inverted index as the central data structures in information retrieval. In this chapter, we employ a number of compression techniques for the two data structures which are essential for efficient information retrieval systems.

One benefit of compression is immediately clear. We will need less disk space. As we will see, compression ratios of 1:4 are easy to achieve, potentially cutting the cost of storing the index by 75%.

There are two more subtle benefits of compression. The first is increased use of caching. Search systems use some parts of the dictionary and the index much more than others. For example, if we cache the posting list of a frequently used query term w, then responding to that query reduces to a simple memory lookup. With compression, we can fit a lot more information into main memory. Instead of having to expend a disk seek when processing a query with w, we instead access its posting list in memory and decompress it. As we will see below, there are compression schemes with simple and efficient decompression, so that the penalty of having to decompress the posting list is small. As a result, we are able to decrease the response time of the IR system substantially. Since memory is a more expensive resource than disk space, increased speed due to caching – rather than decreased space requirements – is often the prime motivator for compression.

The second more subtle advantage of compression is faster transfer of data from disk to memory. Fast decompression algorithms run so fast on modern hardware that the total time of transferring a compressed chunk of data and then decompressing it is less than transferring the same chunk of data in uncompressed form. (This is true for large chunks of data – for a few kilobytes transfer time is dominated by seek time.) For instance, we can reduce I/O time by loading a much smaller compressed posting list, even when you add on the cost of decompression. So in most cases, the retrieval system will run faster on compressed posting lists than on uncompressed posting lists.

If the main goal of compression is to conserve disk space, then the speed of compression algorithms is of no concern. But for improved cache utiliza-

	term types			non-positional postings			tokens (= number of position entries in postings)		
	size	Δ%	%T	size	Δ%	%T	size	Δ%	%T
unfiltered	484,494			109,971,179			197,879,290		
no numbers	473,723	−2	−2	100,680,242	−8	−8	179,158,204	−9	−9
case folding	391,523	−17	−19	96,969,056	−3	−12	179,158,204	−0	−9
30 stop words	391,493	−0	−19	83,390,443	−14	−24	121,857,825	−31	−38
150 stop words	391,373	−0	−19	67,001,847	−30	−39	94,516,599	−47	−52
stemming	322,383	−17	−33	63,812,300	−4	−42	94,516,599	−0	−52

► **Table 5.1** The effect of preprocessing on the number of term types, non-positional postings, and positional postings for RCV1. "Δ%" indicates the reduction in size from the previous line, except that "30 stop words" and "150 stop words" both use "case folding" as their reference line. "%T" is the cumulative reduction (from unfiltered). We performed stemming with the Porter stemmer (Chapter 2, page 32).

tion and faster disk-to-memory transfer times decompression speeds must be high. Otherwise we will not be able to gain the intended speed advantages. The compression algorithms we discuss in this chapter are highly efficient and can therefore serve all three purposes of index compression.

This chapter first gives a statistical characterization of the distribution of the entities we want to compress – terms and postings in large collections (Section 5.1). We then look at compression of the dictionary, using the dictionary-as-a-string method and blocked storage (Section 5.2). Section 5.3 describes two techniques for compressing the postings file, variable byte encoding and γ encoding.

5.1 Statistical properties of terms in information retrieval

As in the last chapter, we will use Reuters-RCV1 as our model collection (see Table 4.2, page 64). We give some term and postings statistics for the collection in Table 5.1. "Δ%" indicates the reduction in size from the previous line. "%T" is the cumulative reduction from unfiltered.

The table shows that the number of term types is the main factor in determining the size of the dictionary. The number of non-positional postings is an indicator of the expected size of the non-positional index of the collection. The expected size of a positional index is related to the number of positions it must encode. Columns 2–4 of Table 5.1 show how many positions there are in RCV1 for different levels of preprocessing.

POSTING In this chapter, we define a *posting* as a docID in a posting list. For example, the posting list (6; 20, 45, 100), where 6 is the termID of the list's term, contains 3 postings. As discussed in Section 2.3.2 (page 39), postings in most

search systems also contain frequency and position information; but we will only cover simple docID postings in this chapter to simplify the discussion. See Section 5.4 for references that go beyond this simplified model.

In general, the statistics in Table 5.1 show that preprocessing affects the size of the dictionary and the number of non-positional postings greatly. Stemming and case folding reduce the number of term types (or distinct terms) by 17% each and the number of non-positional postings by 4% and 3%, respectively. The treatment of the most frequent words is also important. The *rule of 30* states that the 30 most common words account for 30% of the tokens in written text (31% in the table). Eliminating the 150 commonest words from indexing (as stop words; cf. Section 2.2.2, page 26) will cut 25–30% of the non-positional postings. But, while a stop list of 150 words reduces the number of postings by a quarter, this size reduction does not carry over to the size of the compressed index. As we will see later in this chapter, the posting lists of frequent words require only a few bits per posting after compression.

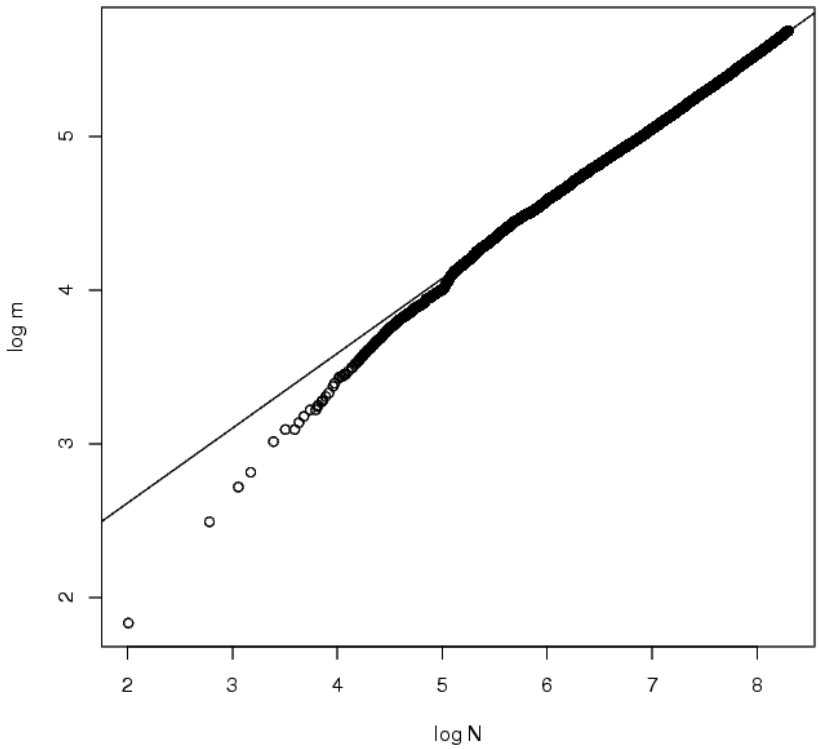
RULE OF 30

The deltas in the table are in a range typical of large collections. Note, however, that the percentage reductions can be very different for some text collections. For example, for a collection of web pages with a high proportion of French text, stemming or lemmatization would reduce vocabulary size much more than the Porter stemmer does for an English-only collection since French is a morphologically richer language than English.

The compression techniques we describe in the remainder of this chapter are *lossless*, that is, all information is preserved. Better compression ratios can be achieved with *lossy compression*, which discards some information. Case folding, stemming and stop word elimination are forms of lossy compression. Similarly, the vector space model (Chapter 6) and dimensionality reduction techniques like Latent Semantic Indexing (Chapter 18) create compact representations from which we cannot fully restore the original collection. Lossy compression makes sense when the "lost" information is unlikely ever to be used by the search system. For example, web search is characterized by a large number of documents, short queries, and users who only look at the first few pages of results. As a consequence, we can discard postings of documents that would only be used for hits far down the list. Thus, there are retrieval scenarios where lossy methods can be used for compression without any reduction in effectiveness.

LOSSLESS COMPRESSION
LOSSY COMPRESSION

Before introducing techniques for compressing the dictionary, we want to estimate the number of term types M in a collection. It is sometimes said that languages have a vocabulary of a certain size. The second edition of the Oxford English Dictionary (OED) defines more than 600,000 words. But the size of the OED cannot be equated with the size of the vocabulary in IR. The OED does not include most names of people, locations, products and scientific entities like genes. These names still need to be included in the inverted index, so our users can search for them.



► **Figure 5.1** Heaps' law. Vocabulary size M as a function of collection size T (number of tokens) for Reuters-RCV1. For these data, the line $\log_{10} M = 0.49 * \log_{10} T + 1.64$ is the best least squares fit. Thus, $k = 10^{1.64} \approx 44$ and $b = 0.49$.

5.1.1 Heaps' law: Estimating the number of term types

HEAPS' LAW

A better way of getting a handle on M is *Heaps' law*, which estimates vocabulary size as a function of collection size:

$$M = kT^b \tag{5.1}$$

where T is the number of tokens in the collection. Typical values for the parameters k and b are: $30 \leq k \leq 100$ and $b \approx 0.5$. The motivation for Heaps' law is that the simplest possible relationship between collection size and vocabulary size is linear in log-log space and the assumption of linearity is usually born out in practice as shown in Figure 5.1 for Reuters-RCV1. In this case, the fit is excellent for $T > 10^5 = 100{,}000$, for the parameter values $b = 0.49$ and $k = 44$. For example, for the first 1,000,020 tokens Heaps' law

predicts 38,323 term types:

$$44 \times 1{,}000{,}020^{0.49} \approx 38{,}323$$

The actual number is 38,365 term types, very close to the prediction.

The parameter k is quite variable because vocabulary growth depends a lot on the nature of the collection and how it is processed. Case-folding and stemming reduce the growth rate of the vocabulary, whereas including numbers and spelling errors will significantly increase it. Regardless of the values of the parameters for a particular collection, Heaps' law suggests that: (i) the dictionary size will continue to increase with more documents in the collection, rather than a maximum vocabulary size being reached, and (ii) the size of the dictionary will be quite large for large collections. These two hypotheses have been empirically shown to be true of large text collections (Section 5.4). So dictionary compression is important for an effective information retrieval system.

5.1.2 Zipf's law: Modeling the distribution of terms

We also want to understand how terms are distributed across documents. This will help us characterize the properties of the algorithms for compressing posting lists in Section 5.3.

ZIPF'S LAW A commonly used model of the distribution of terms in a collection is *Zipf's law*. It states that, if term 1 is the most common term in the collection, term 2 the next most common etc, then the collection frequency cf_i of the ith most common term is proportional to $1/i$:

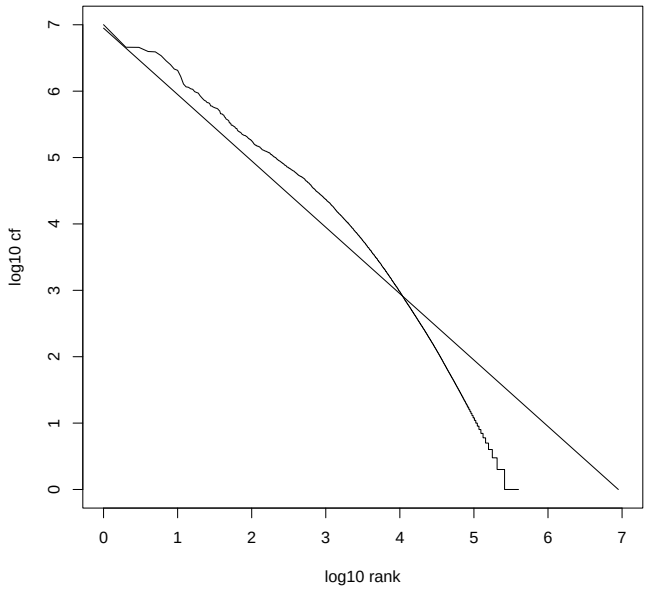
$$\text{cf}_i \propto \frac{1}{i} \tag{5.2}$$

So if the most frequent term occurs cf_1 times, then the second most frequent term has half as many occurrences, the third most frequent term a third as many occurrences, etc. The intuition is that frequency decreases very rapidly with rank. Equation 5.2 is one of the simplest ways of formalizing such a rapid decrease and it has been found to be a reasonably good model.

Equivalently, we can write Zipf's law as $f(i) = ci^k$ or as $\log f(i) = \log c + k \log i$ (where $k = -1$ and c is a constant to be defined below). It is therefore a *power law* with exponent $k = -1$. See Chapter 19, page 377, for another power law characterizing the distribution of links on web pages.

POWER LAW

The log-log graph in Figure 5.2 plots the collection frequency of a term as a function of its rank for Reuters-RCV1. A line with slope -1, corresponding to the Zipf function $\log f(i) = \log c - \log i$, is also shown. The fit of the data to the law is not particularly good, but good enough to serve as a model for term distributions in our calculations in Section 5.3.



► **Figure 5.2** Zipf's law for Reuters-RCV1. Frequency is plotted as a function of frequency rank for the terms in the collection. The line is the distribution predicted by Zipf's law (weighted least squares fit, intercept is 6.95).

5.2 Dictionary compression

This section presents a series of dictionary representations that achieve increasingly higher compression ratios. The dictionary is small compared to the postings file as suggested by Table 5.1. So why compress it if it is responsible for only a small percentage of the overall space requirements of the IR system?

One of the main determinants of response time of an IR system is the number of disk seeks necessary to process a query. If parts of the dictionary are on a disk, then many more disk seeks are necessary in query evaluation. Thus, the main goal of compressing the dictionary is to fit it in main memory, or at least a large portion of it, in order to support high query throughput. While dictionaries of very large collections will fit into the memory of a standard desktop machine, this is not true of many other application scenarios. For example, an enterprise search server for a large corporation may have to index

	term	freq.	pointer to posting list
	a	656,265	⟶
	aachen	65	⟶
	...	...	...
	zulu	221	⟶
space needed:	40 bytes	4 bytes	4 bytes

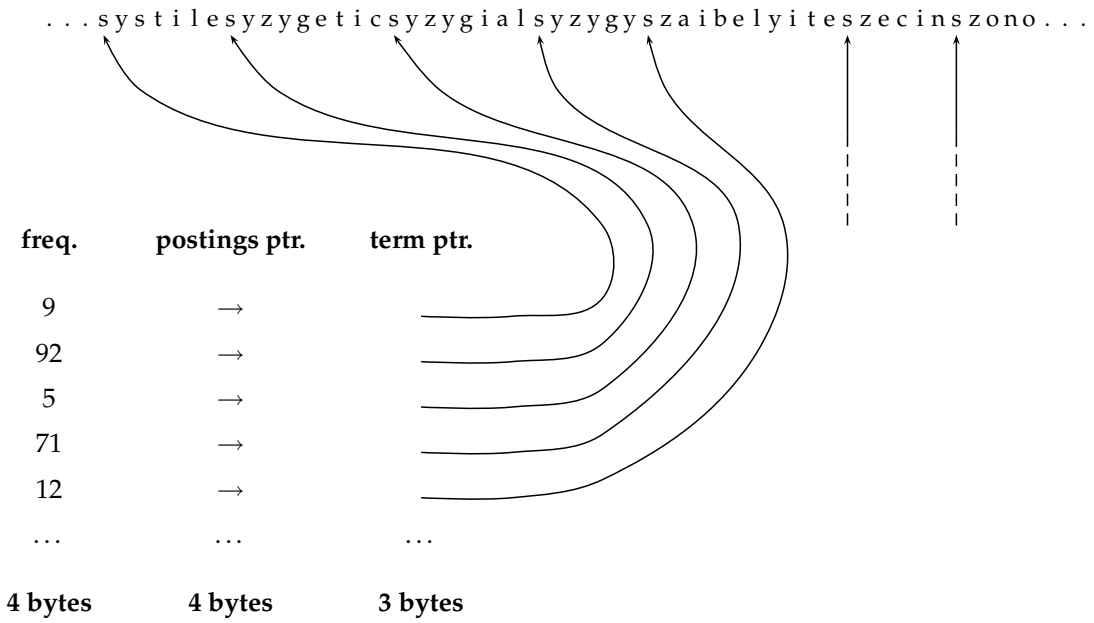
► **Figure 5.3** Storing the dictionary as an array of fixed-width entries.

a multi-terabyte collection with a comparatively large vocabulary because of the presence of documents in many different languages. We also want to be able to design search systems for limited hardware such as mobile phones and onboard computers. Other reasons for wanting to conserve memory are fast startup time and having to share resources with other applications. The search system on your PC must get along with the memory-hogging word processing suite you are using at the same time.

5.2.1 Dictionary-as-a-string

The simplest data structure for the dictionary is to store the lexicographically ordered list of all terms in an array of fixed-width entries as shown in Figure 5.3. Assuming a Unicode representation, we allocate 2×20 bytes for the term itself (since few terms have more than 20 characters in English), 4 bytes for its document frequency and 4 bytes for the pointer to its posting list. 4-byte pointers resolve a 4 GB address space. For large collections like the web, we need to allocate more bytes per pointer. We look up terms in the array by binary search. For Reuters-RCV1, we need $M \times (2 \times 20 + 4 + 4) = 400{,}000 \times 48 = 19.2$ MB for storing the dictionary in this scheme.

Using fixed-width entries for terms is clearly wasteful. The average length of a term in English is about 8 characters, so on average we are wasting 12 characters (or 24 bytes) in the fixed-width scheme. Also, we have no way of storing terms with more than 20 characters like hydrochlorofluorocarbons and supercalifragilisticexpialidocious. We can overcome these shortcomings by storing the dictionary terms as one long string of characters, as shown in Figure 5.4. The pointer to the next term is also used to demarcate the end of the current term. As before, we locate terms in the data structure by way of binary search in the (now smaller) table. This scheme saves us 60% compared to fixed-width storage – 24 bytes on average of the 40 bytes we allocated for terms before. However, we now also need to store term pointers. The term pointers resolve $400{,}000 \times 8 = 3.2 \times 10^6$ positions, so they need to be $\log_2 3{,}200{,}000 \approx 22$ bits or 3 bytes long.



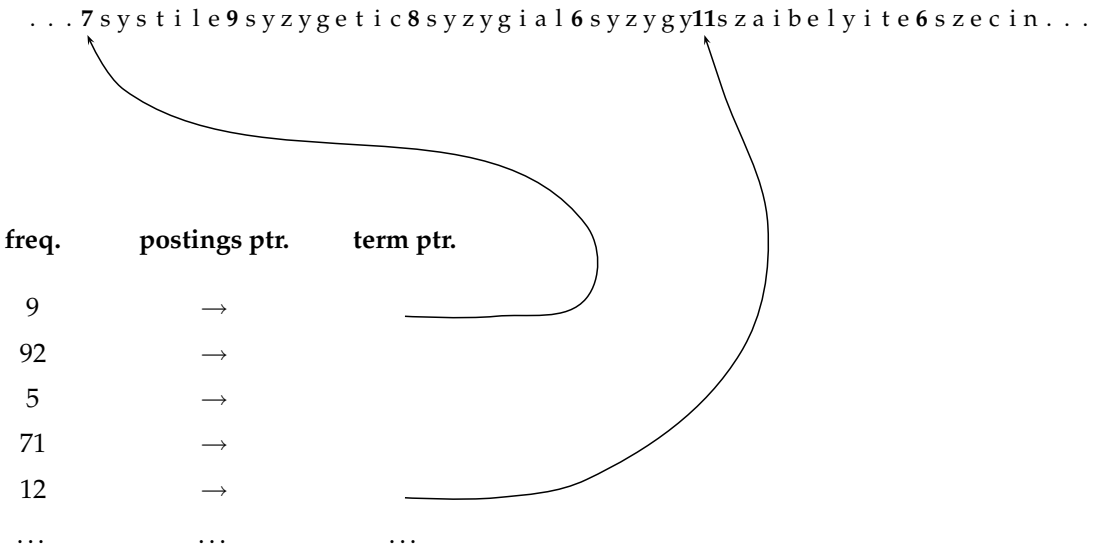
► **Figure 5.4** Dictionary-as-a-string storage. Pointers mark the end of the preceding term and the beginning of the next. For example, the first three terms in this example are systile (frequency 9), syzygetic (frequency 92) and syzygial (frequency 5).

In this new scheme, we need 400,000 $\times$ $(4 + 4 + 3 + 2 \times 8)$ $=$ 10.8 MB for the Reuters-RCV1 dictionary: 4 bytes each for frequency and postings pointer, 3 bytes for the term pointer, and 2×8 bytes on average for the term. So we have reduced the space requirements by almost half from 19.2 MB to 10.8 MB.

5.2.2 Blocked storage

We can further compress the dictionary by grouping terms in the string into blocks of size k and keeping a term pointer only for the first term of each block (see Figure 5.5). We store the length of the term in the string as an additional byte at the beginning of the term. We thus eliminate $k - 1$ term pointers, but need an additional k bytes for storing the length of each term. For $k = 4$, we save $(k - 1) \times 3 = 9$ bytes for term pointers, but need an additional $k = 4$ bytes for term lengths. So the total space requirements for the dictionary of Reuters-RCV1 are reduced by 5 bytes per 4-term block, or a total of 400,000 $\times$ $1/4 \times 5 = 0.5$ MB bringing us down to 10.3 MB.

By increasing the block size k, we get better compression. However, there



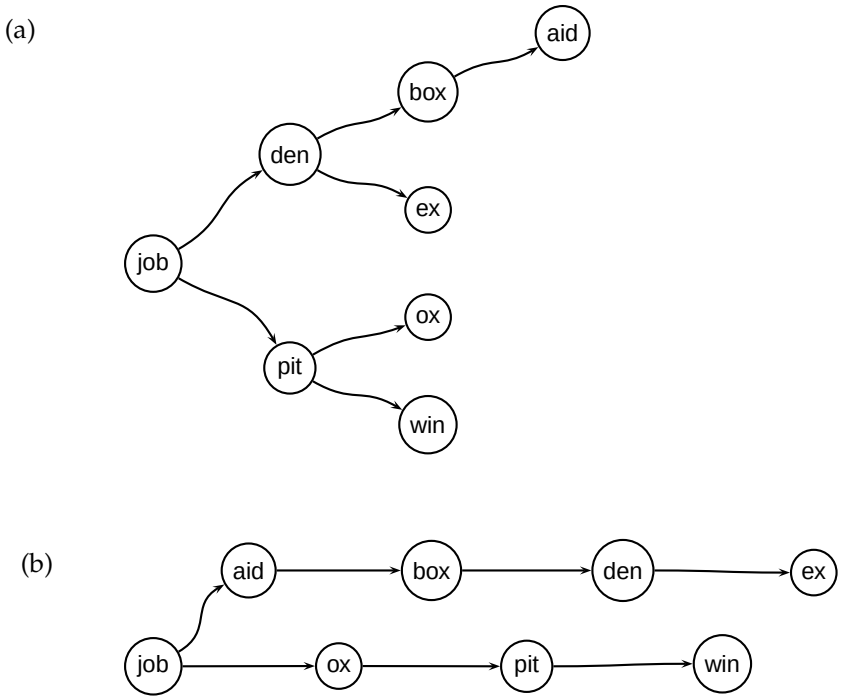
► **Figure 5.5** Blocked storage with four terms per block. The first block consists of systile, syzygetic, syzygial, and syzygy with lengths 7, 9, 8 and 6 characters, respectively. Each term is preceded by a byte encoding its length that indicates how many bytes to skip to reach subsequent terms.

is a tradeoff between compression and query processing speed. Searching the uncompressed eight-term dictionary in Figure 5.6 (a) takes on average $(4+3+2+3+1+3+2+3)/8 \approx 2.6$ steps, assuming each term is equally likely to come up in a query. For example, finding the first two terms, aid and box, takes 4 and 3 steps, respectively. With blocks of size $k = 4$, we need $(2+3+4+5+1+2+3+4)/8 = 3$ steps on average, 20% more (Figure 5.6, b). By increasing k, we can get the size of the compressed dictionary arbitrarily close to the minimum of $400{,}000 \times (4+4+1+2\times 8) = 10$ MB, but query processing becomes prohibitively slow for large values of k.

FRONT CODING

One source of redundancy in the dictionary we have not exploited yet is the fact that consecutive entries in an alphabetically sorted list share common prefixes. This observation leads to *front coding* as shown in Figure 5.7. A common prefix is identified for a subsequence of the term list and then referred to with a special character. In the case of Reuters, front coding saves another 2.4 MB.

Other schemes with even greater compression rely on minimal perfect hashing, i.e., a hash function that maps M terms onto $[1,\ldots,M]$ without collisions. However, we cannot adapt perfect hashes incrementally because each new term causes a collision and therefore requires the creation of a new



► **Figure 5.6** Search of the uncompressed dictionary (a) and a dictionary compressed by blocking with $k = 4$ (b).

One block in blocked compression ($k = 4$) ...
8 a u t o m a t a **8** a u t o m a t e **9** a u t o m a t i c **10** a u t o m a t i o n

⇓

... further compressed with front coding.
8 a u t o m a t ∗ a **1** ⋄ e **2** ⋄ i c **3** ⋄ i o n

► **Figure 5.7** Front coding. A sequence of terms with identical prefix ("automat" in this example) is encoded by marking the end of the prefix with ∗ and replacing it with ⋄ in subsequent terms. As before, the first byte of each entry encodes the number of characters.

representation	size in MB
dictionary, fixed-width	19.2
dictionary, term pointers into string	10.8
$\sim$, with blocking, $k = 4$	10.3
$\sim$, with blocking & front coding	7.9

► **Table 5.2** Dictionary compression for Reuters-RCV1.

	encoding	posting list								
the	docIDs	...		283042		283043		283044		283045 ...
	gaps				1		1		1	...
computer	docIDs	...		283047		283154		283159		283202 ...
	gaps				107		5		43	...
arachnocentric	docIDs	252000		500100						
	gaps	252000	248100							

► **Table 5.3** Encoding gaps instead of document ids. For example, we store gaps 14, 107, 5, ..., instead of docIDs 283047, 283154, 283159, ... for computer. The first docID is left unchanged (only shown for arachnocentric).

perfect hash function. Therefore, they are not very usable in a dynamic environment.

Even with the best compression scheme, it may not be feasible to store the entire dictionary in main memory for very large text collections and for hardware with limited memory. If we have to partition the dictionary onto pages that are stored on disk, then we can index the first term of each page using a B-tree. For processing most queries, the search system has to go to disk anyway to fetch the postings. One additional seek for retrieving the term's dictionary page from disk is a significant, but tolerable increase in the time it takes to process a query.

Table 5.2 summarizes the compression achieved by the four dictionary representation schemes.

5.3 Postings file compression

Recall from Table 4.2 (page 64) that Reuters-RCV1 has 800,000 documents, 200 tokens per document, 6 characters per token and 100,000,000 postings where we define a posting in this chapter as a docID in a posting list, that is, excluding frequency and position information. These numbers correspond to line 3 ("case folding") in Table 5.1. So the size of the collection is about 800,000 $\times$ 200 $\times$ 6 bytes = 960 MB. Document identifiers are $\log_2 800{,}000 \approx 20$ bits long. Thus, the size of the uncompressed postings file is 100,000,000 $\times$

docIDs	824	829	215406
gaps		5	214577
VB code	00000110 10111000	10000101	00001101 00001100 10110001

► **Table 5.4** Variable byte (VB) encoding. Gaps are encoded using an integral number of bytes. The first bit, the continuation bit, of each byte indicates whether the code ends with this byte (1) or not (0).

$20/8 = 250$ MB. To reduce its size, we need to devise methods that use fewer than 20 bits per document.

To devise a more efficient representation, we observe that the postings for frequent terms are close together. Imagine going through the documents of a collection one by one and looking for a frequent term like computer. We will find a document containing computer, then we skip a few documents that do not contain it, then there is again a document with the term and so on (see Table 5.3). The key idea is that the *gaps* between postings are short, requiring a lot less space than 20 bits to store. In fact, gaps for the most frequent terms such as the and for are mostly equal to 1. But the gaps for a rare term that occurs only once or twice in a collection (e.g., arachnocentric in Table 5.3) have the same order of magnitude as the docIDs and will need 20 bits. For an economical representation of this distribution of gaps, we need a *variable encoding* method that uses fewer bits for short gaps.

To encode small numbers in less space than large numbers, we look at two types of methods: bytewise compression and bitwise compression. As the names suggest, these methods attempt to encode gaps with the minimum number of bytes and bits, respectively.

5.3.1 Variable byte codes

VARIABLE BYTE ENCODING

CONTINUATION BIT

Variable byte (VB) encoding uses an integral number of bytes to encode a gap. The last 7 bits of a byte are "payload" and encode part of the gap. The first bit of the byte is a *continuation bit*. It is set to 1 for the last byte of the encoded gap and to 0 otherwise. To decode a variable byte code, we read a sequence of bytes with continuation bit 0 terminated by a byte with continuation bit 1. We then extract and concatenate the 7-bit parts. Figure 5.8 gives pseudocode for VB encoding and decoding and Table 5.4 an example of a VB-encoded posting list.[1]

With variable byte compression, the size of the compressed index for Reuters-

1. Note that the origin is 0 in the table. Since we never need to encode a docID or a gap of 0, in practice the origin is usually 1, so that 10000000 encodes 1, 10000101 encodes 6 (not 5 as in the table) etc. We find the origin-0 version easier to explain and understand.

```
VBENCODE(n)
1  bytes ← empty_list
2  while true
3  do PREPEND(bytes, n mod 128)
4     if n < 128
5        then BREAK
6     n ← n div 128
7  bytes[LENGTH(bytes)] += 128
8  return bytes

VBDECODE(bytes)
1  numbers ← empty_list
2  n ← 0
3  for i ← 1 to LENGTH(bytes)
4  do if bytes[i] < 128
5        then n ← 128 × n + bytes[i]
6        else n ← 128 × n + (bytes[i] − 128)
7             APPEND(numbers, n)
8             n ← 0
9  return numbers
```

► **Figure 5.8** Variable byte encoding and decoding. The functions div and mod compute integer division and remainder after integer division, respectively. Prepend adds an element to the beginning of a list.

RCV1 is 116 MB, a more than 50% reduction of the size of the uncompressed index (Table 5.6).

NIBBLE

The same general idea can also be applied to larger or smaller units: 32-bit words, 16-bit words, and 4-bit words or *nibbles*. Larger words further decrease the amount of bit manipulation necessary at the cost of less effective (or no) compression. Word sizes smaller than bytes get even better compression ratios at the cost of more bit manipulation. In general, bytes offer a good compromise between compression ratio and speed of decompression.

For most information retrieval systems variable byte codes offer an excellent tradeoff between time and space. They are also simple to implement – most of the alternatives referred to in Section 5.4 below are more complex. But if disk space is a scarce resource, we can achieve better compression ratios by using bit-level encodings, in particular two closely related encodings: γ codes, which we will turn to next, and δ codes (Exercise 5.9).

number	unary code	length	offset	γ code
0	0			
1	10	0		0
2	110	10	0	10,0
3	1110	10	1	10,1
4	11110	110	00	110,00
9	1111111110	1110	001	1110,001
13		1110	101	1110,101
24		11110	1000	11110,1000
511		111111110	11111111	111111110,11111111
1025		11111111110	0000000001	11111111110,0000000001

► **Table 5.5** Some examples of unary and γ codes. Unary codes are only shown for the smaller numbers. Commas in γ codes are for readability only and are not part of the actual codes.

5.3.2 γ codes

Variable byte codes use an adaptive number of *bytes* depending on the size of the gap. Bit-level codes adapt the length of the code on the finer grained *bit* level. The simplest bit-level code is *unary code*. The unary code of n is a string of n 1's followed by a 0 (see the first two columns of Table 5.5). Obviously, this is not a very efficient code, but it will come in handy in a moment.

UNARY CODE

How efficient can a code be in principle? Assuming the 2^n gaps G with $1 \leq G \leq 2^n$ are all equally likely, the optimal encoding uses n bits for each G. So some gaps ($G = 2^n$ in this case) cannot be encoded with fewer than $\log_2 G$ bits. Our goal is to get as close to this lower bound as possible.

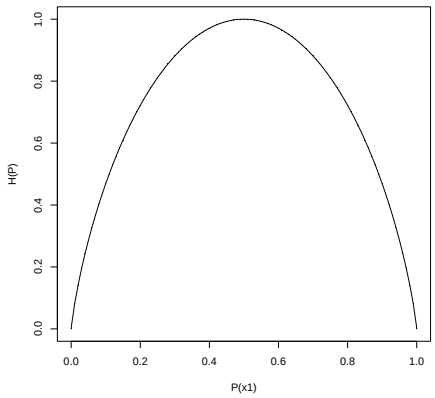
γ ENCODING

A method that is within a factor of optimal is γ *encoding*. γ codes implement variable length encoding by splitting the representation of a gap G into a pair of *length* and *offset*. *Offset* is G in binary, but with the leading 1 removed.[2] For example, for 13 (binary 1101) *offset* is 101. *Length* encodes the length of *offset* in unary code. For 13, the length of *offset* is 3 bits, which is 1110 in unary. The γ code of 13 is therefore 1110101. The right hand column of Table 5.5 gives some examples of γ codes.

A γ code is decoded by first reading the unary code up to the 0 that terminates it, e.g., the four bits 1110 when decoding 1110101. Now we know how long the offset is: 3. The offset 101 can then be read correctly and the 1 that was chopped off in encoding is prepended: $101 \rightarrow 1101 = 13$.

The length of *offset* is $\lfloor \log_2 G \rfloor$ bits and the length of *length* is $\lfloor \log_2 G \rfloor + 1$ bits, so the length of the entire code is $2 \times \lfloor \log_2 G \rfloor + 1$. γ codes are always

2. We assume here that G has no leading 0s. If there are any, they are removed before deleting the leading 1.



► **Figure 5.9** Entropy $H(P)$ as a function of $P(x_1)$ for a sample space with two outcomes x_1 and x_2.

of odd length and they are within a factor of 2 of what we claimed to be the optimal encoding length $\log_2 G$. We derived this optimum from the assumption that the 2^n gaps between 1 and 2^n are equiprobable. But this need not be the case. In general, we do not know the probability distribution over gaps a priori.

ENTROPY

The characteristic of a discrete probability distribution[3] P that determines its coding properties (including whether a code is optimal) is its *entropy* $H(P)$, which is defined as follows:

$$H(P) = -\sum_{x \in X} P(x) \log_2 P(x)$$

where X is the set of all possible numbers we need to be able to encode (and therefore $\sum_{x \in X} P(x) = 1.0$). Entropy is a measure of uncertainty as shown in Figure 5.9 for a probability distribution P over two possible outcomes, i.e., $X = \{x_1, x_2\}$. Entropy is maximized ($H(P) = 1$) for $P(x_1) = P(x_2) = 0.5$ when uncertainty about which x_i will appear next is largest; and minimized ($H(P) = 0$) for $P(x_1) = 1, P(x_2) = 0$ (or $P(x_1) = 0, P(x_2) = 1$) when there is absolute certainty.

It can be shown that the lower bound for the expected length $E(L)$ of a code L is $H(P)$ if certain conditions hold (see Section 5.4 for references). It

3. Readers who want to review basic concepts of probability theory may want to consult Rice (2006) or Ross (2006). Note that we are interested in probability distributions over integers (gaps, frequencies etc.), but that the coding properties of a probability distribution are independent of whether the outcomes are integers or something else.

can further be shown that for $1 < H(P) < \infty$, γ encoding is within a factor of 3 of this optimal encoding, approaching 2 for large $H(P)$:

$$\frac{E(L_\gamma)}{H(P)} \leq 2 + \frac{1}{H(P)} \leq 3$$

What is remarkable about this result is that it holds for any probability distribution P. So without knowing anything about the properties of the distribution of gaps, we can apply γ codes and be certain that they are within a factor of ≈ 2 of the optimal code for distributions of large entropy. A code like γ-code with the property of being within a factor of optimal for an arbitrary distribution P is called *universal*.

UNIVERSAL CODE

In addition to universality, γ codes have two other properties that are useful for index compression. First, they are *prefix-free*, i.e., no γ code is the prefix of another. This means that there is always a unique decoding of a sequence of γ-codes – and we do not need delimiters between them, which would decrease the efficiency of the code. The second property is that γ codes are *parameter-free*. For many other efficient codes, we have to fit a model (e.g., the binomial distribution) to the distribution of gaps in the index. This complicates the implementation of compression and decompression. In decompression, the parameters need to be stored and retrieved. And in dynamic indexing, the distribution of gaps can change, so that the original parameters are no longer appropriate. These problems are avoided with a parameter-free code.

PREFIX-FREE

PARAMETER-FREE

How much compression of the inverted index do γ codes achieve? To answer this question we use the model of term distribution we introduced in the last section, Zipf's law. We first derive the collection frequency of the ith term from Zipf's law. The collection frequency cf_i is proportional to the inverse of the rank i, that is, there is a constant c such that:

$$\text{cf}_i = \frac{c}{i} \tag{5.3}$$

We can choose c such that the cf_i are relative frequencies and sum to 1:

$$1 = \sum_{i=1}^{M} \frac{c}{i} = c \sum_{i=1}^{M} \frac{1}{i} = c\, H_M \tag{5.4}$$

$$c = \frac{1}{H_M} \tag{5.5}$$

where M is the number of distinct terms and H_M is the Mth harmonic number.[4] Reuters-RCV1 has $M = 400{,}000$ distinct terms and $H_M \approx \ln M$, so we

4. Note that, unfortunately, the conventional symbol for both entropy and harmonic number is H. Context should make clear which is meant in this chapter.

	N documents
Lc most frequent terms	
	N gaps of 1 each
Lc next most frequent terms	
	$N/2$ gaps of 2 each
Lc next most frequent terms	
	$N/3$ gaps of 3 each
...	...

► **Figure 5.10** Stratification of terms for estimating the size of a γ encoded inverted index.

have

$$c = \frac{1}{H_M} \approx \frac{1}{\ln M} = \frac{1}{\ln 400{,}000} \approx \frac{1}{13}$$

Thus the ith term has a relative frequency cf_i of roughly $1/(13i)$, and the expected average number of occurrences of term i in a document of length L_{ave} is:

$$L\frac{c}{i} \approx \frac{200 \times \frac{1}{13}}{i} \approx \frac{15}{i}$$

where we interpret cf_i as a term occurrence probability. Recall that 200 is the average number of tokens per document in RCV1 (Table 4.2).

Now we have derived term statistics that characterize the distribution of terms in the collection and, by extension, the distribution of gaps in the posting lists. From these statistics, we can calculate the space requirements for an inverted index compressed with γ encoding. We first stratify the vocabulary into blocks of size $Lc = 15$. On average, term i occurs $15/i$ times per document. So the average number of occurrences $\overline{f}$ per document is $1 \leq \overline{f}$ for terms in the first block, corresponding to a total number of N gaps per term. The average is $\frac{1}{2} \leq \overline{f} < 1$ for terms in the second block, corresponding to $N/2$ gaps per term, and $\frac{1}{3} \leq \overline{f} < \frac{1}{2}$ for terms in the third block, corresponding to $N/3$ gaps per term etc. (We take the lower bound because it simplifies subsequent calculations. As we will see, the final estimate is too pessimistic even with this assumption.) We will make the somewhat unrealistic assumption that all gaps for a given term have the same size as shown in Figure 5.10. Assuming such a uniform distribution of gaps, we then have gaps of size 1 in block 1, gaps of size 2 in block 2, etc.

Encoding the N/j gaps of size j with γ codes, the number of bits needed for the posting list of a term in the jth block (corresponding to one row in the figure) is:

$$\begin{aligned} \textit{bits-per-row} &= \frac{N}{j} \times (2 \times \lfloor \log_2 j \rfloor + 1) \\ &\approx \frac{2N \log_2 j}{j} \end{aligned}$$

To encode the entire block, we need $(2NLc \log_2 j)/j$ bits. There are $M/(Lc)$ blocks, so the postings file as a whole will take up:

$$\sum_{j=1}^{\frac{M}{Lc}} \frac{2NLc \log_2 j}{j} \tag{5.6}$$

For Reuters-RCV1, $\frac{M}{Lc} \approx 400{,}000/15 \approx 27{,}000$ and

$$\sum_{j=1}^{27{,}000} \frac{2 \times 10^6 \times 15 \log_2 j}{j} \approx 224 \text{ MB} \tag{5.7}$$

So the postings file of the compressed inverted index for our 960 MB collection has a size of 224 MB, one fourth the size of the original collection.

When we run γ compression on Reuters-RCV1, the actual size of the compressed index is even lower: 101 MB, a bit more than a tenth of the size of the collection. The reason for the discrepancy between predicted and actual value is that (i) Zipf's law is not a very good approximation of the actual distribution of term frequencies for Reuters-RCV1 and (ii) gaps are not uniform. The Zipf model predicts an index size of 251 MB for the unrounded numbers from Table 4.2. If term frequencies are generated from the Zipf model and a compressed index is created for these artificial terms, then the compressed size is 254 MB. So to the extent that the assumptions about the distribution of term frequencies are accurate, the predictions of the model are correct.

Table 5.6 summarizes the compression techniques covered in this chapter. The term incidence matrix (Figure 1.1, page 4) for Reuters-RCV1 has size $400{,}000 \times 800{,}000 = 40 \times 8 \times 10^9$ bits or 40 GB. The numbers were the collection (3600 MB and 960 MB) are for the encoding of RCV1 of CD, which uses one byte per character, not Unicode.

γ codes achieve great compression ratios – about 15% better than variable byte codes for Reuters-RCV1. But they are expensive to decode. This is because many bit-level operations – shifts and masks – are necessary to decode a sequence of γ codes as the boundaries between codes will usually be somewhere in the middle of a machine word. As a result, query processing is more

representation	size in MB
dictionary, fixed-width	19.2
dictionary, term pointers into string	10.8
$\sim$, with blocking, $k = 4$	10.3
$\sim$, with blocking & front coding	7.9
collection (text, xml markup etc)	3600.0
collection (text)	960.0
term incidence matrix	4000.0
postings, uncompressed (32-bit words)	400.0
postings, uncompressed (20 bits)	250.0
postings, variable byte encoded	116.0
postings, γ encoded	101.0

► **Table 5.6** Index and dictionary compression for Reuters-RCV1. The compression ratio depends on the proportion of actual text in the collection. RCV1 contains a large amount of XML markup. Using the two best compression schemes, γ encoding and blocked storage, the ratio collection size to compressed index is therefore especially small for RCV1: $(101 + 7.9)/3600 \approx 0.03$.

expensive for γ codes than for variable byte codes. Whether variable byte or γ encoding is more advantageous for an application depends on the relative weights we give to conserving disk space versus maximizing query response time.

The compression ratio for the index in Table 5.6 is about 25%: 400 MB (uncompressed, machine word-aligned postings) vs. 101 MB (γ) and 116 MB (VB). This shows that both γ and VB codes meet the objectives we stated in the beginning of the chapter. Index compression substantially improves time and space efficiency of indexes by reducing the amount of disk space needed, increasing the amount of information that can be kept in the cache, and speeding up data transfers from disk to memory.

5.4 References and further reading

Heaps' law was introduced by Heaps (1978). See also Baeza-Yates and Ribeiro-Neto (1999). A detailed study of vocabulary growth in large collections is (Williams and Zobel 2005). Zipf's law is due to Zipf (1949). Witten and Bell (1990) investigate the quality of the fit obtained by the law. Other term distribution models, including K mixture and two-poisson model, are discussed by (Manning and Schütze 1999, ch. 15). Carmel et al. (2001), Büttcher and Clarke (2006) and Blanco and Barreiro (2007) show that lossy compression can achieve good compression with no or no significant decrease in retrieval effectiveness.

Dictionary compression is covered in detail by (Witten et al. 1999, ch. 4), which is recommended as additional reading.

Subsection 5.3.1 is based on Scholer et al. (2002). They find that variable byte codes process queries twice as fast as both bit-level compressed indexes and uncompressed indexes with a 30% penalty in compression ratio compared to the best bit-level compression method. They also show that compressed indexes can be superior to uncompressed indexes not only in disk usage, but also in query processing speed. Compared to VB codes, "variable nibble" codes showed 5%–10% better compression and up to a third worse retrieval effectiveness in one experiment (Anh and Moffat 2005). Trotman (2003) also recommends using VB codes unless disk space is at a premium. In recent work, Anh and Moffat (2005; 2006a), Zukowski et al. (2006) have constructed word-aligned binary codes that are both faster in decompression and at least as efficient as VB codes.

δ codes (Exercise 5.9) and γ codes were introduced by Elias (1975) who proved that both codes are universal. In addition, δ codes are asymptotically optimal for $H(P) \rightarrow \infty$. δ codes perform better than γ codes if large numbers (greater than 15) dominate. A good introduction to information theory, including the concept of entropy, is (Cover and Thomas 1991). While Elias codes are only asymptotically optimal, arithmetic codes (Witten et al. 1999, sec. 2.4) can be constructed to be arbitrarily close to the optimum $H(P)$ for any P.

Several additional index compression techniques are covered by Witten et al. (1999) (Sections 3.3 and 3.4 and Chapter 5). They recommend using parameterized methods for index compression, methods that explicitly model the probability distribution of gaps for each term. For example, they show that *Golomb codes* achieve better better compression ratios than γ codes for large collections. Moffat and Zobel (1992) compare several parameterized methods, including LLRUN (Fraenkel and Klein 1985).

GOLOMB CODES

Different considerations apply to the compression of term frequencies and word positions than to the compression of docIDs in posting lists. See Scholer et al. (2002) and Zobel and Moffat (2006). Zobel and Moffat (2006) is recommended in general as an in-depth and up-to-date tutorial on inverted indexes, including index compression.

This chapter only looks at index compression for Boolean retrieval. For ranked retrieval (Chapter 6), it is advantageous to order postings according to term frequency instead of docID. During query processing, the scanning of many posting lists can then be terminated early because smaller weights do not change the ranking of the highest ranked k documents found so far. Document length is precomputed and stored separately in ranked retrieval. It is not a good idea to precompute and store weights in the index (as opposed to frequencies) because they cannot be compressed as well as integers. See Persin et al. (1996) and Anh and Moffat (2006b) for representing the im-

IMPACT portance of a term by its term frequency or by a discretized weight or *impact* (see (Section 7.1.5, page 132)).

Document compression is also important in an efficient information retrieval system. de Moura et al. (2000) and Brisaboa et al. (2007) describe compression schemes that allow direct searching of terms and phrases in the compressed text, which is infeasible with standard text compression utilities like gzip and compress.

5.5 Exercises

Exercise 5.1

Estimate the space usage of the Reuters dictionary with blocks of size $k = 8$ and $k = 16$ in blocked dictionary storage.

Exercise 5.2

Estimate the time needed for term lookup in the compressed dictionary of Reuters with block sizes of $k = 4$ (Figure 5.6, b), $k = 8$ and $k = 16$ What is the slowdown compared to $k = 1$ (Figure 5.6, a)?

Exercise 5.3

Assuming one machine word per posting, what is the size of the uncompressed (non-positional) index for different tokenizations based on Table 5.1. How do these numbers compare with Table 5.6?

Exercise 5.4

Compute variable byte codes for the numbers in Tables 5.3 and 5.5.

Exercise 5.5

Compute variable byte and γ codes for the posting list 777, 17743, 294068, 31251336. Use gaps instead of docIDs where possible. Write binary codes in 8-bit blocks.

Exercise 5.6

Consider the posting list $< 4, 10, 11, 12, 15, 62, 63, 265, 268, 270, 400 >$ with a corresponding list of document gaps $< 4, 6, 1, 1, 3, 47, 1, 202, 3, 2, 130 >$. Assume that the length of the posting list is stored separately, so the system knows when a posting list is complete. Using variable byte encoding: (i) What is the largest gap you can encode in 1 byte? (ii) What is the largest gap you can encode in 2 bytes? (iii) How many bytes will the above posting list require under this encoding? (Count only space for encoding the sequence of numbers.)

Exercise 5.7

A little trick is to notice that a gap cannot be of length 0 and that the stuff left to encode after shifting cannot be 0. Based on these observations: (i) Suggest a modification to variable byte encoding that allows you to encode slightly larger gaps in the same amount of space. (ii) What is the largest gap you can encode in 1 byte? (iii) What is the largest gap you can encode in 2 bytes? (iv) How many bytes will the posting list in Exercise 5.6 require under encoding? (Count only space for encoding the sequence of numbers.)

Exercise 5.8

From the following sequence of γ coded gaps, reconstruct first the gap sequence and then the postings sequence: 1110001110101011111101101111011.

Exercise 5.9

δ-CODES

γ-codes are relatively inefficient for large numbers (e.g., 1025 in Table 5.5) as they encode the length of the offset in inefficient unary code. *δ-codes* differ from γ-codes in that they encode the first part of the code (*length*) in γ-code instead of unary code. The encoding of *offset* is the same. For example, the δ-code of 7 is 10,0,11 (again, we add commas for readability). 10,0 is the γ-code for *length* (2 in this case) and the encoding of *offset* (11) is unchanged. (i) Compute the δ-codes for the other numbers in Table 5.5. For what range of numbers is the δ-code shorter than the γ-code? (ii) γ code beats variable byte code in Table 5.6 because the index contains stop words and thus many small gaps. Show that variable byte code is more compact if larger gaps dominate. (iii) Compare the compression ratios of δ code and variable byte code for a distribution of gaps dominated by large gaps.

Exercise 5.10

We have defined unary codes as being "10": sequences of 1s terminated by a 0. Interchanging the roles of 0s and 1s yields an equivalent "01" unary code. When this 01 unary code is used, the construction of a γ-code can be stated as follows: 1. Write G down in binary using $b = \lfloor \log_2 j \rfloor + 1$ bits. 2. Prepend $(b - 1)$ 0s. Show that this method produces a well-defined alternative γ-code.

Exercise 5.11

Unary code is not a universal code in the sense defined above. However, there exists a distribution over gaps for which unary code is optimal. Which distribution is this?

Exercise 5.12

Give some examples of terms that violate the assumption that gaps all have the same size (which we made when estimating the space requirements of a γ encoded index). What are general characteristics of these terms?

Exercise 5.13

If a term's distribution is not uniform and its gaps are of variable size, will that increase or decrease the size of the γ-compressed posting list?

Exercise 5.14

Work out the sum in Equation 5.7 and show it adds up to about 251 MB. Use the numbers in Table 4.2, but do not round Lc, c and the number of vocabulary blocks.

Exercise 5.15

Go through the above calculation of index size and explicitly state all the approximations that were made to arrive at Expression 5.6.

Exercise 5.16

For a collection of your choosing determine the number of documents and terms and the average length of a document. (i) How large is the inverted index predicted to be by Equation 5.6? (ii) Implement an indexer that creates a γ-compressed inverted index for the collection. How large is the actual index? (iii) Implement an indexer that uses variable byte encoding. How large is the variable byte encoded index?

γ encoded gap sequence of run 1	1110110111111001011111111110100011111001
γ encoded gap sequence of run 2	1111101000011111100010001111111001000011111010101

► **Table 5.7** Two gap sequences to be merged in block merge indexing.

Exercise 5.17

To be able to hold as many postings as possible in main memory, it is a good idea to compress intermediate index files during index construction. (i) This makes merging runs in block merge indexing more complicated. As an example, work out the γ encoded merged sequence of the gaps in Table 5.7. (ii) Index construction is more space-efficient when using compression. Would you also expect it to be faster?

Exercise 5.18

Show that the size of the vocabulary is finite according to Zipf's law and infinite according to Heaps' law. Given this, can we derive Heaps' law from Zipf's law?

6 *Term weighting and vector space models*

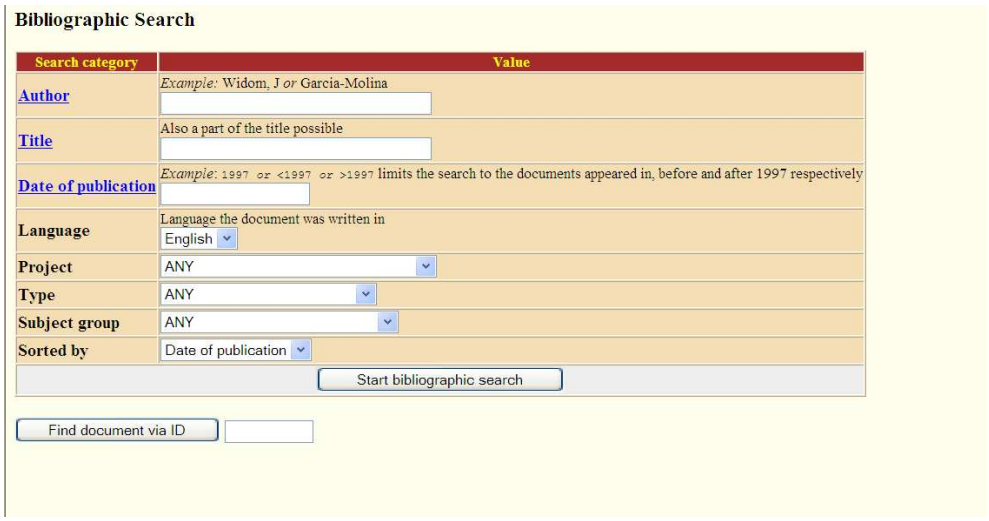
Thus far we have dealt with indexes that support Boolean queries: a document either matches or does not match a query. In the case of large document collections, the resulting number of matching documents can be far in excess of the number a human user could possibly sift through. Accordingly, it is essential for search engines to rank-order the documents matching a query. To do this, an engine computes, for each matching document, a score with respect to the query at hand. In this chapter we initiate the study of assigning a score to a (query, document) pair. We first introduce parametric and zone indexes, which score documents by weighting differently the various parts of a document where a query term occurs; in the process we extend the applicability of inverted indexes to scoring. We then consider the problem of gauging the importance of a term in a document, based on the statistics of occurrence of the term in the document. By viewing each document as a vector of such importance weights, we compute a score between a query and each document. Chapter 7 develops computational aspects of such scoring, and related topics.

6.1 Parametric and zone indexes

We have thus far viewed a document as a sequence of terms. In fact, most documents in the real world have additional structure. Digital documents generally encode, in machine-recognizable form, certain *metadata* associated with each document. By metadata, we mean specific forms of data about a document, such as its author(s), title and date of publication. This metadata would generally include *fields* such as the date of creation and the format of the document, and often the author and possibly the title of the document. Consider queries of the form "find documents authored by William Shakespeare in 1601, containing the phrase alas poor Yorick". Query processing then consists as usual of postings merges, except that we may merge postings from text as well as parametric indexes. Where the field values can be or-

METADATA

FIELD



► **Figure 6.1** Parametric search. In this example we have a collection with fields allowing us to select publications by zones such as Author and fields such as Language.

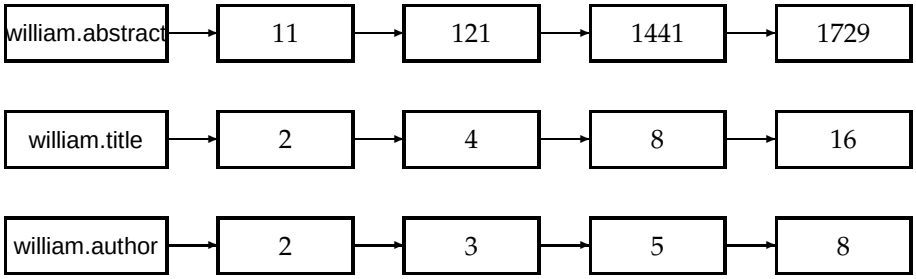
dered (as in the case of dates, for instance) we additionally build a search tree on the ordered universe of values to support range queries. Figure 6.1 illustrates this. Some of the fields may assume ordered values, such as dates; in the example query above, the year 1601 is one such field value. The engine may support querying ranges on such ordered values; to this end, a structure like a B-tree may be used on the field's dictionary.

ZONE

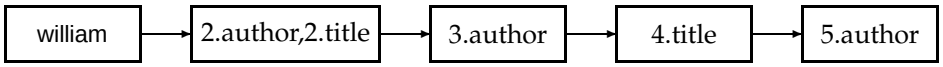
Zones are similar to fields, except the contents of a zone can be an arbitrary body of text. Whereas a field may assume a relatively small set of values, a zone can be thought of as an unbounded amount of text. For instance, document titles and abstracts are generally treated as zones. We may build a separate inverted index for each zone of a document, to support queries such as "find documents with merchant in the title and william in the author list and the phrase gentle rain in the body". This has the effect of building an index that looks like Figure 6.2.

In fact, we can reduce the size of the dictionary by encoding the zone in which a term occurs in the postings. In Figure 6.3 for instance, we show how occurrences of william in the title and author zones of various documents are encoded. Such an encoding is useful when the size of the dictionary is a concern (because we require the dictionary to fit in main memory). But there is another important reason why the encoding of Figure 6.3 is useful: the efficient computation of scores using a technique we will call *weighted zone*

WEIGHTED ZONE SCORING



► **Figure 6.2** Basic zone index ; zones are encoded as extensions of dictionary entries.



► **Figure 6.3** Zone index in which the zone is encoded in the postings rather than the dictionary.

scoring.

6.1.1 Weighted zone scoring

Given a Boolean query q and a document d, weighted zone scoring assigns to the pair (q, d) a score in the interval $[0, 1]$, by computing a linear combination of *zone scores*, where each zone of the document contributes a Boolean value. More specifically, consider a set of documents each of which has ℓ (identical) zones. Let $w_1, \ldots, w_\ell \in [0, 1]$ such that $\sum_{i=1}^{\ell} w_i = 1$. For $1 \leq i \leq \ell$, let s_i be the Boolean score denoting a match (or absence thereof) between q and the ith zone. For instance, the Boolean score from a zone could be 1 if all the query term(s) occur in that zone, and zero otherwise; indeed, it could be any Boolean function that maps the presence of query terms in a zone to $0, 1$. Then, the weighted zone score is defined to be

$$\sum_{i=1}^{\ell} w_i s_i. \tag{6.1}$$

```
ZONESCORE(q1, q2)
 1  int scores[N] = 0
 2  constant w[ℓ]
 3  p1 ← postings(q1)
 4  p2 ← postings(q2)
 5  // scores[] is an array with a score entry for each document, initialized to zero.
 6  //p1 and p2 are initialized to point to the beginning of their respective postings.
 7  //Assume w[] is initialized to the respective zone weights.
 8  while p1 ≠ NIL and p2 ≠ NIL
 9  do if docID[q1] = docID[q2]
10        then WEIGHTEDZONE(score[p1, p2, docID[p1]])
11             p1 ← next[p1]
12             p2 ← next[p2]
13        else if docID[p1] < docID[p2]
14                then p1 ← next[p1]
15                else p2 ← next[p2]
16  return scores
```

► **Figure 6.4** Algorithm for computing the weighted zone score from two postings lists. WeightedZone (not shown here) is assumed to compute the inner loop of Equation 6.1.

✎ **Example 6.1:** Consider the query shakespeare in a collection in which each document has three zones: *author, title* and *body*. The Boolean score function for a zone takes on the value 1 if the query term shakespeare is present in the zone, and zero otherwise. Weighted zone scoring in such a collection would require three weights w_1, w_2 and w_3, respectively corresponding to the *author, title* and *body* zones. Suppose we set $w_1 = 0.2, w_2 = 0.3$ and $w_3 = 0.5$ (so that the three weights add up to 1); this corresponds to an application in which a match in the *author* zone is least important to the overall score, the *title* zone somewhat more, and the *body* contributes as much as either *author* and *title*.

Thus if the term shakespeare were to appear in the *title* and *body* zones but not the *author* zone of a document, the score of this document would be 0.8.

How do we implement the computation of weighted zone scores? A simple approach would be to compute the score for each document in turn, adding in all the contributions from the various zones. However, we now show how we may compute weighted zone scores as in Equation (6.1) directly from inverted indexes. The algorithm of Figure 6.4 treats the case when the query q is a two-term query consisting of query terms q_1 and q_2, and the Boolean function is AND: 1 if both query terms are present in a zone and 0 otherwise. Following the description of the algorithm, we describe the extension to more complex queries and Boolean functions.

The reader may have noticed the close similarity between this algorithm and that in Figure 1.6. Indeed, they represent the same postings traversal, except that instead of merely adding a document to the set of results for a Boolean AND query, we now compute a score for each such document. Some literature refers to the array scores[] above as a set of *accumulator*accumulators. The reason for this will be clear as we consider more complex Boolean functions than the AND; thus we may assign a non-zero score to a document even if it does not contain all query terms.

ACCUMULATOR

6.1.2 Learning weights

How do we determine the weights w_i for weighted zone scoring? These weights could be determined by an expert; but increasingly, these weights are "learned" using training examples that have been judged editorially. This latter methodology falls under a general class of approaches to scoring and ranking in information retrieval, known as *machine-learned relevance*.

MACHINE-LEARNED RELEVANCE

1. We are provided with a set of *training examples*, each of which is a pair consisting of a query and a document, together with a relevance judgment for that document on that query. In the simplest form, the relevance judgments are *Relevant* or *Non-relevant*. More sophisticated implementations of the methodology make use of more nuanced judgments.

2. The weights w_i are then "learned" from these examples, in order that the learned scores approximate the given training examples.

For weighted zone scoring, the process may be viewed as learning a linear function of the Boolean match scores contributed by the various zones. The expensive component of this methodology is the availability of user-generated relevance judgments from which to learn the weights, especially in a collection that changes frequently (such as the Web). We now detail a simple example that illustrates how, we can reduce the problem of learning the weights w_i to a simple optimization problem.

We now consider a simple case of weighted zone scoring, where each document has a *title* zone and a *body* zone. Given a query q and a document d, we use the given Boolean match function to compute Boolean variables $s_T(d,q)$ and $s_B(d,q)$, depending on whether the title (respectively, body) zone of d match query q. For instance, the algorithm in Figure 6.4 uses an AND of the query terms for this Boolean function. We will compute a score between 0 and 1 for each (document, query) pair using $s_T(d,q)$ and $s_B(d,q)$ by using a constant $w \in [0,1]$, as follows:

$$score(d,q) = w \cdot s_T(d,q) + (1-w)s_B(d,q). \tag{6.2}$$

Example	DocID	Query	s_T	s_B	Judgment
Φ_1	37	linux	1	1	Relevant
Φ_2	37	penguin	0	1	Non-relevant
Φ_3	238	system	0	1	Relevant
Φ_4	238	penguin	0	0	Non-relevant
Φ_5	1741	kernel	1	1	Relevant
Φ_6	2094	driver	0	1	Relevant
Φ_7	3191	driver	1	0	Non-relevant

► **Figure 6.5** An illustration of training examples.

We now describe how to determine the constant w from a set of *training examples*, each of which is a triple of the form $\Phi_t = (d_t, q_t, r(d_t, q_t))$. In each training example, a given training document d_t and a given training query q_t are assessed by a human editor who delivers a relevance judgment $r(d_t, q_t)$ that is either *Relevant* or *Non-relevant*. This is illustrated in Figure 6.5, where seven training examples are shown.

For each training example Φ_t we have Boolean values $s_T(d_t, q_t)$ and $s_B(d_t, q_t)$ that we use to compute a score from (6.2)

$$score(d_t, q_t) = w \cdot s_T(d_t, q_t) + (1 - w)s_B(d_t, q_t). \tag{6.3}$$

We now compare this computed score to the human relevance judgment for the same document-query pair (d_t, q_t); to this end, we will quantize each *Relevant* judgment as a 1 and each *Non-relevant* judgment as a 0. Suppose that we define the error of the scoring function with weight w as

$$\varepsilon(w, \Phi_t) = (r(d_t, q_t) - score(d_t, q_t))^2,$$

where we have quantized the editorial relevance judgment to 0 or 1. Then, the total error of a set of training examples is given by

$$\sum_{\Phi_t} \varepsilon(w, \Phi_t). \tag{6.4}$$

The problem of learning the constant w from the given training examples then reduces to picking the value of w that minimizes the total error in (6.4).

Picking the best value of w in (6.4) in the formulation of Section 6.1.3 reduces to the problem of minimizing a quadratic function of w over the interval $[0, 1]$. This reduction is detailed in Section 6.1.3.

6.1.3 The optimal weight w

We begin by noting that for any training example Φ_t for which $s_T(d_t, q_t) = 0$ and $s_B(d_t, q_t) = 1$, the score computed by Equation (6.2) is $1 - w$. In similar

s_T	s_B	Score
0	0	0
0	1	$1 - w$
1	0	w
1	1	1

► **Figure 6.6** The four possible combinations of s_T and s_B.

fashion, we may write down the score computed by Equation (6.2) for the three other possible combinations of $s_T(d_t, q_t)$ and $s_B(d_t, q_t)$; this is summarized in Figure 6.6.

Let n_{01r} (respectively, n_{01i}) denote the number of training examples for which $s_T(d_t, q_t) = 0$ and $s_B(d_t, q_t) = 1$ and the editorial judgment is *Relevant* (respectively, *Non-relevant*). Then the contribution to the total error in Equation (6.4) from training examples for which $s_T(d_t, q_t) = 0$ and $s_B(d_t, q_t) = 1$ is

$$[1 - (1 - w)]^2 n_{01r} + [0 - (1 - w)]^2 n_{01i}.$$

By writing in similar fashion the error contributions from training examples of the other three values of $s_T(d_t, q_t)$ and $s_B(d_t, q_t)$ (and extending the notation in the obvious manner), the total error corresponding to Equation (6.4) is

$$(n_{01r} + n_{10i})w^2 + (n_{10r} + n_{01i})(1 - w)^2 + n_{00r} + n_{11i}. \tag{6.5}$$

By differentiating Equation (6.5) with respect to w and setting the result to zero, it follows that the optimal value of w is

$$\frac{n_{10r} + n_{01i}}{n_{10r} + n_{10i} + n_{01r} + n_{01i}}. \tag{6.6}$$

Exercise 6.1

When using weighted zone scoring, is it necessary for all zones to use the same Boolean match function?

Exercise 6.2

In Worked Example 6.1 above with weights $w_1 = 0.2, w_2 = 0.31$ and $w_3 = 0.49$, what are all the distinct score values a document may get?

Exercise 6.3

Rewrite the algorithm in Figure 6.4 to the case of more than two query terms.

Exercise 6.4

Write pseudocode for the function WeightedZone for the case of two postings lists in Figure 6.4.

Exercise 6.5

Apply Equation 6.6 to the sample training set in Figure 6.5 to estimate the best value of w for this sample.

Exercise 6.6

For the value of w estimated in Exercise 6.5, compute the weighted zone score for each (query, document) example. How do these scores relate to the relevance judgments (quantized to 0/1)?

Exercise 6.7

Why does the expression for w in (6.6) not involve training examples in which $s_T(d_t, q_t)$ and $s_B(d_t, q_t)$ have the same value?

6.2 Term frequency and weighting

Thus far, scoring has hinged on whether or not a query term is present in a zone within a document. We take the next logical step: a document or zone that mentions a query term more often has more to do with that query and therefore should receive a higher score. To motivate this we introduce the notion of a *free text query*: a query in which the terms of the query are typed freeform into the search interface, without any connecting search operators (such as Boolean operators). This query style, which is extremely popular on the web, views the query as simply a set of terms. A plausible scoring mechanism then is to compute a score that is the sum, over the query terms, of the match scores between each term and the document. How do we determine such a match score between a query term and each document?

FREE TEXT QUERY

To this end, we assign to each term in a document a *weight* for that term, that depends on the number of occurrences of the term in the document. The simplest approach is to assign the weight to be equal to the number of occurrences of the term t in document d. This weighting scheme is referred to as *term frequency* and is denoted $\text{tf}_{t,d}$, with the subscripts denoting the term and the document in order.

TERM FREQUENCY

For a document d, the set of weights (determined by the tf weighting function above, or indeed any weighting function that maps the number of occurrences of t in d to a positive real value) may be viewed as a vector, with one component for each distinct term. In this view of a document, known in the literature as the *bag of words model*, the exact ordering of the terms in a document is ignored. The vector view only retains information on the number of occurrences. Thus, the document "Mary is quicker than John" is, in this view, identical to the document "John is quicker than Mary". Nevertheless, it seems intuitive that two documents with similar vector representations are similar in content. We will develop this intuition further in Section 6.4. Before doing so we first study the question: are all words in a document equally important? Clearly not; in Section 2.2.2 (page 26) we looked at the

BAG OF WORDS

Word	cf	df
try	10422	8760
insurance	10440	3997

► **Figure 6.7** Collection frequency (cf) and document frequency (df) behave differently.

idea of *stop words* – words that we decide not to index at all, and therefore do not contribute in any way to retrieval and scoring.

6.2.1 Inverse document frequency

Raw term frequency as above suffers from a critical problem: all terms are considered equally important when it comes to assessing relevancy on a query. In fact, as discussed in Chapter 5, certain terms have little or no discriminating power in determining relevance. For instance, a collection of documents on the insurance industry is likely to have the term insurance in almost every document. To this end, we introduce a mechanism for attenuating the effect of terms that occur too often in the collection to be meaningful for relevance determination. An immediate idea is to scale down the term weights of terms with high *collection frequency*, defined to be the total number of occurrences of a term in the collection. The idea would be to reduce the tf weight of a term by a factor that grows with its collection frequency.

Instead, it is more commonplace to use for this purpose the *document frequency* df_t, defined to be the number of documents in the collection that contain a term t. The reason to prefer df to cf is illustrated in Figure 6.7, where a simple example shows that collection frequency (cf) and document frequency (df) can behave rather differently. In particular, the cf values for both try and insurance are roughly equal, but their df values differ significantly. Intuitively, we want the few documents that contain insurance to get a higher boost for a query on insurance than the many documents containing try get from a query on try.

How is the document frequency df of a term used to scale its weight? Denoting as usual the total number of documents in a collection by N, we define the *inverse document frequency* (idf) of a term t as follows:

INVERSE DOCUMENT FREQUENCY

$$\text{idf}_t = \log \frac{N}{\text{df}_t}. \tag{6.7}$$

Thus the idf of a rare term is high, whereas the idf of a frequent term is likely to be low. Figure 6.8 gives an example of idf's in the Reuters collection of 806,791 documents; in this example logarithms are to the base 10. In fact,

term	df_t	idf_t
car	18,165	1.65
auto	6723	2.08
insurance	19,241	1.62
best	25,235	1.5

► **Figure 6.8** Example of idf values. Here we give the idf's of terms with various frequencies in the Reuters collection of 806,791 documents.

as we will see in Exercise 6.12, the precise base of the logarithm is not material to ranking.

6.2.2 Tf-idf weighting

We now combine the above expressions for term frequency and inverse document frequency, to produce a composite weight for each term in each document. The *tf-idf* weighting scheme assigns to term t a weight in document d given by

$$\text{tf-idf}_{t,d} = \text{tf}_{t,d} \times \text{idf}_t. \tag{6.8}$$

In other words, $\text{tf-idf}_{t,d}$ assigns to term t a weight in document d that is

1. highest when t occurs many times within a small number of documents (thus lending high discriminating power to those documents);
2. lower when the term occurs fewer times in a document, or occurs in many documents (thus offering a less pronounced relevance signal);
3. lowest when the term occurs in virtually all documents.

DOCUMENT VECTOR

At this point, we may view each document as a *vector* with one component corresponding to each term in the dictionary, together with a weight for each component that is given by (6.8). For dictionary terms that do not occur in a document, this weight is zero. This vector form will prove to be crucial to scoring and ranking; we will develop these ideas in Section 6.4. As a first step, we introduce the *overlap score measure*: the score of a document d is the sum, over all query terms, of the number of times each of the query terms occurs in d. We can refine this idea so that we add up not the number of occurrences of each query term t in d, but instead the tf-idf weight of each term in d.

$$\text{Score}(q, d) = \sum_{t \in q} \text{tf-idf}_{t,d}. \tag{6.9}$$

	Doc1	Doc2	Doc3
car	27	4	24
auto	3	33	0
insurance	0	33	29
best	14	0	17

► **Figure 6.9** Table of tf values for Exercise 6.10.

Exercise 6.8

Why is the idf of a term always finite?

Exercise 6.9

What is the idf of a term that occurs in every document? Compare this with the use of stop word lists.

Exercise 6.10

Consider the table of term frequencies for 3 documents denoted Doc1, Doc2, Doc3 in Figure 6.9. Compute the tf-idf weights for the terms car, auto, insurance, best, for each document, using the idf values from Figure 6.8.

Exercise 6.11

Can the tf-idf weight of a term in a document exceed 1?

Exercise 6.12

How does the base of the logarithm in (6.7) affect the score calculation in (6.9)? How does the base of the logarithm affect the relative scores of two documents on a given query?

Exercise 6.13

If the logarithm in (6.7) is computed base 2, suggest a simple approximation to the idf of a term.

6.3 Variants in tf-idf functions

A number of alternatives to tf and tf-idf have been considered. We discuss some of the principal ones here; a more complete development is deferred to Chapter 11. We will summarize these alternatives in Section 6.4.3 (page 120).

6.3.1 Sublinear tf scaling

It seems unlikely that twenty occurrences of a term in a document truly carry twenty times the significance of a single occurrence. Accordingly, there has been considerable research into variants of term frequency that go beyond counting the number of occurrences of a term. A common modification is

to use instead the logarithm of the term frequency, which assigns a weight given by

$$\text{wf}_{t,d} = \begin{cases} 1 + \log \text{tf}_{t,d} & \text{if } \text{tf}_{t,d} > 0 \\ 0 & \text{otherwise} \end{cases}. \tag{6.10}$$

In this form, we may replace tf by some other function wf as in (6.10), to obtain:

$$\text{wf-idf}_{t,d} = \text{wf}_{t,d} \times \text{idf}_t. \tag{6.11}$$

Equation (6.9) can then be modified by replacing tf-idf by wf-idf as defined in (6.11). Indeed, we may choose to use any weighting function we want; below we discuss several choices.

6.3.2 Maximum tf normalization

One well-studied technique is to normalize the tf weights of all terms occurring in a document by the maximum tf in that document. For each document d, let $\text{tf}_{\max}(d) = \max_{\tau \in d} \text{tf}_{\tau,d}$, where τ ranges over all terms in d. Then, we compute a normalized term frequency for each term t in document d by

$$\text{ntf}_{t,d} = a + (1-a)\frac{\text{tf}_{t,d}}{\text{tf}_{\max}(d)}, \tag{6.12}$$

where a is a value between 0 and 1 and is generally set to 0.5. The term a in (6.12) is a *smoothing* term whose role is to damp the contribution of the second term – which may be viewed as a scaling down of tf by the largest tf value in d. We will encounter smoothing further in Chapter 13 when discussing classification; but the basic idea is to avoid a large swing in $\text{ntf}_{t,d}$ from modest changes in $\text{tf}_{t,d}$ (say from 1 to 2). The main idea of maximum tf normalization is to mitigate the following anomaly: we observe higher term frequencies in longer documents, merely because longer documents tend to repeat the same words over and over again. To appreciate this, consider the following extreme example: supposed we were to take a document d and create a new document d' by simply appending a copy of d to itself. While d' should be no more relevant to any query than d is, the use of (6.9) would assign it twice as high a score as d. Replacing $\text{tf-idf}_{t,d}$ in (6.9) by $\text{ntf-idf}_{t,d}$ eliminates the anomaly in this example. Maximum tf nomalization does suffer from the following issues:

SMOOTHING

1. A document may contain an outlier term with an unusually large number of occurrences of that term, not representative of the content of that document.
2. More generally, a document in which the most frequent term appears roughly as often as many other terms should be treated differently from one with a more skewed distribution.

	Doc1	Doc2	Doc3
car	0.88	0.09	0.58
auto	0.10	0.71	0
insurance	0	0.71	0.70
best	0.46	0	0.41

► **Figure 6.10** Euclidean normalized tf values for documents in Figure 6.9.

6.3.3 Document length and Euclidean normalization

The above discussion of weighting ignores the length of documents in computing term weights. However, document lengths are material to these weights, for several reasons. First, longer documents will – as a result of containing more terms – have higher tf values. Second, longer documents contain more distinct terms. These factors conspire to raise the scores of longer documents, which (at least for some information needs) is unnatural. Longer terms can broadly be lumped into two categories: (1) *verbose* documents that essentially repeat the same content – in these, the length of the document does not alter the relative weights of different terms; (2) documents covering multiple different topics, in which the search terms probably match small segments of the document but not all of it – in this case, the relative weights of terms are quite different from a single short document that matches the query terms. We will give a more nuanced treatment of compensating for document length in Section 6.4.5.

EUCLIDEAN NORMALIZATION

Instead of normalizing term frequencies or tf-idf weights using the largest tf or tf-idf, as in (6.12), one common form of normalization is *Euclidean normalization*, defined as follows; sometimes Euclidean normalization is used over and above weighting techniques such as maximum tf normalization. Let $w_1, \ldots, w_N$ be the weights of a term in a document. These weights could be tf, tf-idf or a variant such as those in Sections 6.3.1-6.3.2. Then Euclidean normalization divides each of the weights $w_1, \ldots, w_N$ by the common denominator $\sqrt{w_1^2 + \ldots + w_N^2}$.

✎ **Example 6.2:** Consider the documents in Figure 6.9. We now apply Euclidean normalization to the tf values from the table, for each of the three documents in the table. The quantity $\sqrt{w_1^2 + \ldots + w_N^2}$ has the values 30.56, 46.84 and 41.30 respectively for Doc1, Doc2 and Doc3. The resulting Euclidean normalized tf values for these documents are shown in Figure 6.10.

Consider again the overlap score measure of (6.9); we may apply it to the Euclidean normalized tf weights. This has the effect of "normalizing" the contributions of long documents in which the same content (and therefore

terms) are repeated. Consider again a document d' created by taking a document d and appending it to itself. Then, the Euclidean normalized weight of any term is the same in d as well as d'; consequently, the overlap score for any query is the same for d and d'.

6.3.4 Scoring from term weights

We now put together the ideas from the preceding sections to complete our picture of scoring using weights derived from term frequency. The overlap measure of (6.9) is an unweighted sum over query terms of the term weights. We may in fact weight the terms in the query as well, using sublinear tf scaling, idf, normalization, or any combination thereof. We then write (6.9) in the following weighted form:

$$\text{Score}(q,d) = \sum_{t \in q} w_{t,q} \cdot w_{t,d}, \tag{6.13}$$

where $w_{t,q}$ and $w_{t,d}$ are respectively the weights of term t in the query q and in document d.

✎ **Example 6.3:** We now consider the query best car insurance on a fictitious collection with $N = 1{,}000{,}000$ documents where the document frequencies of auto, best, car and insurance are respectively 5000, 50000, 10000 and 1000.

term	query				document			product
	tf	df	idf	$w_{t,q}$	tf	wf	$w_{t,d}$	
auto	0	5000	2.3	0	1	1	0.52	0
best	1	50000	1.3	1.3	0	0	0	0
car	1	10000	2.0	2.0	1	1	0.52	1.04
insurance	1	1000	3.0	3.0	2	1.3	0.68	2.04

In this example the weight of a term in the query is simply the idf; this is reflected in the column header $w_{t,q}$ (the entry for auto is zero because the query does not contain the termauto). For documents, we use logarithmic tf scaling as in (6.10), with no use of idf but with Euclidean normalization. The former is shown under the column headed wf, while the latter is shown under the column headed $w_{t,d}$. Invoking (6.13) now gives a net score of $0 + 0 + 1.04 + 2.04 = 3.08$.

Exercise 6.14

Recall the tf-idf weights computed in Exercise 6.10. Compute the Euclidean normalized document vectors for each of the documents, where each vector has four components, one for each of the four terms.

Exercise 6.15

Verify that the sum of the squares of the components of each of the document vectors in Exercise 6.14 is 1 (to within rounding error). Why is this the case?

Exercise 6.16

With term weights as computed in Exercise 6.14, rank the three documents by computed score for the query car insurance, for each of the following cases of term weighting in the query:

1. The weight of a term is 1 if present in the query, 0 otherwise.
2. Euclidean normalized idf.

6.4 The vector space model for scoring

In Section 2.2.2 (page 26) we developed the notion of a document vector that captures the relative importances of the terms in a document. The representation of a set of documents as vectors in a common vector space is known as the *vector space model* and is fundamental to a host of information retrieval operations ranging from scoring documents on a query, document classification and document clustering. We first develop the basic ideas underlying vector space retrieval; a pivotal step in this development is the view (Section 6.4.2) of queries as vectors in the same vector space as the document collection. Following this we outline techniques for accelerating vector space retrieval; we end this chapter by placing vector space retrieval in perspective to other retrieval mechanisms, such as Boolean retrieval.

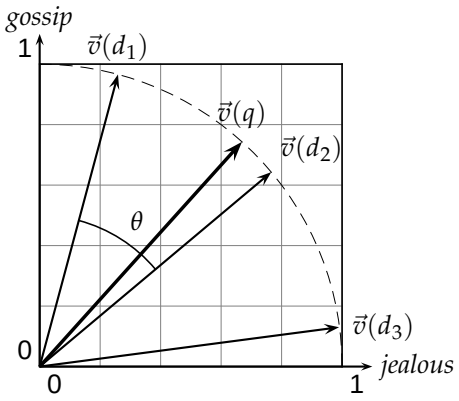
VECTOR SPACE MODEL

6.4.1 Inner products

We denote by $\vec{V}(d)$ the vector derived from document d, with one component in the vector for each dictionary term. Unless otherwise specified, the reader may assume that the components are computed using the tf-idf weighting scheme, although the particular weighting scheme is immaterial to the discussion that follows. The set of documents in a collection then turns into a vector space, with one axis for each term. This representation loses the relative ordering of the terms in each document; recall our example from Section 6.2 (page 110), where we pointed out that the documents *Mary is quicker than John* and *John is quicker than Mary* are identical in such a *bag of words* representation.

How do we quantify the similarity between two documents in this vector space? A first attempt might consider the magnitude of the vector difference between two document vectors. This measure suffers from a drawback: two documents with very similar term distributions can have a significant vector difference simply because one is much longer than the other. Thus the relative distributions of terms may be identical in the two documents, but the absolute term frequencies of one may be far larger.

To compensate for the effect of document length, the standard way of quantifying the similarity between two documents d_1 and d_2 is to compute



► **Figure 6.11** Cosine similarity illustrated. $\text{sim}(d_1, d_2) = \cos\theta$.

COSINE SIMILARITY

the *cosine similarity* of their vector representations $\vec{V}(d_1)$ and $\vec{V}(d_2)$

$$\text{sim}(d_1, d_2) = \frac{\vec{V}(d_1) \cdot \vec{V}(d_2)}{|\vec{V}(d_1)||\vec{V}(d_2)|}, \tag{6.14}$$

where the numerator represents the *inner product* (also known as the dot product) of the vectors $\vec{V}(d_1)$ and $\vec{V}(d_2)$, while the denominator is the products of their lengths. The effect of the denominator is to *length-normalize* the vectors $\vec{V}(d_1)$ and $\vec{V}(d_2)$ to unit vectors $\vec{v}(d_1) = \vec{V}(d_1)/|\vec{V}(d_1)|$ and $\vec{v}(d_2) = \vec{V}(d_2)/|\vec{V}(d_2)|$. We can then rewrite (6.14) as

LENGTH-NORMALIZE

$$\text{sim}(d_1, d_2) = \vec{v}(d_1) \cdot \vec{v}(d_2). \tag{6.15}$$

Thus, (6.15) can be viewed as the inner product of the normalized versions of the two document vectors. This measure is the cosine of the angle θ between the two vectors, shown in Figure 6.11. What use is the similarity measure $\text{sim}(d_1, d_2)$? Given a document d (potentially one of the d_i in the collection), consider searching for the documents in the collection most similar to d. Such a search is useful in a system where a user may identify a document and seek others like it – a feature available in the results lists of search engines as a *more like this* feature. We reduce the problem of finding the document(s) most similar to d to that of finding the d_i with the highest inner products (sim values) $\vec{v}(d) \cdot \vec{v}(d_i)$. We could do this by computing the inner products between $\vec{v}(d)$ and each of $\vec{v}(d_1), \ldots, \vec{v}(d_N)$, then picking off the highest resulting sim values.

✎ **Example 6.4:** Figure 6.12 shows the number of occurrences of three terms (affection, jealous and gossip) in each of the following three novels: Jane Austen's *Sense and Sensi-*

term	SaS	PaP	WH
affection	115	58	20
jealous	10	7	11
gossip	2	0	6

► **Figure 6.12** Term frequencies in three novels. The novels are Austen's *Sense and Sensibility, Pride and Prejudice* and Bronte's *Wuthering Heights*.

term	SaS	PaP	WH
affection	0.996	0.993	0.847
jealous	0.087	0.120	0.466
gossip	0.017	0	0.254

► **Figure 6.13** Term vectors for the three novels of Figure 6.12. These are based on raw term frequency only and are normalized as if these were the only terms in the collection. (Since affection and jealous occur in all three documents, their tf-idf weight would be 0 in most formulations.)

bility (SaS) and *Pride and Prejudice* (PaP) and Emily Brontë's *Wuthering Heights* (WH). Of course, there are many other terms occurring in each of these novels. In this example we represent each of these novels as a unit vector in three dimensions, corresponding to these three terms (only); we use raw term frequencies here, with no idf multiplier. The resulting weights are as shown in Figure 6.13.

Now consider the cosine similarities between pairs of the resulting three-dimensional vectors. A simple computation shows that sim($\vec{v}$(SAS), $\vec{v}$(PAP)) is 0.999, whereas sim($\vec{v}$(SAS), $\vec{v}$(WH)) is 0.888; thus, the two books authored by Austen (SaS and PaP) are considerably closer to each other than to Brontë's *Wuthering Heights*. In fact, the similarity between the first two is almost perfect (when restricted to the three terms we consider).

TERM-DOCUMENT MATRIX

Viewing a collection of N documents as a collection of vectors leads to a natural view of a collection as a *term-document matrix*: this is an $M \times N$ matrix whose rows represent the M terms (dimensions) of the N columns, each of which corresponds to a document. As always, the terms being indexed could be stemmed before indexing; for instance, jealous and jealousy would under stemming be considered as a single dimension.

Exercise 6.17

If we were to stem jealous and jealousy to a common stem before setting up the vector space, detail how the definitions of tf and idf should be modified.

6.4.2 Queries as vectors

There is a far more compelling reason to represent documents as vectors: we can also view a *query* as a vector. Consider the query $q =$ jealous gossip.

This query turns into the unit vector $\vec{v}(q) = (0, 0.707, 0.707)$ on the three coordinates of Figures 6.12 and 6.13. The key idea now: to assign to each document d a score equal to the inner product

$$\vec{v}(q) \cdot \vec{v}(d).$$

In the example of Figure 6.13, *Wuthering Heights* is the top-scoring document for this query with a score of 0.509, with *Pride and Prejudice* a distant second with a score of 0.085, and *Sense and Sensibility* last with a score of 0.074. The number of dimensions in general will be far larger than three: it will equal the number M of distinct terms being indexed.

To summarize, by viewing a query as a "bag of words", we are able to treat it as a very short document. As a consequence, we can use the cosine similarity between the query vector and a document vector as a measure of the score of the document for that query. The resulting scores can then be used to select the top-scoring documents for a query. Thus we have

$$\text{score}(q, d) = \frac{\vec{V}(q) \cdot \vec{V}(d)}{|\vec{V}(q)||\vec{V}(d)|}. \tag{6.16}$$

Computing the cosine similarities between the query vector and each document vector in the collection, sorting the resulting scores and selecting the top K documents can be expensive — a single similarity computation can entail an inner product in tens of thousands of dimensions, demanding tens of thousands of arithmetic operations. In Section 7.1 we study how to use an inverted index for this purpose, followed by a series of heuristics for improving on this.

6.4.3 Document and query weighting schemes

Equation (6.16) is fundamental to information retrieval engines that use any form of vector space scoring. Variations from one vector space scoring engine to another hinge on the specific choices of weights in the vectors $\vec{V}(d)$ and $\vec{V}(q)$. Figure 6.14 lists some of the principal weighting schemes in use for each of these vectors, together with a mnemonic for representing a specific combination of weights. The mnemonic for representing a combination of weights takes the form *ddd.qqq* where the first triplet gives the term weighting of the document vector, while the second triplet gives the weighting in the query vector. It is quite common to apply different normalization to the document and the query. The first letter in each triplet specifies the term frequency component of the weighting, the second the document frequency component, and the third the form of normalization used. For example, a very standard baseline weighting scheme is *lnc.ltc*, where the document vector has log-weighted term frequency, no idf (for both effectiveness and

Term frequency		Document frequency		Normalization	
n (natural)	$\mathrm{tf}_{t,d}$	n (no)	1	n (none)	1
l (logarithm)	$1 + \log(\mathrm{tf}_{t,d})$	t (idf)	$\log \frac{N}{\mathrm{df}_t}$	c (cosine)	$\frac{1}{\sqrt{w_1^2+w_2^2+\ldots+w_M^2}}$
a (augmented)	$0.5 + \frac{0.5 \times \mathrm{tf}_{t,d}}{\max_t(\mathrm{tf}_{t,d})}$	p (prob idf)	$\log \frac{N-\mathrm{df}_t}{\mathrm{df}_t}$	u (pivoted unique)	$1/u$ (Section 6.4.5)
L (log ave)	$\frac{1+\log(\mathrm{tf}_{t,d})}{1+\log(\mathrm{ave}_{t \in d}(\mathrm{tf}_{t,d}))}$			b (byte size)	$1/charLeng^{\alpha}$, $\alpha < 1$
b (boolean)	$\mathrm{tf}_{t,d} > 0$				

► **Figure 6.14** Smart notation for tf-idf variants.

efficiency reasons), and cosine normalization, while the query vector uses log-weighted term frequency, idf weighting, and cosine normalization.

6.4.4 Computing vector scores

We now initiate the study of computing the vector space scores for all documents, in response to a query. In a typical setting we have a collection of documents each represented by a vector, a free text query represented by a vector, and a positive integer K. We seek the K documents of the collection with the highest vector space scores on the given query. Typically, we seek these K top documents in ordered by decreasing score; for instance many search engines use $K = 10$ to retrieve and rank-order the first page of the ten best results. Here we give the basic algorithm for this computation; we develop a fuller treatment of efficient techniques and approximations in Chapter 7.

Figure 6.15 gives the basic algorithm for computing vector space scores. The array Length holds the lengths (normalization factors) for each of the N documents, while the the array Scores holds the scores for each of the documents. When the scores are finally computed in Step 11, all that remains in Step 12 is to pick off the K documents with the highest scores.

The outermost loop beginning Step 3 repeats the updating of Scores, iterating over each query term t in turn. In Step 5 we calculate the weight in the query vector for term t. Steps 6-8 update the score of each document by adding in the contribution from term t. For this purpose, it would appear necessary to store, with each postings entry, the weight $w_{t,q}$. In fact this is wasteful, since storing this weight may require a floating point number. Two ideas help alleviate this space problem. First, if we are using inverse document frequency, we need not precompute idf_t; it suffices to store N/df_t at the head of the postings for t. Second, we store the term frequency $tf_{t,d}$ for each postings entry. Particularly when using logarithmic term weighting, we may

```
COSINESCORE(q)
 1  float Scores[N] = 0
 2  Initialize Length[N]
 3  for each query term t
 4  do
 5      calculate w_{t,q} and fetch postings list for t
 6      for each pair(d, tf_{t,d}) in postings list
 7      do
 8          add wf_{t,d} × w_{t,q} to Scores[d]
 9          Read the array Length[d]
10  for  each d
11  do Divide Scores[d] by Length[d]
12      return Top K components of Scores[]
```

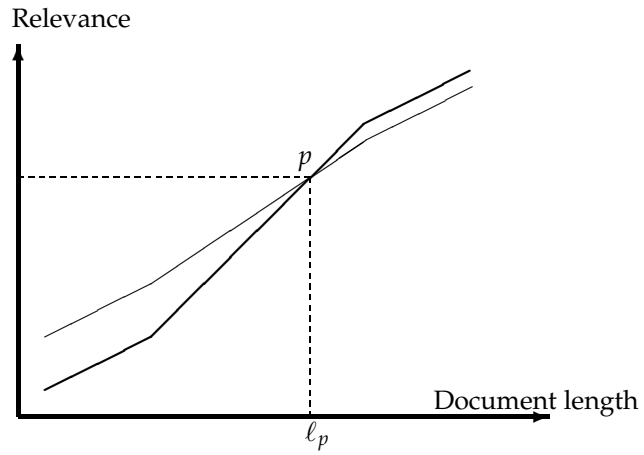
► **Figure 6.15** The basic algorithm for computing vector space scores.

store this logarithm rather than the raw term frequency $tf_{t,d}$, saving further storage. Finally, Step 12 extracts the top K scores – this requires a priority queue data structure, often implemented using a heap. Such a heap takes no more than $2N$ comparisons to construct, following which each of the K top scores can be extracted from the heap at a cost of $O(\log N)$ comparisons.

Note that the general algorithm of Figure 6.15 does not prescribe a specific implementation of how we traverse the postings lists of the various query terms; we may traverse them one term at a time as in the loop beginning at Step 3, or we could in fact traverse them concurrently as in Figure 1.6. We will say more about this in Section 7.1.5.

6.4.5 Pivoted normalized document length

In Section 6.4.1 we normalized each document vector by the Euclidean length of the vector, so that all document vectors turned into unit vectors. In doing so, we eliminated all information on the length of the original document. However, in Section 6.3.3 we argued that the length of the a document (independent of its content) can directly affect the relevance of a document. Compensating for this phenomenon is a form of document length normalization that is independent of term and document frequencies. To this end, we introduce a form of normalizing the vector representation of a document, so that the resulting "normalized" documents are not necessarily of unit length. Then, when we compute the inner product score between a (unit) query vector and such a normalized document, the score is skewed to account for the



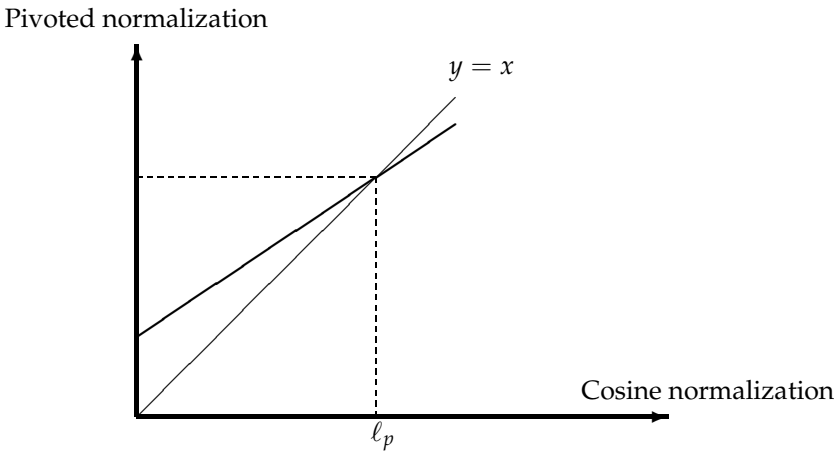
► **Figure 6.16** Pivoted document length normalization.

PIVOTED DOCUMENT LENGTH NORMALIZATION

effect of document length on relevance. This form of compensation for document length is known as *pivoted document length normalization*.

Consider a document collection together with an ensemble of queries for that collection. Suppose that we were given, for each query q and for each document d, a Boolean judgment of whether or not d is relevant to the query q; in Chapter 8 we will see how to procure such a set of relevance judgments for a query ensemble and a document collection. Given this set of relevance judgments, we may compute a *probability of relevance* as a function of document length, averaged over all queries in the ensemble. The resulting plot may look like the curve drawn in thick lines in Figure 6.16. To compute this curve, we bucket documents by length and compute the fraction of relevant documents in each bucket, then plot this fraction against the median document length of each bucket. (Thus even though the "curve" in Figure 6.16 appears to be continuous, it is in fact a histogram of discreet buckets of document length.)

On the other hand, the curve in thin lines shows what might happen with the same documents and query ensemble if we were to use relevance as prescribed by cosine normalization (6.16) – thus, cosine normalization has a tendency to distort the computed relevance vis-à-vis the true relevance, at the expense of longer documents. The thin and thick curves crossover at a point p corresponding to document length ℓ_p, which we refer to as the *pivot length*; dashed lines mark this point on the $x-$ and $y-$ axes. The idea of pivoted



► **Figure 6.17** Implementing pivoted document length normalization by linear scaling.

document length normalization would then be to "rotate" the cosine normalization curve counter-clockwise about p so that it more closely matches the relevance vs. document length curve. As mentioned at the beginning of this section, we do so by using in (6.16) a normalization factor for each document vector $\vec{V}(d)$ that is not the Euclidean length of that vector, but instead one that is larger than the Euclidean length for documents of length less than ℓ_p, and smaller for longer documents.

To this end, we first note that the normalizing term for $\vec{V}(d)$ in the denominator of (6.16) is the L_2 norm (length) of $\vec{V}(d)$. In the simplest implementation of pivoted document length normalization, we still use a linear normalization factor in the denominator, but one of slope < 1 as in Figure 6.17. In this figure, the $x-$ axis represents the document length (and therefore the cosine normalization factor used in (6.14)). The $y-$axis represents the pivoted normalization factor we instead use. Notice the following aspects of the thick line representing pivoted length: (1) it is linear in the document length and has an equation of the form $a|\vec{V}(d)| + b$; (2) its slope is $a < 1$ and (3) it crosses the $y = x$ line at ℓ_p. Because the pivoted normalization factor is linear, we may view this as a linear scaling of the document vector, but by a quantity $a|\vec{V}(d)| + b$ other than $|\vec{V}(d)|$.

Of course, pivoted document length normalization is not appropriate for

	query					document			
word	tf	wf	df	idf	q_i = wf-idf	tf	wf	d_i = normalized wf	$q_i \cdot d_i$
digital			10,000						
video			100,000						
cameras			50,000						

► **Table 6.1** Cosine computation for Exercise 6.19.

all applications. For instance, in a collection of answers to frequently asked questions (say, at a customer service website), relevance may have little to do with document length. In other cases the dependency may be more complex than can be accounted for by a simple linear pivoted normalization. In such cases, document length can be used as a feature in the machine learning based scoring approach of Section 6.1.2.

Exercise 6.18

EUCLIDEAN DISTANCE One measure of the similarity of two unit vectors is the *Euclidean distance* (or L_2 distance) between them:

$$|\vec{x} - \vec{y}| = \sqrt{\sum_{i=1}^{M}(x_i - y_i)^2}$$

Given a query q and documents $d_1, d_2, \ldots$, we may rank the documents d_i in order of increasing Euclidean distance from q. Show that if q and the d_i are all normalized to unit vectors, then the rank ordering produced by Euclidean distance is identical to that produced by cosine similarities.

Exercise 6.19

Compute the vector space similarity between the query "digital cameras" and the document "digital cameras and video cameras" by filling out the empty columns in Table 6.1. Assume N = 10,000,000, logarithmic term weighting (wf columns) for query and document, idf weighting for the query only and cosine normalization for the document only. Treat and as a stop word. Enter term counts in the tf columns. What is the final similarity score?

Exercise 6.20

Show that for the query affection, the relative ordering of the scores of the three documents in Figure 6.13 is the reverse of the ordering of the scores for the query jealous gossip.

Exercise 6.21

In turning a query into a unit vector in Figure 6.13, we assigned equal weights to each of the query terms. What other principled approaches are plausible?

Exercise 6.22

Consider the case of a query term that is not in the set of M indexed terms. How would one adapt the vector space representation to handle this case?

Exercise 6.23

Refer to the tf and idf values for four terms and three documents in Exercise 6.10. Compute the two top scoring documents on the query best car insurance for each of the following weighing schemes: (i) `nnn.atc`; (ii) `ntc.atc`.

Exercise 6.24

Suppose that the word coyote does not occur in the collection used in Exercises 6.10 and 6.23. How would one compute `ntc.atc` scores for the query coyote insurance?

References and further reading

Chapter 7 develops the computational aspects of vector space scoring. Luhn (1957; 1958) describes some of the earliest reported applications of term weighting. His paper dwells on the importance of medium frequency terms (terms that are neither too commonplace nor too rare) and may be thought of as anticipating tf-idf and related weighting schemes. Spärck Jones (1972) builds on this intuition through detailed experiments showing the use of inverse document frequency in term weighting. A series of extensions and theoretical justifications of idf are due to Salton and Buckley (1988a) Robertson and Spärck Jones (1976a), Robertson and Spärck Jones (1976b), Croft and Harper (1979) and Papineni (2001). Robertson maintains a web page (http://www.soi.city.ac.uk/~ser/idf.html) containing the history of idf, including soft copies of early papers that predated electronic versions of journal article. Singhal et al. (1996a) develop pivoted document length normalization. Probabilistic language models (Chapter 11) develop weighting techniques that are more nuanced than tf-idf; the reader will find this development in Section 11.4.2.

We observed that by assigning a weight for each term in a document, a document may be viewed as a vector of term weights, one for each term in the collection. The SMART information retrieval system at Cornell (Salton 1971b) due to Salton and colleagues was perhaps the first to view a document as a vector of weights. We will develop this view further in Chapter 7. The basic computation of cosine scores as described in Section 6.4.4 is due to Zobel and Moffat (2006).

The Smart notation for tf-idf term weighting schemes in Figure 6.14 is presented in (Salton and Buckley 1988b, Singhal et al. 1996a;b). Not all versions of the notation are consistent; we most closely follow (Singhal et al. 1996b).

7 Computing scores in a complete search system

Chapter 6 developed the theory underlying term weighting in documents for the purposes of scoring, leading up to vector space models and the basic cosine scoring algorithm of Section 6.4.4 (page 121).

7.1 Efficient scoring and ranking

We begin by recapping the algorithm of Figure 6.15. For a query such as $q =$ jealous gossip, two observations are immediate:

1. The unit vector $\vec{v}(q)$ has only two non-zero components.
2. These non-zero components are equal – in this case, both equal 0.707. Indeed, such equality holds for any query in which no term is repeated.

For the purpose of ranking the documents matching this query, we are really interested in the relative (rather than absolute) scores of the documents in the collection. To this end, it suffices to compute the cosine similarity from each document unit vector $\vec{v}(d)$ to $\vec{V}(q)$ (in which all non-zero components of the query vector are set to 1), rather than to the unit vector $\vec{v}(q)$. For any two documents d_1, d_2

$$\vec{V}(q) \cdot \vec{v}(d_1) > \vec{V}(q) \cdot \vec{v}(d_2) \Leftrightarrow \vec{v}(q) \cdot \vec{v}(d_1) > \vec{v}(q) \cdot \vec{v}(d_2). \tag{7.1}$$

For any document d, the cosine similarity $\vec{V}(q) \cdot \vec{v}(d)$ is the weighted sum, over all terms in the query q, of the weights of those terms in d. This in turn can be computed by a postings intersection: we walk through the postings in the inverted index for the terms in q, accumulating the total score for each document – very much as in processing a Boolean query, except we assign a positive score to each document that appears in any of the postings being traversed. As mentioned in Section 6.4.4 we maintain an idf value for each dictionary term and a tf value for each postings entry, generally in logarithmic form. This scheme computes a score for every document in the postings

of any of the query terms; the total number of such documents may be considerably smaller than N.

Given these scores (some of which could exceed 1), the final step before presenting results to a user is to pick out the K highest-scoring documents. While one could sort the complete set of scores, a better approach is to use a heap to retrieve only the top K documents in order. Where J is the number of documents with non-zero cosine scores, constructing such a heap can be performed in $2J$ comparison steps, following which each of the K highest scoring documents can be "read off" the heap with $\log J$ comparison steps.

7.1.1 Inexact top K document retrieval

Thus far, we have focused on retrieving precisely the K highest-scoring documents for a query. We now consider schemes by which we produce K documents that are *likely* to be among the K highest scoring documents for a query. In doing so, we hope to dramatically lower the cost of computing the K documents we output, without materially altering the user's perceived relevance of the top K results. The vector space (or any variant) score we compute is a proxy estimate of the user's relevance perception, rather than an exact measure. As a consequence, in most applications it suffices to retrieve K documents whose scores are very close to those of the K best. In the sections that follow we detail schemes that retrieve K such documents while potentially avoiding computing scores for most of the N documents in the collection.

Such inexact top-K retrieval is not necessarily, from the user's perspective, a bad thing. The top K documents by the cosine measure are already not necessarily the K best for the query: this is because cosine similarity is only a proxy for the user's perceived relevance. Below we give heuristics using which we are likely to retrieve K documents with cosine scores close to those of the top K documents; from the standpoint of the user's perception, these may not be noticeably less relevant than the top K. The principal cost in computing the output stems from computing cosine similarities between the query and a large number of documents. Having a large number of documents in contention also increases the selection cost in the final stage of culling the top K documents from a heap. We now consider a series of ideas designed to eliminate a large number of documents from consideration. The heuristics have the following two-step scheme:

1. Find a set A of documents that are contenders, where $K \ll |A| \ll N$. A does not necessarily contain the K top-scoring documents for the query, but is likely to have many documents with scores near those of the top K.

2. Return the K top-scoring documents in A.

From the descriptions of these ideas it will be clear that many of them require parameters to be tuned to the collection and application at hand; pointers to experience in setting these parameters may be found at the end of this chapter.

7.1.2 Index elimination

For a multi-term query q, it is clear we only consider documents containing at least one of the query terms. We can take this a step further using additional heuristics:

1. We only consider documents containing terms whose idf exceeds a preset threshold. Thus, in the postings traversal, we only traverse the postings for terms with high idf. This has a fairly significant benefit: the postings lists of low-idf terms are generally long; with these removed from contention, the set of documents for which we compute cosines is greatly reduced. One way of viewing this heuristic: low-idf terms are treated as stop words and do not contribute to scoring. For instance, on the query catcher in the rye, we only traverse the postings for catcher and rye.

2. We only consider documents that contain many (and as a special case, all) of the query terms. This can be accomplished by viewing the query as a conjunctive query; during the postings traversal, we only compute scores for documents containing all (or many) of the query terms. A danger of this scheme is that by requiring all (or even many) query terms to be present in a document before considering it for cosine computation, we may end up with fewer than K candidate documents in the output. This issue will discussed further in Section 7.2.1.

7.1.3 Champion lists

The idea of *champion lists* (sometimes also called *fancy lists*) is to precompute, for each term t in the dictionary, the set of the r documents with the highest weights for t; the value of r is chosen in advance. For tf-idf weighting, these would be the r documents with the highest tf values for term t. We call this set of r documents the *champion list* for term t.

Now, given a query q we take the union of the champion lists for each of the terms comprising q to create a set A. We now restrict cosine computation to only the documents in A. A critical parameter in this scheme is the value r, which is highly application dependent. Intuitively, r should be large compared with K, especially if we use any form of the index elimination described above. One issue here is that the value r is set at the time of index construction, whereas K is application dependent and may not be available

until the query is received; as a result we may (as in the case of index elimination) find ourselves with a set A that has fewer than K documents. Note that there is no reason to have the same value of r for all terms in the dictionary; it could for instance be set to be higher for rarer terms.

7.1.4 Static quality scores and ordering

STATIC QUALITY SCORES

We now further develop the idea of champion lists above, in the somewhat more general setting of *static quality scores*. In many search engines, we have available a measure of quality $g(d)$ for each document d that is query-independent and thus *static*. This quality measure may be viewed as a number between zero and one. For instance, in the context of news stories on the web, $g(d)$ may be derived from the number of favorable reviews of the story by web surfers. Chapter 4, page 73 provides further discussion on this topic, as does Chapter 21 in the context of web search.

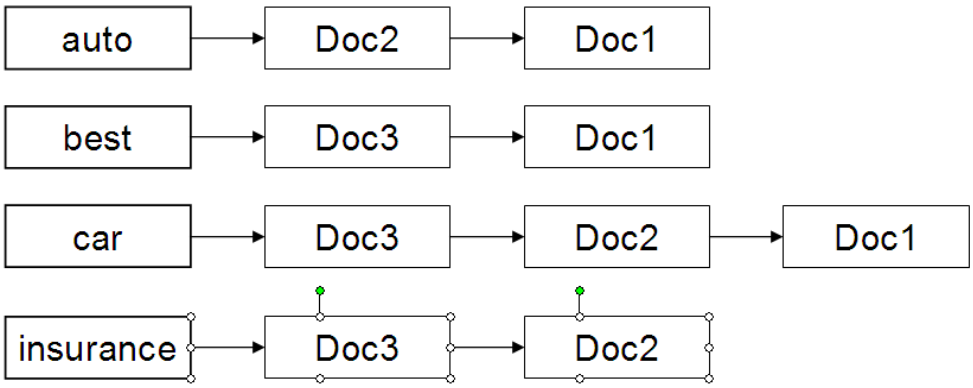
The net score for a document d is some combination of $g(d)$ together with the query-dependent score induced (say) by (6.16). The precise combination may be determined by the learning methods of Section 6.1.2 but for the purposes of our exposition here, let us envision a linear combination:

$$\text{net-score}(q,d) = g(d) + \frac{\vec{V}(q)\cdot\vec{V}(d)}{|\vec{V}(q)||\vec{V}(d)|}. \tag{7.2}$$

In this simple form, the static quality $g(d)$ and the query-dependent score from (6.14) have equal contributions, assuming each is between 0 and 1. Other relative weightings are possible; the effectiveness of the heuristics below will depend on the specific relative weighting. We will discuss the choice of relative weighting further in Section 7.2.4, building on the ideas developed in Section 6.1.2.

First, consider ordering the documents in the postings list for each term by decreasing value of $g(d)$. Note that this allows us to perform the postings merge of Chapter 1. In order to perform the merge by a single pass through the postings of each query term we relied in Chapter 1 on the postings being ordered by document ID's. But in fact, we only required that all postings be ordered by a single common ordering; here we rely on the $g(d)$ values to provide this common ordering. This is illustrated in Figure 7.1.

The first idea is a direct extension of champion lists: for a well-chosen value r, we maintain for each term t a *global champion list* of the r documents with the highest values for $g(d) + \text{tf-idf}_{t,d}$. The list itself is, like all the postings lists considered so far, sorted by a common order (either by document ID's or by static quality). Then at query time, we only compute the net scores (7.2) for documents in the union of these global champion lists. Intuitively, this has the effect of filtering out documents with large net scores.



► **Figure 7.1** Statically quality-ordered indexes. In this example we assume that Doc1, Doc2 and Doc3 respectively have static quality scores $g(1) = 0.25, g(2) = 0.5, g(3) = 1$.

We conclude the discussion of global champion lists with one further idea. We maintain for each term t two postings lists consisting of disjoint sets of documents, each sorted by $g(d)$ values. The first list, which we call *high*, contains the m documents with the highest tf values for t. The second list, which we call *low*, contains all other documents containing t. When processing a query, we first scan only the high lists of the query terms, computing net scores for any document on the high lists of all (or more than a certain number of) query terms. If we obtain scores for K documents in the process, we terminate. If not, we continue the scanning into the low lists, scoring documents in all (or many) of these postings lists. This idea is developed further in Section 7.2.1.

Exercise 7.1

When discussing champion lists above, we simply used the r documents with the largest tf values to create the champion list for t. But when considering global champion lists, we used idf as well, identifying documents with the largest values of $g(d) + \text{tf-idf}_{t,d}$. Why do we differentiate between these two cases?

Exercise 7.2

If we were to only have one-term queries, explain why the use of global champion lists with $r = K$ suffices for identifying the K highest scoring documents. What is a simple modification to our design of global champion lists if we were to only have s-term queries for any fixed integer $s > 1$?

Exercise 7.3

Explain how the common global ordering by $g(d)$ values in all high and low lists helps make the final step above efficient.

Exercise 7.4

Consider again the data of Exercise 6.23 with `nnn.atc` for the query-dependent scoring. Suppose that we were given static quality scores of 1 for Doc1 and 2 for Doc2. Determine under Equation (7.2) what ranges of static quality score for Doc3 result in it being the first, second or third result for the query best car insurance.

7.1.5 Impact ordering

Thus far, all the postings lists described order the documents consistently by some common ordering: typically by document ID but in Section 7.1.4 by static quality scores. As noted at the end of Section 6.4.4, such a common ordering supports the concurrent traversal of all of the query terms' postings lists, computing the score for each document as we encounter it. We will now introduce a technique for inexact top-K retrieval in which the postings are not all ordered by a common ordering, thereby precluding such a concurrent traversal. We will therefore require scores to be "accumulated" one term at a time as in the basic scheme of Figure 6.15.

The idea is to order the documents d in the postings list of term t by decreasing order of $tf_{t,d}$. Thus, the ordering of documents will vary from one postings list to another, and we cannot compute scores by a concurrent traversal of the postings lists of all query terms. Given postings lists ordered by decreasing order of $tf_{t,d}$, two ideas have been found to significantly lower the number of documents for which we accumulate scores: (1) when traversing the postings list for a query term t, we stop after considering a prefix of the postings list – either after a fixed number of documents r have been seen, or after the value of $tf_{t,d}$ has dropped below a threshold; (2) we consider the query terms in decreasing order of idf, so that the query terms likely to contribute the most to the final scores are considered first. This latter idea too can be adaptive at the time of processing a query: as we get to query terms with lower idf, we can determine whether to proceed based on the changes in document scores from processing the previous query term. If these changes are minimal, we may omit accumulation from the remaining query terms, or alternatively process shorter prefixes of their postings lists.

Note that these ideas form a common generalization of the methods introduced above in Section 7.1.2, Section 7.1.3 and Section 7.1.4. We may also implement a version of static ordering in which each postings list is ordered by an additive combination of static and query-dependent scores. We would again lose the consistency of ordering across postings, thereby having to process query terms one at time accumulating scores for all documents as we go along. Depending on the particular scoring function, the postings list for a document may be ordered by other quantities than term frequency; under this more general setting, this idea is known as impact ordering.

Exercise 7.5

Sketch the frequency-ordered postings for the data in Figure 6.9.

Exercise 7.6

Let the static quality scores for Doc1, Doc2 and Doc3 in Figure 6.10 be respectively 0.25, 0.5 and 1. Sketch the postings for impact ordering when each postings list is ordered by the sum of the static quality score and the Euclidean normalized tf values in Figure 6.10.

7.1.6 Cluster pruning

In *cluster pruning* we have a preprocessing step during which we cluster the document vectors. Then at query time, we consider only documents in a small number of clusters as candidates for which we compute cosine scores. Specifically, the preprocessing step is as follows:

1. Pick $\sqrt{N}$ documents at random from the collection. Call these *leaders*.
2. For each document that is not a leader, we compute its nearest leader.

We refer to documents that are not leaders as *followers*. Intuitively, in the partition of the followers induced by the use of $\sqrt{N}$ randomly chosen leaders, the expected number of followers for each leader is $\simeq N/\sqrt{N} = \sqrt{N}$. Next, query processing proceeds as follows:

1. Given a query q, find the leader L that is closest to q. This entails computing cosine similarities from q to each of the $\sqrt{N}$ leaders.
2. The candidate set A consists of L together with its followers. We compute the cosine scores for all documents in this candidate set.

The use of randomly chosen leaders for clustering is fast and likely to reflect the distribution of the document vectors in the vector space: a region of the vector space that is dense in documents is likely to produce multiple leaders and thus a finer partition into sub-regions.

Variations of cluster pruning introduce additional parameters b_1 and b_2, both of which are positive integers. In the pre-processing step we attach each follower to its b_1 rather than one closest leader. At query time we consider the b_2 leaders closest to the query q. Clearly, the basic scheme above corresponds to the case $b_1 = b_2 = 1$. Further, increasing b_1 or b_2 increases the likelihood of finding K documents that are more likely to be in the set of true top-scoring K documents, at the expense of more computation. We reiterate this approach when describing clustering in Chapter 16 (page 314).

Exercise 7.7

The nearest-neighbor problem in the plane is the following: given a set of N data points on the plane, we preprocess them into some data structure such that, given a query point Q, we seek the point in N that is closest to Q in Euclidean distance. Clearly cluster pruning can be used as an approach to the nearest-neighbor problem

in the plane, if we wished to avoid computing the distance from Q to every one of the query points. Devise a simple example on the plane so that with two leaders, the answer returned by cluster pruning is incorrect (it is not the data point closest to Q).

7.2 Components of a basic information retrieval system

In this section we combine the ideas developed so far to describe a rudimentary search system that retrieves and scores documents. In doing so we develop some further ideas that help improve the relevance of returned results as perceived by users. This leads us to the next level of development of machine-learned relevance. Following this, we will put together all of these elements to outline a complete system, then finish with a treatment of how various querying interact with one another.

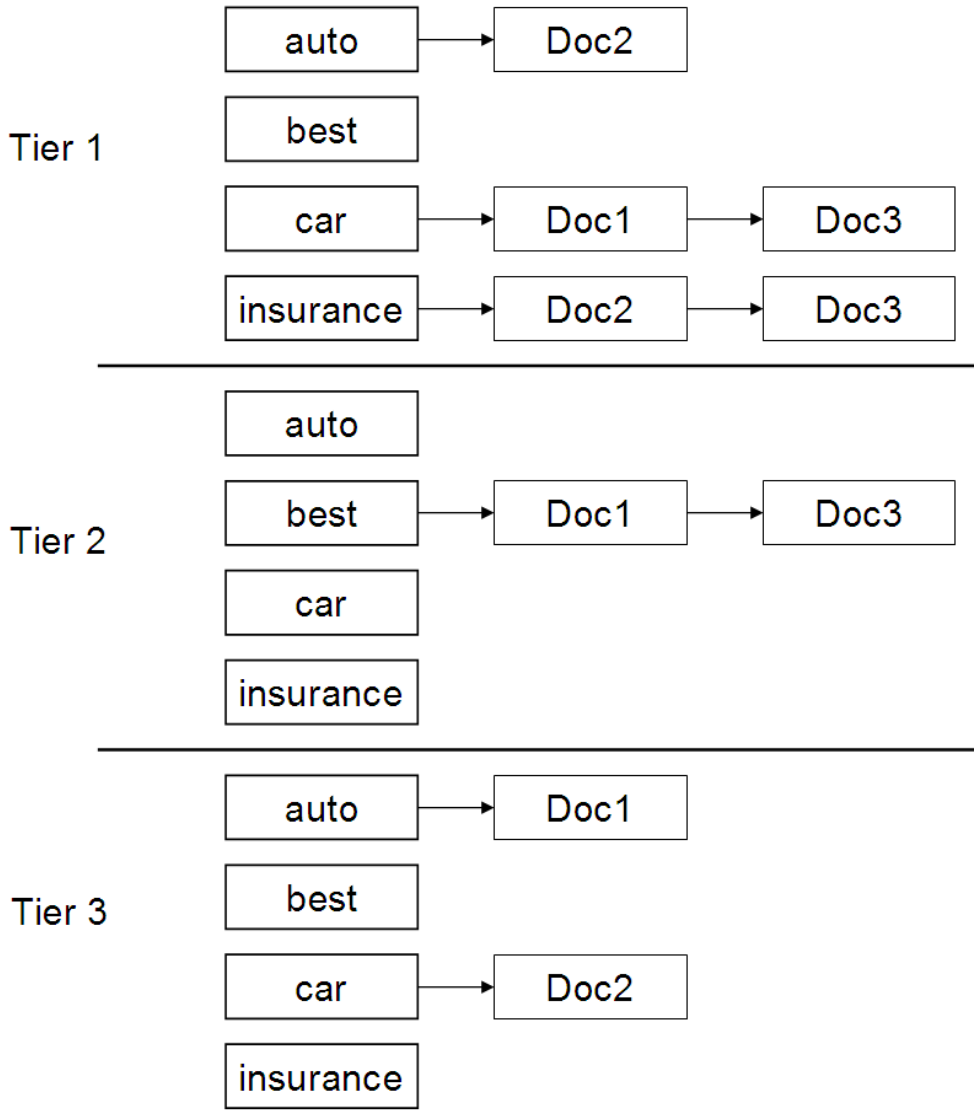
7.2.1 Tiered indexes

We mentioned in Section 7.1.2 that when using devices such as index elimination in pursuit of inexact top-K retrieval, we may occasionally find ourselves with a set A of contenders that has fewer than K documents. A common solution to this issue is the user of *tiered indexes*, which may be viewed as a generalization of champion lists. We illustrate this idea in Figure 7.2, where we represent the documents and terms of Figure 6.9. In this example we set a tf threshold of 20 for tier 1 and 10 for tier 2, meaning that the tier 1 index only has postings entries with tf values exceeding 20, while the tier 2 index only has postings entries with tf values exceeding 10. In this example we have chosen to order the postings entries within a tier by document ID.

TIERED INDEXES

7.2.2 Query-term proximity

Especially for free-text queries on the web (Chapter 19), users prefer a document in which most or all of the query terms most or all of the query terms appear close to each other, because this is evidence that the document has a section about what they are interested in. Consider a query with two or more query terms, $t_1, t_2, \ldots, t_k$. Let ω be the width of the smallest window in a document d that contains all the query terms, measured in the number of words in the window. For instance, if the document were to simply consist of the sentence The quality of mercy is not strained, the smallest window for the query strained mercy would be 4. In cases where the document does not contain all of the query terms, we can set ω to be some enormous number. Intuitively, the smaller that ω is, the better that d matches the query. We could also consider variants in which only words that are not stop words are considered in computing ω. Such proximity-weighted scoring functions are



► **Figure 7.2** Tiered indexes. If we fail to get K results from tier 1, query processing "falls back" to tier 2, and so on. Within each tier, postings are ordered by document ID.

a departure from pure cosine similarity and closer to the "soft conjunctive" semantics that Google and other web search engines evidently use.

PROXIMITY WEIGHTING

How can we design such a *proximity-weighted* scoring function to depend on ω? The simplest answer relies on a "hand coding" technique we introduce below in Section 7.2.3; a more scalable approach goes back to Section 6.1.2 – we treat the integer ω as yet another feature in the scoring function, whose importance is assigned by the methodology of Section 6.1.2. We will develop this approach further in Section 7.2.4 below.

Exercise 7.8

Explain how the postings merge first introduced in Section 1.3 can be adapted to find the smallest integer ω that contains all query terms.

Exercise 7.9

Adapt this procedure to work when not all query terms are present in a document.

7.2.3 Designing parsing and scoring functions

Common search interfaces, particulary for consumer-facing search applications on the web, tend to mask query operators from the end user. The intent is to hide the complexity of these operators from the largely non-technical audience for such applications, inviting free-text queries. Given such interfaces, how should a search equipped with indexes for various retrieval operators treat a query such as rising interest rates? More generally, given the various factors we have studied that could affect the score of a document, how should we combine these features?

The answer of course depends on the user population, the query distribution and the collection of documents. Typically, a *query parser* is used to translate the user-specified keywords into a query with various operators that is executed against the underlying indexes. Sometimes, this execution can entail multiple queries against the underlying indexes; for our example, the query parser may issue a stream of queries:

1. Run the user-generated query string as a phrase query. Rank them by vector space scoring using as query the vector consisting of the 3 terms rising interest rates.

2. If fewer than ten documents contain the phrase rising interest rates, run the two 2-term phrase queries rising interest and interest rates; rank these using vector space scoring, as well.

3. If we still have fewer than ten results, run the vector space query consisting of the three individual query terms.

Each of these steps (if invoked) may yield a list of scored documents, for each of which we compute a score. This score must combine contributions from vector space scoring, static quality, proximity weighting and potentially other factors. How do we devise a query parser and how do we devise the aggregate scoring function? The answer depends on the setting. In many enterprise settings we have application builders who make use of a toolkit of available scoring operators, along with a query parsing layer, with which to manually configure the scoring function as well as the query parser. Such application builders make use of the available zones, metadata and knowledge of typical documents and queries to tune the parsing and scoring. In collections whose characteristics change infrequently (in an enterprise application, significant changes in collection and query characteristics typically happen with infrequent events such as the introduction of new document formats or document management systems, or a merger with another company). Web search on the other hand is faced with a constantly changing document collection with new characteristics being introduced all the time. It is also a setting in which the number of scoring factors can run into the hundreds, making hand-tuned scoring a difficult exercise. To address this, it is becoming increasingly common to use machine-learned scoring, extending the ideas we introduced in Section 6.1.2.

7.2.4 Machine-learned scoring

In this section we generalize the methodology of Section 6.1.2 to *machine learn* the scoring function. In Section 6.1.2 we considered a case where we had to combine Boolean indicators of relevance; here we consider more general factors to further develop the notion of machine-learned relevance. In particular, the factors we now consider go beyond Boolean functions of query term presence in document zones, as in Section 6.1.2.

We develop the ideas using a setting in which we have a scoring function that is a linear combination of two factors: (1) the vector space cosine similarity between query and document and (2) the minimum window width ω within which the query terms lie. Thus we have a factor that depends on the statistics of query terms in the document as a bag of words, and another that depends on proximity weighting. We focus on this two-factor development of the ideas because it retains the generality of many more factors, while remaining simple enough to visualize.

As in Section 6.1.2 we are provided with a set of *training examples*, each of which is a pair consisting of a query and a document, together with a relevance judgment for that document on that query that is either *Relevant* or *Non-relevant*. For each such example we can compute the vector space cosine similarity, as well as the window width ω. The result is a training set as shown in Figure 7.3, which resembles Figure 6.5 from Section 6.1.2.

Example	DocID	Query	Cosine score	ω	Judgment
Φ_1	37	linux operating system	0.032	3	Relevant
Φ_2	37	penguin logo	0.02	4	Non-relevant
Φ_3	238	operating system	0.043	2	Relevant
Φ_4	238	runtime environment	0.004	2	Non-relevant
Φ_5	1741	kernel layer	0.022	3	Relevant
Φ_6	2094	device driver	0.03	2	Relevant
Φ_7	3191	device driver	0.027	5	Non-relevant
...	...	...	...	...	...

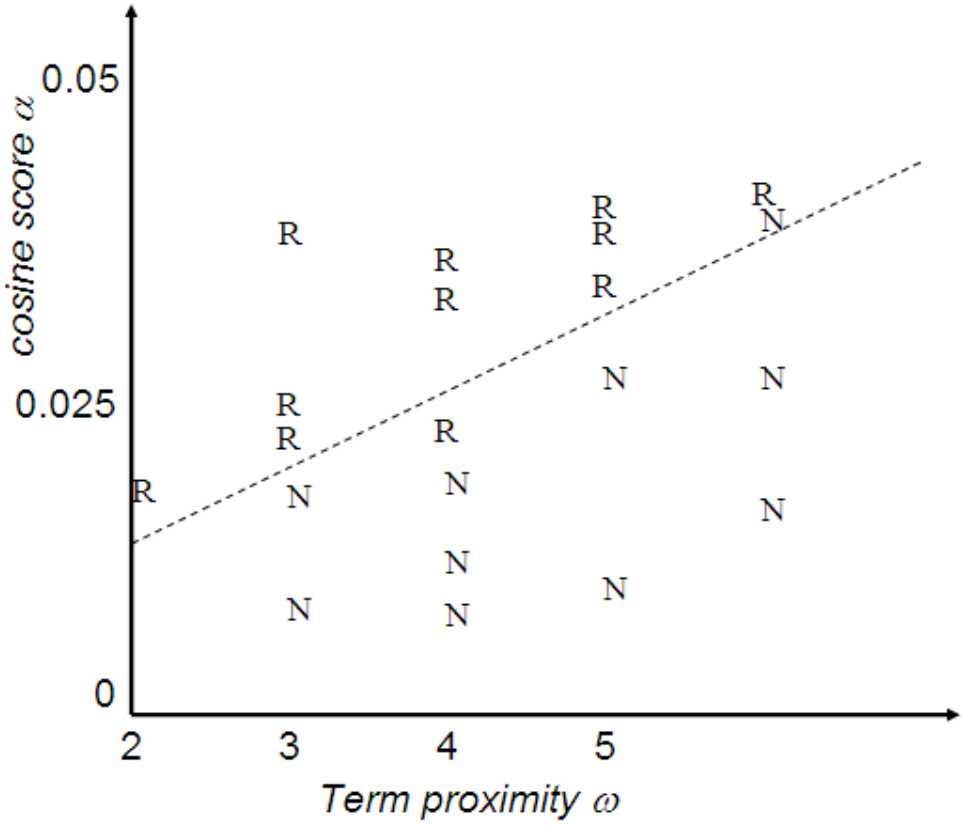
► **Figure 7.3** Training examples for machine-learned scoring.

The two numerical factors (cosine score denoted α and window width ω) are called *features* in the setting of machine learning, which we will explore further beginning Chapter 13. If we were once again to quantify the judgment Relevant as a 1 and Non-relevant as 0, we seek a scoring funtion that combines the values of the features to generate a value that is 0 or 1. We wish this function to be in agreement with our set of training examples as far as possible. Without loss of generality, our linear combination of features has the form

$$Score(\alpha, \omega) = a\alpha + b\omega + c, \tag{7.3}$$

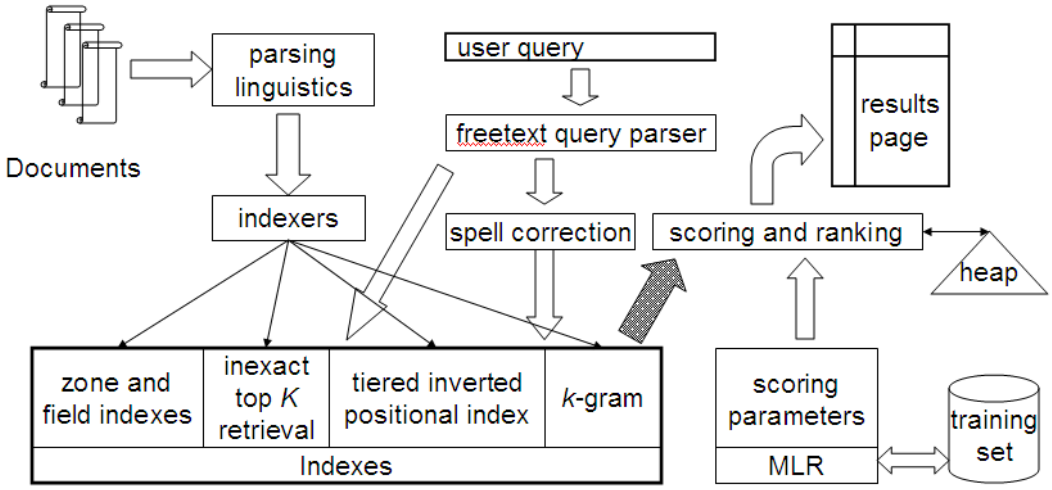
with the coefficients a, b, c to be learned from the training data. While it is now possible to formulate this as an error minimization problem as we did in Section 6.1.2, it is instructive to visualize the geometry of Equation (7.3). First, note that the examples in Figure 7.3 can be plotted on a two-dimensional plane with axes corresponding to the cosine score α and the window width ω. This is depicted in Figure 7.4.

In this setting, the function $Score(\alpha, \omega)$ from Equation (7.3) represents a plane "hanging above" Figure 7.4. Ideally this plane (in the direction perpendicular to the page containing Figure 7.4) assumes values close to 1 above the points marked R, and values close to 0 above the points marked N. Since a plane is unlikely to assume only values close to 0 or 1 above the training sample points, we make use of *thresholding*: given any query and document for which we wish to determine relevance, we pick a value θ and if $Score(\alpha, \omega) > \theta$ we declare the document to be Relevant, else we declare the document to be Non-relevant. This is equivalent to the following: consider the line passing through the plane $Score(\alpha, \omega)$ whose height is θ above the page containing Figure 7.4. Project this line down onto Figure 7.4; this might look like the dashed line in Figure 7.4. Then, any subsequent query/document pair that falls below the dashed line in Figure 7.4 is deemed Non-relevant; above the dashed line, Relevant.



► **Figure 7.4** A collection of training examples. Each R denotes a training example labeled Relevant, while each N is a training example labeled Non-relevant.

Thus, the problem of making a binary Relevant/Non-relevant judgment given training examples as above turns into one of learning the dashed line in Figure 7.4 separating Relevant training examples from the Non-relevant ones. Being in the α-ω plane, this line can be written as a linear equation involving α and ω, with two parameters (slope and intercept). The problem of finding such a line has a rich mathematical basis and is studied in a very general form in Chapter 15. Indeed, it has a ready generalization to functions on more than two variables – thus allowing us to not only consider (as here) α and ω, but simultaneously a host of other scoring features such as static quality, zone contributions, document length and so on. Provided we can build a sufficiently rich collection of training samples, we can thus alto-



► **Figure 7.5** A complete search system. Data paths are shown primarily for a free-text query.

gether avoid hand-tuning score functions as in Section 7.2.3. The bottleneck of course is the ability to maintain a suitably representative set of training examples, whose relevance assessments must be made by experts.

Exercise 7.10

Plot the first 7 rows of Figure 7.3 in the α-ω plane to produce a figure like that in Figure 7.4.

Exercise 7.11

Write down the equation of a line in the α-ω plane separating the R's from the N's.

Exercise 7.12

Give a training example (consisting of values for α, ω and the relevance judgment) that when added to the training set makes it impossible to separate the R's from the N's using a line in the α-ω plane.

7.2.5 Putting it all together

We have now studied all the components necessary for a basic search system that supports freetext queries as well as Boolean, zone and field queries. We briefly review how the various pieces fit together into an overall system; this is depicted in Figure 7.5.

In this figure, documents stream in from the left for parsing and linguistic processing (language detection, tokenization and stemming). The resulting

stream of tokens is fed to a bank of indexers that create a bank of indexes including zone and field indexes, (tiered) positional indexes, indexes for spell-correction and other tolerant retrieval, and structures for accelerating inexact top-K retrieval. A freetext user query (top center) is sent down to the indexes both directly and as for generating spell-correction candidate; as noted in Chapter 3 the latter may optionally be invoked only when the original query fails to retrieve enough results. Retrieved documents (dark arrow) are passed to a scoring module that computes scores based on machine-learned ranking (MLR), then rendered as a results page.

7.2.6 Interaction between vector space and other retrieval methods

We conclude this chapter by discussing how the vector space scoring model relates to the query operators we have studied in earlier chapters. The relationship should be viewed at two levels: in terms of the expressiveness of queries that a sophisticated user may pose, and in terms of the index that supports the evaluation of the various retrieval methods. In building a search engine, we may opt to support multiple query operators for an end user. In doing so we need to understand what components of the index can be shared for executing various query operators, as well as how to handle user queries that mix various query operators.

Vector space scoring supports so-called free-text retrieval, in which a query is specified as a set of words without any query operators connecting them. It allows documents matching the query to be scored and thus ranked, unlike the Boolean, wildcard and phrase queries studied earlier. Classically, the interpretation of such free-text queries was that at least one of the query terms be present in any retrieved document. However more recently, modern web search engines such as Google have popularized the notion that a set of terms typed into their query boxes (thus on the face of it, a free-text query) carries the semantics of a conjunctive query that only retrieves documents containing all or most query terms.

Boolean retrieval

Clearly a vector space index can be used to answer Boolean queries, but not vice versa, as long as the weight of a term t in the vector representation of document d is non-zero whenever term t occurs in document d. There is no easy way of combining vector space and Boolean queries from a user's standpoint: vector space queries are fundamentally a form of *evidence accumulation*, where the presence of more query terms in a document adds to the score of a document. Boolean retrieval on the other hand, requires a user to specify a formula for *selecting* documents through the presence (or absence) of specific

combinations of keywords, without inducing any relative ordering among them.

Wildcard queries

Wildcard and vector space queries require different indexes, except at the basic level that both can be implemented using postings and a dictionary (e.g., a dictionary of trigrams for wildcard queries). If a search engine allows a user to specify a wildcard operator as part of a free-text query (for instance, the query rom* restaurant), we may interpret the wildcard component of the query as spawning multiple terms in the vector space (in this example, rome and roman would be two such terms) all of which are added to the query vector. The vector space query is then executed as usual, with matching documents being scored and ranked; thus a document containing both rome and roma is likely to be scored higher than another containing only one of them. The exact score ordering will of course depend on the relative weights of each term in matching documents.

Phrase queries

The representation of documents as vectors is fundamentally lossy: the relative order of terms in a document is lost in the encoding of a document as a vector. Even if we were to try and somehow treat every biword as a term (and thus an axis in the vector space, a questionable encoding as the weights on different axes not independent), notions such as idf would have to be extended to such biwords. Thus an index built for vector space retrieval cannot, in general, be used for phrase queries. Moreover, there is no way of demanding a vector space score for a phrase query — we only know the relative weights of each term in a document.

On the query german shepherd, we could use vector space retrieval to identify documents heavy in these two terms, with no way of prescribing that they occur consecutively. Phrase retrieval, on the other hand, tells us of the existence of the phrase german shepherd in a document, without any indication of the relative frequency or weight of this phrase. While these two retrieval paradigms (phrase and vector space) consequently have different implementations in terms of indexes and retrieval algorithms, they can in some cases be combined usefully, as detailed below.

7.3 References and further reading

Heuristics for fast query processing with early termination are described by Anh et al. (2001), Garcia et al. (2004), Anh and Moffat (2006b), Persin et al.

(1996). Cluster pruning is investigated by Chierichetti et al. (2007). Champion lists are developed in Brin and Page (1998), Long and Suel (2003). While these heuristics are well-suited to free-text queries that can be viewed as vectors, they complicate phrase queries; see Anh and Moffat (2006c) for an index structure that supports both weighted and Boolean / phrase searches. Carmel et al. (2001) Clarke et al. (2000) and Song et al. (2005) treat the use of query term proximity in assessing relevance. Pioneering work on learning of ranking functions was done by Fuhr (1989), Fuhr and Pfeifer (1994), Cooper et al. (1994), Bartell (1994), Bartell et al. (1998) and by Cohen et al. (1998).

8 *Evaluation in information retrieval*

We have seen in the preceding chapters many alternatives in designing an IR system. How do we know which of these techniques are effective in which applications? Should we use stop lists? Should we stem? Should we use inverse document frequency weighting? Information retrieval has developed as a highly empirical discipline, requiring careful and thorough evaluation to demonstrate the superior performance of novel techniques on representative document collections.

In this chapter we begin with a discussion of measuring the effectiveness of IR systems (Section 8.1) and the test collections that are most often used for this purpose (Section 8.2). We then present the straightforward notion of relevant and nonrelevant documents and the formal evaluation methodology that has been developed for evaluating unranked retrieval results (Section 8.3). This includes explaining the kinds of evaluation measures that are standardly used for retrieval and related tasks like categorization and why they are appropriate. We then extend these notions and develop further measures for evaluating ranked retrieval results (Section 8.4) and discuss developing reliable and informative test collections (Section 8.5).

We then step back to introduce the notion of user utility, and how it is approximated by the use of document relevance (Section 8.6). At the end of the day, the key measure is user happiness. Speed of response and the size of the index are factors in user happiness. It seems as if relevance of results is the most important factor: blindingly fast, useless answers do not make a user happy. However, user perceptions do not always coincide with system designers' notions of quality. For example, user happiness commonly depends very strongly on user interface design issues, including the layout, clarity, and responsiveness of the user interface, which are independent of the quality of the results returned. We touch on other measures of the quality of a system, in particular the generation of high-quality result summary snippets, which strongly influence user utility, but are not measured in the basic relevance ranking paradigm (Section 8.7).

8.1 Evaluating information retrieval systems and search engines

To measure ad hoc information retrieval effectiveness in the standard way, we need a test collection consisting of three things:

1. A test document collection
2. A test suite of information needs, expressible as queries
3. A set of relevance judgements, standardly a binary assessment of either *relevant* or *not relevant* for each query-document pair.

RELEVANCE

GOLD STANDARD

GROUND TRUTH

The standard approach to information retrieval system evaluation revolves around the notion of *relevant* and *not relevant* documents. With respect to a user information need, a document is given a binary classification as either relevant or not relevant. This decision is refered to as the *gold standard* or *ground truth* judgement of relevance. The test document collection and suite of information needs need to be of a reasonable size: you need to average performance over fairly large test sets, as results are very variable over different documents and information needs.

INFORMATION NEED

Relevance is assessed relative to an information need, *not* a query. For example, an information need might be:

> I'm looking for information on whether drinking red wine is more effective at reducing your risk of heart attacks than white wine.

This might be translated into a query such as:

wine AND red AND white AND heart AND attack AND effective

A document is relevant if it addresses the stated information need, not because it just happens to contain all the words in the query. This distinction is often misunderstood in practice, because the information need is not overt. But, nevertheless, an information need is present. If I type python into a web search engine, I might be wanting to know where I can purchase a pet python. Or I might be wanting information on the programming language Python. From a one word query, it is very difficult for a system to know what my information need is. But, nevertheless, I have one, and can judge the returned results on the basis of their relevance to it. To do a system evaluation, we require an overt expression of an information need, which can be used for judging returned documents as relevant or not relevant. At this point, we make a simplification: you could reasonably think that relevance is a scale, with some documents highly relevant and others marginally so. But for the moment, we will use just a binary decision of relevance. We discuss the reasons for using binary relevance judgements and alternatives in Section 8.5.1.

8.2 Standard test collections

Here is a list of the most standard test collections and evaluation series. We focus particularly on test collections for ad hoc information retrieval system evaluation, but also mention a couple of similar test collections for text classification.

CRANFIELD The *Cranfield* collection. The pioneering test collection in allowing precise quantative metrics of information retrieval effectiveness. Collected in the United Kingdom starting in the late 1950s, it contains 1398 abstracts of aerodynamics journal articles, a set of 225 queries, and exhaustive relevance judgements.

TREC *TREC*. The U.S. National Institute of Standards and Technology (NIST) has run a large IR test bed evaluation series since 1992. Within this framework, there have been many tracks over a range of different test collections, but the best known test collections are the ones used for the TREC Ad Hoc track during the first 8 TREC evaluations between 1992 and 1999. In total, these test collections comprise 6 CDs containing 1.89 million documents (mainly, but not exclusively, newswire articles) and relevance judgements for 450 information needs, which are specified in detailed text passages. Individual test collections are defined over different subsets of this data. For example, taken together, TREC 1–3 provide 150 information needs over 742,000 newswire and magazine articles and government abstracts, and TREC 6–8 provide 150 information needs over 515,000 Foreign Broadcast Information Service articles. Because the test document collections are so large, there are no exhaustive relevance judgements. Rather, NIST assessor's relevance judgements have been gathered only for the documents that were among the top-k returned for some system which was entered in the TREC evaluation in which the information need was first used.

GOV2 In more recent years, NIST has done evaluations on larger document collections, including the 25 million page *GOV2* web page collection. From the beginning, the NIST test document collections were orders of magnitude larger than anything available to researchers previously. Nevertheles, the size of GOV2 is still more than 2 orders of magnitude smaller than the current size of the document collections indexed by the large web search companies.

NTCIR NII Test Collections for IR Systems (*NTCIR*). The NTCIR project has built various test collections of similar sizes to the TREC collections, focusing on East Asian language and cross-language information retrieval. See: http://research.nii.ac.jp/ntcir/data/data-en.html

CLEF Cross Language Evaluation Forum (*CLEF*). This evaluation series has concentrated on European languages and cross-language information retrieval. See: http://www.clef-campaign.org/

REUTERS Reuters-21578 and Reuters-RCV1. For text classification, the most used test collection has been the Reuters-21578 collection of 21578 newswire articles; see Chapter 13, page 261. More recently, Reuters released the much larger Reuters Corpus Volume 1 (RCV1), consisting of 806,791 documents; see Chapter 4, page 63. It is probably a better basis for future research.

20 NEWSGROUPS *20 Newsgroups*. This is another widely used text classification collection, collected by Ken Lang. It consists of 1000 articles from each of 20 Usenet newsgroups (the newsgroup name being regarded as the category). After the removal of duplicate articles, as it is usually used, it contains 18941 articles.

8.3 Evaluation of unranked retrieval sets

Given these ingredients, how is system effectiveness measured? The two most frequent and basic measures for information retrieval effectiveness are precision and recall. These are first defined for the simple case where an IR system returns a set of documents for a query. We will see later how to extend these notions to ranked retrieval situations.

PRECISION *Precision* (P) is the fraction of retrieved documents that are relevant

$$\text{Precision} = \frac{\#(\text{relevant items retrieved})}{\#(\text{retrieved items})} = P(\text{relevant}|\text{retrieved}) \tag{8.1}$$

RECALL *Recall* (R) is the fraction of relevant documents that are retrieved

$$\text{Recall} = \frac{\#(\text{relevant items retrieved})}{\#(\text{relevant items})} = P(\text{retrieved}|\text{relevant}) \tag{8.2}$$

These notions can be made clear by examining the following contingency table:

(8.3)

	Relevant	Not relevant
Retrieved	true positives (tp)	false positives (fp)
Not retrieved	false negatives (fn)	true negatives (tn)

Then:

$$\begin{aligned} P &= tp/(tp+fp) \\ R &= tp/(tp+fn) \end{aligned} \tag{8.4}$$

ACCURACY

An obvious alternative that may occur to the reader is to judge an information retrieval system by its *accuracy*, that is, the fraction of its classifications that are correct. In terms of the contingency table above, accuracy $= (tp + tn)/(tp + fp + fn + tn)$. This seems plausible, since there are two actual classes, relevant and not relevant, and an information retrieval system can be thought of as a two class classifier which attempts to label them as such (it retrieves the subset of documents which it believes to be relevant). Precisely this measure is the effectiveness measure often used for evaluating machine learning classification problems.

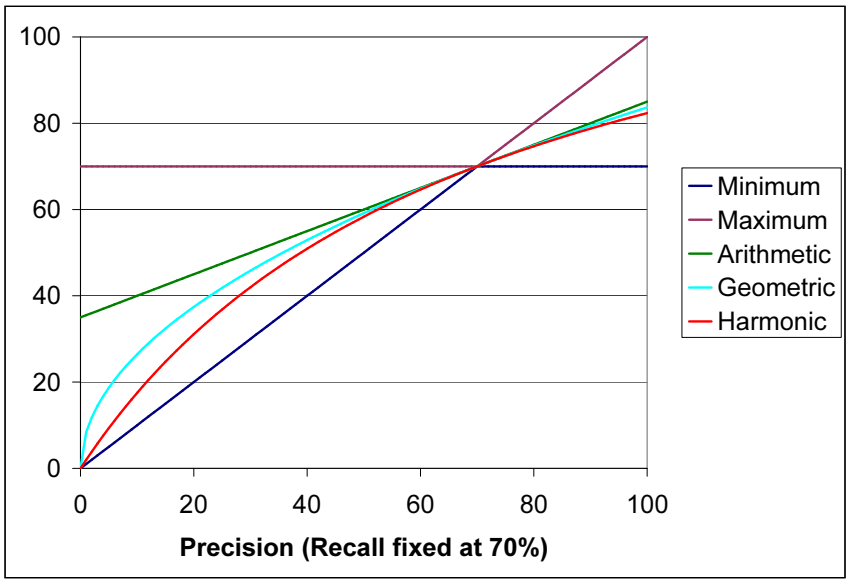
There is a good reason why accuracy is not an appropriate measure for information retrieval problems. In almost all circumstances, the data is extremely skewed: normally over 99.9% of the documents are in the not relevant category. In such circumstances, a system tuned to maximize accuracy will almost always declare every document not relevant. Even if the system is quite good, trying to label some documents as relevant will almost always lead to an unacceptably high rate of false positives. However, this behavior is completely unsatisfying to an information retrieval system user. Users are always going to want to see some documents, and can be assumed to have a certain tolerance for seeing some false positives providing that they get some useful information. The measures of precision and recall concentrate the evaluation on the return of true positives, asking what percentage of the relevant documents have been found and how many false positives have also been returned.

The advantage of having the two numbers for precision and recall is that one is more important than the other in many circumstances. Typical web surfers would like every result on the first page to be relevant (high precision) but have not the slightest interest in knowing let alone looking at every document that is relevant. In contrast, various professional searchers such as paralegals and intelligence analysts are very concerned with trying to get as high recall as possible, and will tolerate fairly low precision results in order to get it. Nevertheless, the two quantities clearly trade off against one another: you can always get a recall of 1 (but very low precision) by retrieving all documents for all queries! Recall is a non-decreasing function of the number of documents retrieved. On the other hand, in a good system, precision usually decreases as the number of documents retrieved is increased. In general we want to get some amount of recall while tolerating only a certain percentage of false positives.

F MEASURE

A single measure that trades off precision versus recall is the *F measure*, which is the weighted harmonic mean of precision and recall:

$$F = \frac{1}{\alpha\frac{1}{P} + (1-\alpha)\frac{1}{R}} = \frac{(\beta^2+1)PR}{\beta^2 P + R} \quad \text{where} \quad \beta^2 = \frac{1-\alpha}{\alpha} \tag{8.5}$$



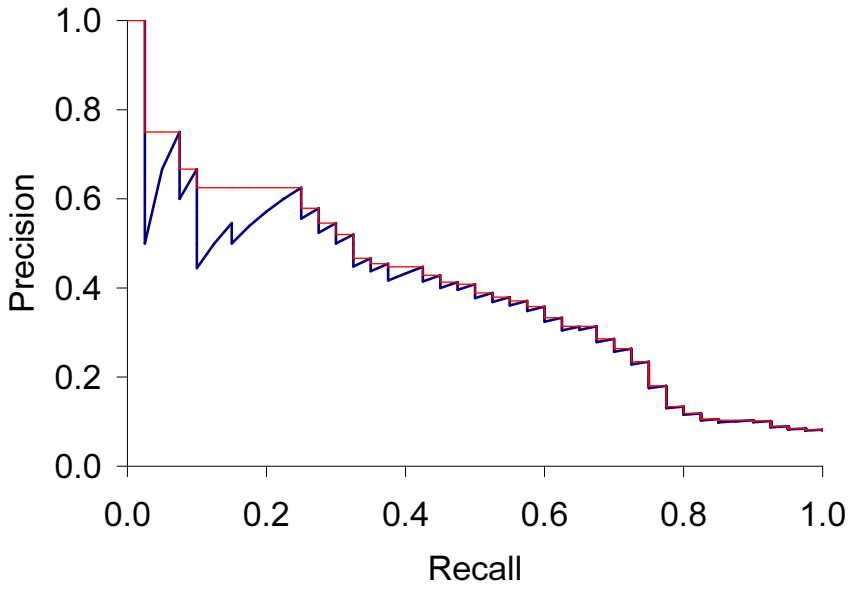
► **Figure 8.1** Graph comparing the harmonic mean to other means. The graph shows a slice through the calculation of various means of precision and recall for the fixed recall value of 70%. The harmonic means is always less than either the arithmetic or geometric mean, and often quite close to the minimum of the two numbers. When the precision is also 70%, all the measures coincide.

The weighting $\alpha \in [0, 1]$, and so the ratio of weights $\beta^2 \in [0, \infty]$. The default balanced F measure equally weights precision and recall, which means making $\alpha = 1/2$ or $\beta = 1$. It is commonly written as F_1, which is short for $F_{\beta=1}$, even though the formulation in terms of α more transparently exhibits the F measure as a weighted harmonic mean. When using $\beta = 1$, the formula on the right simplifies to:

$$F_{\beta=1} = \frac{2PR}{P+R} \tag{8.6}$$

However, using an even weighting is not the only choice. Values of $\beta < 1$ emphasize precision, while values of $\beta > 1$ emphasize recall. For example, a value of $\beta = 3$ or $\beta = 5$ might be used if recall is to be emphasized. Recall, precision, and the F measure are inherently measures between 0 and 1, but they are also very commonly written as percentages, on a scale between 0 and 100.

Why do we use a harmonic mean rather than the more usual average (arithmetic mean)? Recall that we can always get 100% recall by just returning all documents, and therefore we can always get a 50% arithmetic



► **Figure 8.2** Precision/Recall graph.

mean by the same process. This strongly suggests that the arithmetic mean is an unsuitable measure to use. In contrast, if we assume that 1 document in 10000 is relevant to the query, the harmonic mean score of this strategy is 0.02%. The harmonic mean, the third of the classical Pythagorean means, is always less than or equal to the arithmetic mean and the geometric mean. When the values of two numbers differ greatly, the harmonic mean is closer to their minimum than to their arithmetic mean; see Figure 8.1.

8.4 Evaluation of ranked retrieval results

Precision, recall, and the F measure are set-based measures. They are computed using unordered sets of documents. We need to extend these measures (or to define new measures) if we are to evaluate the ranked retrieval results that are now standard in information retrieval. In a ranking context, appropriate sets of retrieved documents are naturally given by the top k retrieved documents. For each such set, precision and recall values can be plotted to give a *precision-recall curve*, such as the one shown in Figure 8.2. Precision-recall curves have a distinctive saw-tooth shape: if the $(k+1)^{\text{th}}$ document retrieved is nonrelevant then recall is the same as for the top k documents, but precision has dropped. If it is relevant, then both precision and recall

PRECISION-RECALL CURVE

Recall	Interp. Precision
0.0	1.00
0.1	0.67
0.2	0.63
0.3	0.55
0.4	0.45
0.5	0.41
0.6	0.36
0.7	0.29
0.8	0.13
0.9	0.10
1.0	0.08

► **Table 8.1** Calculation of 11-point Interpolated Average Precision. This is for the precision-recall curve shown in Figure 8.2.

increase, and the curve jags up and to the right. It is often useful to remove these jiggles and the standard way to do this is with an interpolated precision: the interpolated precision p_{interp} at a certain recall level r is defined as the highest precision found for any recall level $q \geq r$:

$$p_{interp}(r) = max_{r' \geq r} p(r') \tag{8.7}$$

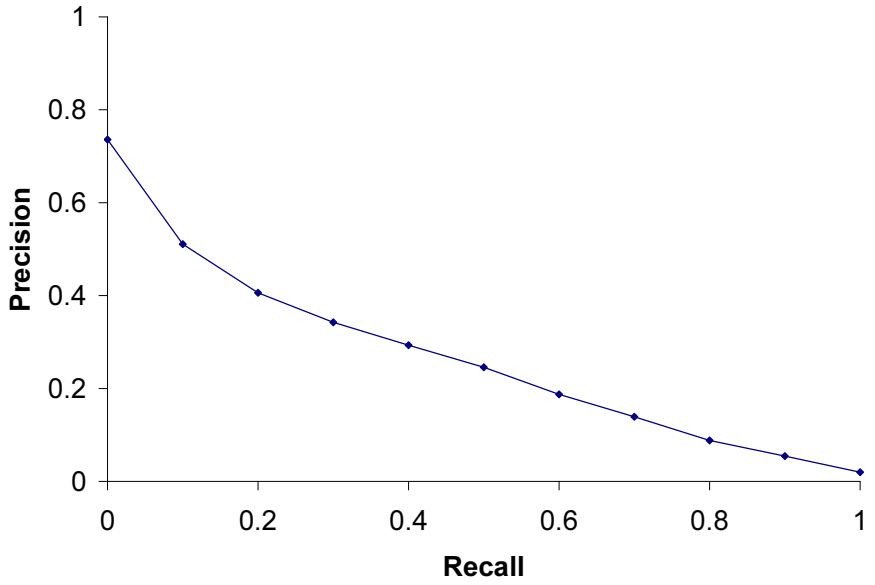
The justification is that almost anyone would be prepared to look at a few more documents if it would increase the percentage of the viewed set that were relevant (that is, if the precision of the larger set is higher). Interpolated precision is shown by a thinner line in Figure 8.2. With this definition, the interpolated precision at a recall of 0 is well-defined.

Examining the entire precision-recall curve is often very informative, but there is often a desire to boil this information down to a few numbers, or perhaps even a single number. The traditional way of doing this (used for instance in the first 8 TREC Ad Hoc evaluations) is the *11-point interpolated average precision*. For each information need, the interpolated precision is measured at the 11 recall levels of 0.0, 0.1, 0.2, . . . , 1.0. For the precision-recall curve in Figure 8.2, these 11 values are shown in Table 8.1. For each recall level, we then calculate the arithmetic mean of the interpolated precision at that recall level for each information need in the test collection. A composite precision-recall curve showing 11 points can then be graphed. Figure 8.3 shows an example graph of such results from a representative good system at TREC 8.

11-POINT INTERPOLATED AVERAGE PRECISION

In recent years, other measures have become more common. Most standard among the TREC community is *Mean Average Precision* (MAP), which

MEAN AVERAGE PRECISION



► **Figure 8.3** Averaged 11-Point Precision/Recall graph across 50 queries for a representative TREC system. The Mean Average Precision for this system is 0.2553.

provides a single-figure measure of quality across recall levels. For one information need, Average Precision is the average of the precision value obtained for the top set of k documents existing after each relevant document is retrieved, and this value is then averaged over information needs. That is, if the set of relevant documents for an information need $q_j \in Q$ is $\{d_1, \ldots d_{m_j}\}$ and R_k is the set of ranked retrieval results from the top result until you get to document d_k, then

$$\text{MAP}(Q) = \frac{1}{|Q|} \sum_{j=1}^{|Q|} \frac{1}{m_j} \sum_{k=1}^{m_j} \text{Precision}(R_k) \tag{8.8}$$

When a relevant document is not retrieved at all, the precision value in the above equation is taken to be 0. For one information need, the average precision approximates the area under the uninterpolated precision-recall curve, and so the MAP is roughly the average area under the precision-recall curve for a set of queries.

Using MAP, fixed recall levels are not chosen, and there is no interpolation. The MAP value for a test collection is the arithmetic mean of MAP values for individual information needs. (This has the effect of weighting each information need equally in the final reported number, even if many

documents are relevant to some queries whereas very few are relevant to other queries.) Calculated MAP scores normally vary widely across information needs when measured for the same system, for instance, between 0.1 and 0.7. Indeed, there is normally more agreement in MAP for an individual information need across systems than for MAP scores for different information needs for the same system. This means that a set of test information needs must be large and diverse enough to be representative of system effectiveness across different queries.

PRECISION AT k

The above measures factor in precision at all recall levels. For many prominent applications, particularly web search, this may not be highly relevant to users. What matters is rather how many good results there are on the first page or the first three pages. This leads to measuring precision at fixed low levels of retrieved results, such as 10 or 30 documents. This is referred to as "Precision at k", for example "Precision at 10". It has the advantage of not requiring any estimate of the size of the set of relevant documents but the disadvantage that it does not average well, since the total number of relevant documents for a query has a strong influence on precision at k.

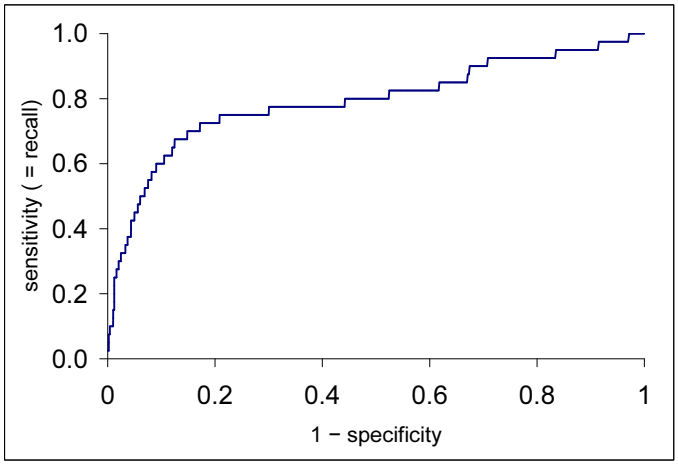
R-PRECISION

An alternative, which alleviates this problem, is *R-precision*. It requires having a set of known relevant documents of size *Rel*, from which we calculate the precision of the top *Rel* documents returned. (This relevant set may be incomplete, such as when this set is formed by examining the pooled top k results of particular systems in a set of experiments.) This measure adjusts for the size of the set of relevant documents: A perfect system could score 1 on this metric for each query, whereas, even a perfect system could only achieve a precision at 20 of 0.4 if there were only 8 documents in the collection relevant to an information need. Averaging this measure across queries thus makes more sense. This measure is harder to explain to naive users than Precision at k but easier to explain than MAP. If there are *Rel* relevant documents for a query, we examine the top *Rel* results of a system, and find that r are relevant, then by definition, not only is the precision (and hence R-precision) r/Rel, but the recall of this result set is also r/Rel. Thus, R-precision turns out to be identical to the *break-even point*, another sometimes used measure, defined in terms of this equality relationship holding. Like the Precision at k, R-precision describes only one point on the precision-recall curve, rather than attempting to summarize effectiveness across the curve, and it is somewhat unclear why you should be interested in the break-even point rather than either the best point on the curve (the point with maximal F-measure) or a retrieval level of interest to a particular application (Precision at k). Nevertheless, R-precision turns out to be highly correlated with MAP empirically, despite measuring only a single point on the curve.

BREAK-EVEN POINT

ROC CURVE

Another concept sometimes used in evaluation is an *ROC curve* ("ROC" stands for "Receiver Operating Characteristics", but knowing that doesn't help most people). An ROC curve plots the true positive rate or sensitiv-



► **Figure 8.4** The ROC curve corresponding to the precision-recall curve in Figure 8.2.

SENSITIVITY

SPECIFICITY

ity against the false positive rate or (1 − specificity). Here, *sensitivity* is just another term for recall and the false positive rate is given by $fp/(fp + tn)$. Figure 8.4 shows the ROC curve corresponding to the precision-recall curve in Figure 8.2. An ROC curve always goes from the bottom left to the top right of the graph. For a good system, the graph climbs steeply on the left side. For unranked retrieval sets in IR, *specificity*, given by $tn/(fp + tn)$, was not seen as such a useful notion. Because the set of true negatives is always so large, its value would be almost 1 for all information needs (and, correspondingly, the value of the false positive rate would be almost 0). That is, the "interesting" part of Figure 8.2 is 0 <recall< 0.4, a part which is compressed to a small corner of Figure 8.4. But an ROC curve could make sense if looking over the full retrieval spectrum, and it provides another way of looking at the data. In many fields, a common aggregate measure is to report the area under the ROC curve, which is the ROC analog of the Average Precision measure. Precision-recall curves are sometimes loosely referred to as ROC curves. This is understandable, but not accurate.

8.5 Assessing relevance

To properly evaluate a system, your test information needs must be germane to the documents in the test document collection, and appropriate for predicted usage of the system. These information needs are best designed by

		Judge 2 Relevance		
		Yes	No	Total
Judge 1 Relevance	Yes	300	20	320
	No	10	70	80
	Total	310	90	400

Observed proportion of the times the judges agreed
$P(A) = (300 + 70)/400 = 370/400 = 0.925$
Pooled marginals
$P(nonrelevant) = (80 + 90)/(400 + 400) = 170/800 = 0.2125$
$P(relevant) = (320 + 310)/(400 + 400) = 630/800 = 0.7878$
Probability that the two judges agreed by chance
$P(E) = P(nonrelevant)^2 + P(relevant)^2 = 0.2125^2 + 0.7878^2 = 0.665$
Kappa measure
$\kappa = (P(A) - P(E))/(1 - P(E)) = (0.925 - 0.665)/(1 - 0.665) = 0.776$

▶ **Table 8.2** Calculating the kappa statistic.

domain experts. Using random query terms as an information need is generally not a good idea because typically they will not resemble the actual query distribution.

Given information needs and documents, you need to collect relevance assessments. This is a time-consuming and expensive process involving human beings. For tiny collections like Cranfield, exhaustive judgements of relevance for each query and document pair were obtained; for large modern collections, it is usual to determine relevance of only a subset of documents for each query, where the subset usually contains the top documents returned by each system being evaluated and additional documents gathered by human beings searching on likely keywords. Good practice is to collect the relevance judgements of two human judges working independently, and then for disagreements to be adjudicated, commonly in a discussion between the two original judges and a third senior judge. Such dual assessment raises the question as to whether human judgements of relevance are reliable and consistent.

KAPPA MEASURE

In the social sciences, a common measure for agreement between judges is the *Kappa measure*. It is designed for categorical judgments and corrects a simple agreement rate for the rate of chance agreement.

$$Kappa = \frac{P(A) - P(E)}{1 - P(E)} \tag{8.9}$$

where $P(A)$ is the proportion of the times the judges agreed, and $P(E)$ is the proportion of the times they would be expected to agree by chance. There

are choices in how the latter is estimated: if we simply say we are making a two-class decision and examine nothing more, then the expected chance agreement rate is 0.5. However, normally the class distribution assigned is skewed, and it is usual to use *marginal* statistics to calculate expected agreement.[1] There are still two ways to do it depending on whether one pools the marginal distribution across judges or uses the marginals for each judge separately; both forms have been used, but we present the pooled version because it is more conservative in the presence of systematic differences in coding across coders. The calculations are shown in Table 8.2. The kappa value will be 1 if two judges always agree, 0 if they agree only at the rate given by chance, and negative if they are worse than random. If there are more than two judges, it is normal to calculate an average pairwise kappa value. As a rule of thumb, a kappa value above 0.8 is taken as good agreement, a kappa value between 0.67 and 0.8 is taken as fair agreement, and agreement below 0.67 is seen as data providing a dubious basis for an evaluation, though the precise cutoffs depend on the purposes for which the data will be used.

MARGINAL

Interjudge agreement of relevance has been measured within the TREC evaluations and for medical IR collections (Hersh et al. 1994). Using the above rules of thumb, the level of agreement normally falls in the range of "fair" (0.67–0.8). The fact that human agreement on a binary relevance judgement is quite modest is one reason for not requiring more fine-grained relevance labeling from the test set creator. To answer the question of whether IR evaluation results are valid despite the variation of individual assessors' judgements, people have experimented with evaluations taking one or other of two judges' opinions as the gold standard. The choice can make a considerable absolute difference to reported scores, but has in general been found to have little impact on the relative performance of different systems, that is, to their ranking.

8.5.1 Document relevance: critiques and justifications of the concept

The advantage of system evaluation, as enabled by the standard model of relevant and nonrelevant documents, is that we have a fixed setting in which we can manipulate parameters and carry out comparative experiments. Such formal testing is much less expensive and allows clearer diagnosis of the effect of changing parameters than doing user studies of retrieval effectiveness. Indeed, once we have a formal measure that we have confidence in, we can proceed to optimize effectiveness by machine learning methods, rather than doing experiments by hand. Of course, if the formal measure poorly de-

1. For a contingency table, a marginal statistic is formed by summing a row or column. The marginal $a_{i.k} = \sum_j a_{ijk}$.

scribes what users actually want, doing this will not be effective in improving user satisfaction. Our perspective is that, in practice, the standard formal measures for IR evaluation, although a simplification, are good enough, and recent work in optimizing formal evaluation measures in IR has succeeded brilliantly. There are numerous examples of techniques developed in formal evaluation settings, which improve effectiveness in operational settings, such as the development of document length normalization methods within the context of TREC (Sections 6.4.5 and 11.4.2) and machine learning methods for adjusting parameter weights in ranking (Section 6.1.2).

That is not to say that there are not problems latent within the abstractions used. The relevance of one document is treated as independent of the relevance of other documents in the collection. (This assumption is actually built into most retrieval systems – documents are scored against queries, not against each other – as well as being assumed in the evaluation methods.) Assessments are binary: there aren't any nuanced assessments of relevance. Relevance of a document to an information need is treated as an absolute, objective decision, but judgements of relevance are subjective, varying across people as we discussed above, and, in practice, human assessors are also imperfect measuring instruments, susceptible to failures of understanding and attention. We also have to assume that users' information needs do not change as they start looking at retrieval results. Any results based on one collection are heavily skewed by the choice of collection, queries, and relevance judgment set: the results may not translate from one domain to another or to a different user population.

Some of these problems may be fixable. A number of recent evaluations, including INEX, some TREC tracks, and NCTIR have adopted a ordinal notion of relevance with documents divided into 3 or 4 classes, distinguishing slightly relevant documents from highly relevant documents. See Section 10.4 (page 198) for a detailed discussion of how this is implemented in the INEX evaluations.

MARGINAL RELEVANCE

One clear problem with the relevance-based assessment that we have presented is the distinction between Relevance vs. *Marginal Relevance*: whether a document still has distinctive usefulness after the user has looked at certain other documents (Carbonell and Goldstein 1998). Even if a document is highly relevant, its information can be completely redundant with other documents which have already been examined. The most extreme case of this is documents which are duplicates – a phenomenon that is actually very common on the World Wide Web – but it can also easily occur when several documents provide a similar precis of an event. In such circumstances, marginal relevance is clearly a better measure of utility to the user. Maximizing marginal relevance requires returning documents that exhibit diversity and novelty. One way to approach measuring this is by using distinct facts or entities as evaluation units. This perhaps more directly measures true

utility to the user but doing this makes it harder to create a test collection.

8.6 A broader perspective: System quality and user utility

Formal evaluation measures are at some distance from our ultimate interest in measures of human utility: how satisfied is each user with the results the system gives for each information need that they pose? The standard way to measure human satisfaction is by various kinds of user studies. These might include quantitative measures, both objective, such as time to complete a task, as well as subjective, such as a score for satisfaction with the search engine, and qualitative measures, such as user comments on the search interface. In this section we will touch on other system aspects that allow quantitative evaluation and the issue of user utility.

8.6.1 System issues

There are many practical benchmarks on which to rate an information retrieval system beyond its retrieval quality. These include:

- How fast does it index, that is, how many documents per hour does it index for a certain distribution over document sizes?
- How fast does it search, that is, what is its latency as a function of index size?
- How expressive is its query language? How fast is it on complex queries?
- How large is its document collection, in terms of the number of documents or the collection having information distributed across a broad range of topics?

All these criteria apart from query language expressiveness are straightforwardly *measurable*: we can quantify the speed or size. Various kinds of feature checklists can make query language expressiveness semi-precise.

8.6.2 User utility

What we would really like is a way of quantifying aggregate user happiness, based on the relevance, speed, and user interface of a system. One part of this is understanding the distribution of people we wish to make happy, and this depends entirely on the setting. For a web search engine, happy search users are those who find what they want. One indirect measure of such users is that they tend to return to the same engine. Measuring the rate of return users is thus an effective metric, which would of course be more effective

if you could also measure how much these users used other search engines too. But advertisers are also users of modern web search engines. They are happy if customers click through to their sites and then make purchases. On an eCommerce web site, a user is presumably also at least potentially wanting to purchase something. We can perhaps measure the time to purchase, or the fraction of searchers who become buyers. On a shopfront web site, perhaps both the user's and the store owner's needs are satisified if a purchase is made. Nevertheless, in general, we need to decide whether it is the end user's or the eCommerce site's owner's happiness that we are trying to optimize. Alas, it is the store owner who is paying you.

For an "enterprise" (company, government, or academic) intranet search engine, the relevant metric is more likely to be user productivity: how much time do users spend looking for information that they need. There are also many other practical criteria concerning such matters as information security, which we mentioned in Section 4.6.

User happiness is elusive to measure, and this is part of why the standard methodology uses the proxy of relevance of search results. The standard direct way to get at user satisfaction is to run user studies, where people engage in tasks, and usually various metrics are measured, the participants are observed, and ethnographic interview techniques are used to get qualitative information on satisfaction. User studies are very useful in system design, but they are time consuming and expensive to do. They are also difficult to do well, and expertise is required to design the studies and to interpret the results. We will not discuss the details of human usability testing here.

8.6.3 Refining a deployed system

If an IR system has been built and is being used by a large number of users, the system's builders can evaluate possible changes by deploying variant versions of the system and recording measures that are indicative of user satisfaction with the system as it is used. This method is commonly used by web search engines.

A/B TEST

The most common version of this is *A/B testing*, a term borrowed from the advertising industry. For such a test, precisely one thing is changed between the current system and a proposed system, and a small proportion of traffic (say, 1–10% of users) is randomly directed to the variant system, while most users use the current system. For example, if we wish to investigate a change to the relevance algorithm, we redirect a random sample of users to a variant system and evaluate measures such as the frequency with which people click on the top result, or any result on the first page. (This particular analysis method is referred to as *clickthrough log analysis* or *clickstream mining*. It is further discussed as a method of implicit feedback in Section 9.1.7.)

CLICKTHROUGH LOG ANALYSIS
CLICKSTREAM MINING

The basis of A/B testing is running a bunch of single variable tests (either

in sequence or in parallel): for each test only one parameter is varied from the control (the current live system). It is therefore easy to see whether varying each parameter has a positive or negative effect. Such testing of a live system can easily and cheaply gauge the effect of a change on users, and, with a large enough user base, it is practical to measure even very small positive and negative effects. In principle, more analytic power can be achieved by varying multiple things at once in an uncorrelated (random) way, and doing standard multivariate statistical analysis, such as multiple linear regression. Such techniques are at the heart of the optimization methods discussed in Section 6.1.2. In practice, though, A/B testing is still widely used, because A/B tests are easy to deploy, easy to understand, and easy to explain to management.

8.7 Results snippets

Having chosen or ranked the documents matching a query, we wish to present a results list that will be informative to the user. In many cases the user will not want to examine all the returned documents and so we want to make the results list informative enough that the user can do a final ranking of the documents for themselves based on relevance to their information need.[2] The standard way of doing this is to provide a *snippet*, a short summary of the document, which is designed so as to allow the user to decide its relevance. Typically, the snippet has the document title and a short summary, which is automatically extracted. The question is how to design the summary so as to maximize its usefulness to the user.

SNIPPET

STATIC SUMMARY
DYNAMIC SUMMARY

The two basic kinds of summaries are *static*, which are always the same regardless of the query, and *dynamic* (or query-dependent), which are customized according to the user's information need as deduced from a query. Dynamic summaries attempt to explain why a particular document was retrieved for the query at hand.

A static summary is generally comprised of either or both a subset of the document and metadata associated with the document. The simplest form of summary takes the first two sentences or 50 words of a document, or extracts particular zones of a document, such as the title and author. Instead of zones of a document, the summary can instead use metadata associated with the document. This may be an alternative way to provide an author or date, or may include elements which are designed to give a summary, such as the `description` metadata which can appear in the `meta` element of a web HTML page. This summary is typically extracted and cached at indexing time, in such a way that it can be retrieved and presented quickly

2. There are exceptions, in domains where recall is emphasized. For instance, in many legal disclosure cases, an associate will review *every* document that matches a keyword search.

when displaying search results, whereas, having to access the actual document content might be a relatively expensive operation.

There has been extensive work within natural language processing (NLP) on better ways to do text summarization. Most such work still aims only to choose sentences from the original document to present and concentrates on how to select good sentences. The models typically combine positional factors, favoring the first and last paragraphs of documents and the first and last sentences of paragraphs, with content factors, emphasizing sentences with key terms, which have low document frequency in the collection as a whole, but high frequency and good distribution across the particular document being returned. In sophisticated NLP approaches, the system synthesizes sentences for a summary, either by doing full text generation or by editing and perhaps combining sentences used in the document. For example, it might delete a relative clause or replace a pronoun with the noun phrase that it refers to. This last class of methods remains in the realm of research and is seldom used for search results: it is easier, safer, and often even better to just use sentences from the original document.

Dynamic summaries display one or more "windows" on the document, aiming to present the pieces that have the most utility to the user in evaluating the document with respect to their information need. Usually these windows contain one or several of the query terms, and so are often referred to as *keyword-in-context* (KWIC) snippets, though sometimes they may still be pieces of the text such as the title that are selected for their information value just as in the case of static summarization. Dynamic summaries are generated in conjunction with scoring. If the query is found as a phrase, occurrences of the phrase in the document will be shown as the summary. If not, windows within the document that contain multiple query terms will be selected. Commonly these windows may just stretch some number of words to the left and right of the query terms. This is a place where NLP techniques can usefully be employed: users prefer snippets that read well because they contain complete phrases.

KEYWORD-IN-CONTEXT

Dynamic summaries are generally regarded as greatly improving the usability of IR systems, but they present a complication for IR system design. A dynamic summary cannot be precomputed, but, on the other hand, if a system has only a positional index, then it cannot easily reconstruct the context surrounding search engine hits in order to generate such a dynamic summary. This is one reason for using static summaries. The standard solution to this in a world of large and cheap disk drives is to locally cache all the documents at index time (notwithstanding that this approach raises various legal and information security and control issues that are far from resolved). Then, a system can simply scan a document which is about to appear in a displayed results list to find snippets containing the query words. Beyond simply access to the text, producing a good KWIC snippet requires some

... ***In recent years, Papua New Guinea has faced severe economic difficulties and*** economic growth has slowed, partly as a result of weak governance and civil war, and partly as a result of external factors such as the Bougainville civil war which led to the closure in 1989 of the Panguna mine (at that time the most important foreign exchange earner and contributor to Government finances), the Asian financial crisis, a decline in the prices of gold and copper, and a fall in the production of oil. ***PNG's economic development record over the past few years is evidence that*** governance issues underly many of the country's problems. Good governance, which may be defined as the transparent and accountable management of human, natural, economic and financial resources for the purposes of equitable and sustainable development, flows from proper public sector management, efficient fiscal and accounting mechanisms, and a willingness to make service delivery a priority in practice. ...

► **Figure 8.5** An example of selecting text for a dynamic snippet. This snippet was generated for a document in response to the query new guinea economic development. The figure shows in bold italic where the the selected snippet text occurred in the original document.

care. Given a variety of keyword occurrences in a document, the goal is to choose fragments which are: (i) maximally informative about the discussion of those terms in the document, (ii) self-contained enough as to be easy to read, and (iii) short enough to fit within the normally strict constraints on the space available for summaries.

Generating snippets must be fast since the system is typically generating many snippets for each query that it handles. Rather than caching an entire document, it is common to cache only a generous but fixed size prefix of the document, such as perhaps 10,000 characters. For most common, short documents, the entire document is thus cached, but huge amounts of local storage will not be wasted on potentially vast documents. Their summaries will be based on material in the document prefix, which is in general a useful zone in which to look for a document summary anyway. Secondly, if a document has been updated recently, these changes will not be in the cache (any more than they will be reflected in the index). In these circumstances, neither the index nor the summary will accurately reflect the contents of the document, but it is the differences between the summary and the actual document content that will be more glaringly obvious to the end user.

8.8 References and further reading

Rigorous formal testing of IR systems was first done in the Cranfield experiments, beginning in the late 1950s. A retrospective discussion of the Cranfield test collection and experimentation with it can be found in Cleverdon (1991). The other seminal series of early IR experiments were those on the SMART system by Gerard Salton and colleagues (Salton 1971b; 1991). The TREC evaluations are described in detail in Voorhees and Harman (2005). Online information is available at http://trec.nist.gov/. User studies of IR system effectiveness began more recently (Saracevic and Kantor 1988; 1996).

F MEASURE

The F measure (or, rather its inverse $E = 1 - F$) was introduced in van Rijsbergen (1979). He provides an extensive theoretical discussion which shows how adopting a principle of decreasing marginal relevance (at some point a user will be unwilling to sacrifice a unit of precision for an added unit of recall) leads to the harmonic mean being the appropriate method for combining precision and recall (and hence to its adoption rather than the minimum or geometric mean).

R-PRECISION

R-precision was adopted as the official evaluation metric in the TREC HARD track (Allan 2005). Aslam and Yilmaz (2005) examines its close correlation to MAP. A standard program for evaluating IR systems which computes many measures of ranked retrieval effectiveness is the `trec_eval` program used in the TREC evaluations. It can be downloaded from: http://trec.nist.gov/trec_eval/.

KAPPA STATISTIC

The kappa statistic and its use for language-related purposes is discussed by Carletta (1996). Many standard sources (e.g., Siegel and Castellan 1988) present pooled calculation of the expected agreement, but Di Eugenio and Glass (2004) argues for preferring the unpooled agreement (though perhaps presenting multiple measures). For further discussion of alternative measures of agreement, which may in fact be better, see Lombard et al. (2002) and Krippendorff (2003).

Voorhees (2000) is the standard article for examining variation in relevance judgements and their effects on retrieval system scores and ranking for the TREC Ad Hoc task. She concludes that although the numbers change, the rankings are quite stable. In contrast, Kekäläinen (2005) analyzes some of the later TRECs, exploring a 4-way relevance judgement and the notion of cumulative gain, arguing that the relevance measure used does substantially affect system rankings. See also Harter (1998).

Text summarization has been actively explored for many years. Modern work on sentence selection was initiated by Kupiec et al. (1995). More recent work includes Barzilay and Elhadad (1997) and Jing (2000) (together with a broad selection of work appearing at the yearly DUC conferences and at other NLP venues).

User interfaces for IR and human factors such as models of human information seeking and usability testing are outside the scope of what we cover

in this book. More information on these topics can be found in other textbooks, including (Baeza-Yates and Ribeiro-Neto 1999, ch. 10) and (Korfhage 1997), and collections focused on cognitive aspects (Spink and Cole 2005).

Clickthrough log analysis is studied in (Joachims 2002b, Joachims et al. 2005).

8.9 Exercises

Exercise 8.1 [⋆]

An IR system returns 8 relevant documents, and 10 non-relevant documents. There are a total of 20 relevant documents in the collection. What is the precision of the system on this search, and what is its recall?

Exercise 8.2 [⋆]

The balanced F measure (a.k.a. F_1) is defined as the harmonic mean of precision and recall. What is the advantage of using the harmonic mean rather than "averaging" (using the arithmetic mean)?

Exercise 8.3 [⋆⋆]

Derive the equivalence between the two formulas for F measure shown in Equation (8.5), given that $\alpha = 1/(\beta^2 + 1)$.

Exercise 8.4 [⋆]

What are the possible values for interpolated precision at a recall level of 0?

Exercise 8.5 [⋆⋆]

Must there always be a break-even point between precision and recall? Either show there must be or give a counter-example.

Exercise 8.6 [⋆⋆]

What is the relationship between the value of F_1 and the break-even point?

Exercise 8.7 [⋆⋆]

The Dice coefficient of two sets is a measure of their intersection scaled by their size (giving a value in the range 0 to 1):

$$\text{Dice}(X, Y) = \frac{|X \cap Y|}{|X| + |Y|}$$

Show that the balanced F-measure (F_1) is equal to the Dice coefficient of the retrieved and relevant document sets.

Exercise 8.8 [⋆⋆]

Below is a table showing how two human judges rated the relevance of a set of 12 documents to a particular information need (0 = nonrelevant, 1 = relevant). Let us assume that you've written an IR engine that for this query returns the set of documents {4, 5, 6, 7, 8}.

docID	Judge 1	Judge 2
1	0	0
2	0	0
3	1	1
4	1	1
5	1	0
6	1	0
7	1	0
8	1	0
9	0	1
10	0	1
11	0	1
12	0	1

a. Calculate the kappa measure between the two judges.
b. Calculate precision, recall, and F_1 of your system if a document is considered relevant only if the two judges agree
c. Calculate precision, recall, and F_1 of your system if a document is considered relevant if either judge thinks it is relevant.

Exercise 8.9 [⋆]

Consider an information need for which there are 4 relevant documents in the collection. Contrast two systems run on this collection. Their top 10 results are judged for relevance as follows (the leftmost item is the top ranked search result):

System 1 R N R N N N N N R R

System 2 N R N N R R R N N N

a. What is the (Mean) Average Precision of each system? Which has a higher Average Precision?
b. Does this result intuitively make sense? What does it say about what is important in getting a good MAP score?
c. What is the R-precision of each system? (Does it rank the systems the same as MAP?)

Exercise 8.10 [⋆⋆]

The following list of R's and N's represents relevant (R) and non-relevant (N) returned documents in a ranked list of 20 documents retrieved in response to a query from a collection of 10,000 documents. The top of the ranked list (the document the system thinks is most likely to be relevant) is on the left of the list. This list shows 6 relevant documents. Assume that there are 8 relevant documents in total in the collection.

R R N N N N N N R N R N N N R N N N N R

a. What is the precision of the system on the top 20?

b. What is the F_1 for the set of 20 retrieved documents?

c. What is the uninterpolated precision of the system at 25

d. What is the interpolated precision at 33

e. Assume that these 20 documents are the complete result set of the system. What is the mean average precision (MAP) for the query?

Assume, now, instead, that the system returned the entire 10,000 documents in a ranked list, and these are the first 20 results returned.

f. What is the largest possible (Mean) Average Precision that this system could have?

g. What is the smallest possible (Mean) Average Precision that this system could have?

h. In a set of experiments, only the top 20 results are evaluated by hand. The result in (e) is used to approximate the range (f)–(g). For this example, how large (in absolute terms) can the error for the MAP be by calculating (e) instead of (f) and (g) for this query?

9 *Relevance feedback and query expansion*

SYNONYMY

In most collections, the same concept may be referred to using different words. This issue, known as *synonymy*, has an impact on the recall of most information retrieval systems. For example, you would want a search for aircraft to match plane (but only for references to an *airplane*, not a woodworking plane), and for a search on thermodynamics to match references to heat in appropriate discussions. Users often attempt to address this problem themselves by manually refining a query, as was discussed in Section 1.4; in this chapter we discuss ways in which a system can help with query refining, either fully automatically or with the user in the loop.

The methods for tackling this problem split into two major classes: global methods and local methods. Global methods are techniques for expanding or reformulating query terms independent of the query and results returned from it, so that changes in the query wording will cause the new query to match other semantically similar terms. Global methods include:

- Query expansion/reformulation with a thesaurus or WordNet (Section 9.2.2)
- Query expansion via automatic thesaurus generation (Section 9.2.3)
- Techniques like spelling correction (discussed in Chapter 3)

Local methods adjust a query relative to the documents that initially appear to match the query. The basic methods here are:

- Relevance feedback (Section 9.1)
- Pseudo-relevance feedback, also known as Blind relevance feedback (Section 9.1.6)
- (Global) indirect relevance feedback (Section 9.1.7)

In this chapter, we will mention all of these approaches, but we will concentrate on relevance feedback, which is one of the most used and most successful approaches.

9.1 Relevance feedback and pseudo-relevance feedback

RELEVANCE FEEDBACK

The idea of *relevance feedback* is to involve the user in the retrieval process so as to improve the final result set. In particular, the user gives feedback on the relevance of documents in an initial set of results. The basic procedure is:

- The user issues a (short, simple) query.
- The system returns an initial set of retrieval results.
- The user marks some returned documents as relevant or not relevant.
- The system computes a better representation of the information need based on the user feedback.
- The system displays a revised set of retrieval results.

Relevance feedback can go through one or more iterations of this sort. The process exploits the idea that it may be difficult to formulate a good query when you don't know the collection well, but it is easy to judge particular documents, and so it makes sense to engage in iterative query refinement of this sort. In such a scenario, relevance feedback can also be effective in tracking a user's evolving information need: seeing some documents may lead users to refine their understanding of the information they are seeking.

Image search provides a good example of relevance feedback. Not only is it easy to see the results at work, but this is a domain where a user can easily have difficulty formulating what they want in words, but can easily indicate relevant or non-relevant images. After the user enters an initial query for bike on the demonstration system at:

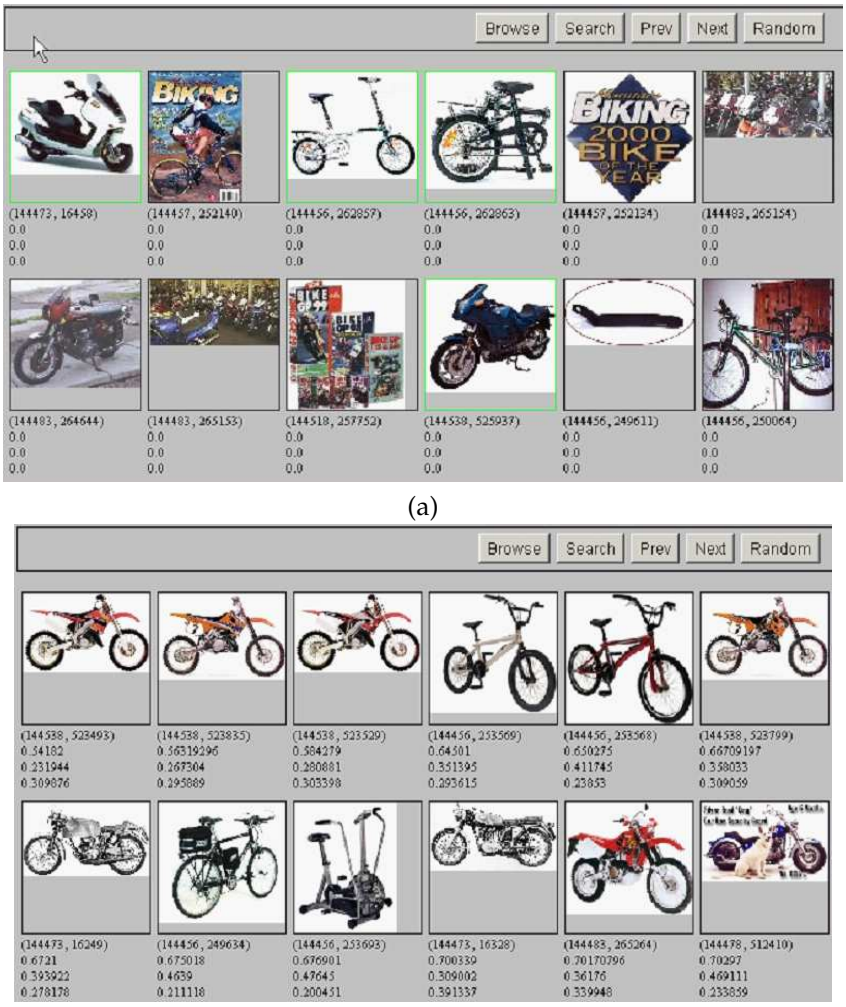
http://nayana.ece.ucsb.edu/imsearch/imsearch.html

the initial results (in this case, images) are returned. In Figure 9.1 (a), the user has selected some of them as relevant. These will be used to refine the query, while other displayed results have no effect on the reformulation. Figure 9.1 (b) then shows the new top-ranked results calculated after this round of relevance feedback.

Figure 9.2 shows a textual IR example where the user wishes to find out about new applications of space satellites.

9.1.1 The Rocchio algorithm for relevance feedback

The Rocchio Algorithm is the classic algorithm for implementing relevance feedback. It models a way of incorporating relevance feedback information into the vector space model of Chapter 7.



► **Figure 9.1** Relevance feedback searching over images. (a) The user views the initial query results for a query of bike, selects the first, third and fourth result in the top row and the fourth result in the bottom row as relevant, and submits this feedback. (b) The users sees the revised result set. Precision is greatly improved. From http://nayana.ece.ucsb.edu/imsearch/imsearch.html (Newsam et al. 2001).

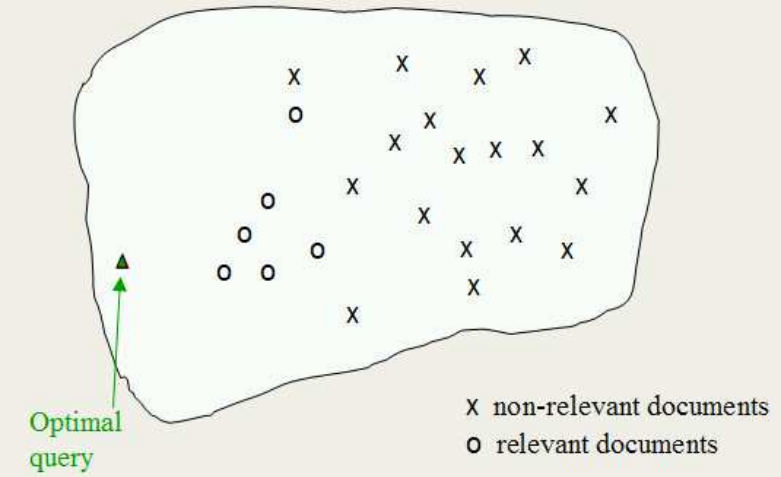
(a) Query: New space satellite applications

(b)
\+ 1. 0.539, 08/13/91, NASA Hasn't Scrapped Imaging Spectrometer
\+ 2. 0.533, 07/09/91, NASA Scratches Environment Gear From Satellite Plan
3. 0.528, 04/04/90, Science Panel Backs NASA Satellite Plan, But Urges Launches of Smaller Probes
4. 0.526, 09/09/91, A NASA Satellite Project Accomplishes Incredible Feat: Staying Within Budget
5. 0.525, 07/24/90, Scientist Who Exposed Global Warming Proposes Satellites for Climate Research
6. 0.524, 08/22/90, Report Provides Support for the Critics Of Using Big Satellites to Study Climate
7. 0.516, 04/13/87, Arianespace Receives Satellite Launch Pact From Telesat Canada
\+ 8. 0.509, 12/02/87, Telecommunications Tale of Two Companies

(c)
2.074 new 15.106 space
30.816 satellite 5.660 application
5.991 nasa 5.196 eos
4.196 launch 3.972 aster
3.516 instrument 3.446 arianespace
3.004 bundespost 2.806 ss
2.790 rocket 2.053 scientist
2.003 broadcast 1.172 earth
0.836 oil 0.646 measure

(d)
* 1. 0.513, 07/09/91, NASA Scratches Environment Gear From Satellite Plan
* 2. 0.500, 08/13/91, NASA Hasn't Scrapped Imaging Spectrometer
3. 0.493, 08/07/89, When the Pentagon Launches a Secret Satellite, Space Sleuths Do Some Spy Work of Their Own
4. 0.493, 07/31/89, NASA Uses 'Warm' Superconductors For Fast Circuit
* 5. 0.492, 12/02/87, Telecommunications Tale of Two Companies
6. 0.491, 07/09/91, Soviets May Adapt Parts of SS-20 Missile For Commercial Use
7. 0.490, 07/12/88, Gaping Gap: Pentagon Lags in Race To Match the Soviets In Rocket Launchers
8. 0.490, 06/14/90, Rescue of Satellite By Space Agency To Cost $90 Million

► **Figure 9.2** Example of relevance feedback on a text collection. (a) The initial query (a). (b) The user marks some relevant documents (shown with a plus sign). (c) The query is then expanded by 18 terms with weights as shown. (d) The revised top results are then shown. A * marks the documents which were judged relevant in the relevance feedback phase.



► **Figure 9.3** The Rocchio optimal query for separating relevant and non-relevant documents.

The underlying theory. We want to find a query vector, denoted as $\vec{q}$, that maximizes similarity with relevant documents while minimizing similarity with non-relevant documents. If C_r is the set of relevant documents and C_{nr} is the set of non-relevant documents, then we wish to find:[1]

$$\vec{q}_{opt} = \arg\max_{\vec{q}}[\text{sim}(\vec{q}, C_r) - \text{sim}(\vec{q}, C_{nr})], \tag{9.1}$$

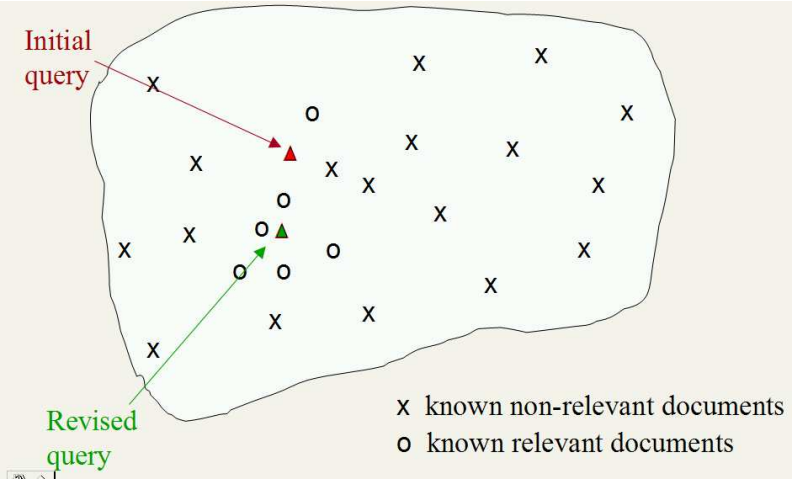
where sim is defined as in Equation 6.14. Under cosine similarity, the optimal query vector $\vec{q}_{opt}$ for separating the relevant and non-relevant documents is:

$$\vec{q}_{opt} = \frac{1}{|C_r|}\sum_{\vec{d}_j \in C_r}\vec{d}_j - \frac{1}{|C_{nr}|}\sum_{\vec{d}_j \in C_{nr}}\vec{d}_j \tag{9.2}$$

That is, the optimal query is the vector difference between the centroids of the relevant and non-relevant documents; see Figure 9.3. However, this observation is not terrribly useful, precisely because the full set of relevant documents is not known: it is what we want to find.

ROCCHIO ALGORITHM **The Rocchio (1971) algorithm.** This was the relevance feedback mecha-

1. In the equation, $\arg\max_x f(x)$ returns a value of x which maximizes the value of the function $f(x)$. Similarly, $\arg\min_x f(x)$ returns a value of x which minimizes the value of the function $f(x)$.



► **Figure 9.4** An application of Rocchio's algorithm. Some documents have been labeled as relevant and non-relevant and the initial query vector is moved in response to this feedback.

nism introduced in and popularized by Salton's SMART system around 1970. In a real IR query context, we have a user query and partial knowledge of known relevant and non-relevant documents. The algorithm proposes using the modified query $\vec{q}_m$:

$$\vec{q}_m = \alpha\vec{q}_0 + \beta\frac{1}{|D_r|}\sum_{\vec{d}_j \in D_r}\vec{d}_j - \gamma\frac{1}{|D_{nr}|}\sum_{\vec{d}_j \in D_{nr}}\vec{d}_j \tag{9.3}$$

where q_0 is the original query vector, D_r and D_{nr} are the set of known relevant and non-relevant documents respectively, and α, β, and γ are weights attached to each term. These control the balance between trusting the judged document set versus the query: if we have a lot of judged documents, we would like a higher β and γ. Starting from q_0, the new query moves you some distance toward the centroid of the relevant documents and some distance away from the centroid of the non-relevant documents. This new query can be used for retrieval in the standard vector space model (see Chapter 7). We can easily leave the positive quadrant of the vector space by subtracting off a non-relevant document's vector. In the Rocchio algorithm, negative term weights are ignored. That is, the term weight is set to 0. Figure 9.4 shows the effect of applying relevance feedback.

Relevance feedback can improve both recall and precision. But, in practice, it has been shown to be most useful for increasing recall in situations

where recall is important. This is partly because the technique expands the query, but it is also partly an effect of the use case: when they want high recall, users can be expected to take time to review results and to iterate on the search. Positive feedback also turns out to be much more valuable than negative feedback, and so most IR systems set $\gamma < \beta$. Reasonable values might be $\alpha = 1$, $\beta = 0.75$, and $\gamma = 0.15$. In fact, many systems, such as the image search system in Figure 9.1, allow only positive feedback, which is equivalent to setting $\gamma = 0$. Another alternative is to use only the marked non-relevant document which received the highest ranking from the IR system as negative feedback (here, $|D_{nr}| = 1$ in Equation (9.3)). While many of the experimental results comparing various relevance feedback variants are rather inconclusive, some studies have suggested that this variant, called *Ide dec-hi* is the most effective or at least the most consistent performer.

IDE DEC-HI

Exercise 9.1

Under what conditions would the modified query q_m in Equation 9.3 be the same as the original query q_0? In all other cases, is q_m closer than q_0 to the centroid of the relevant documents?

Exercise 9.2

Why is positive feedback likely to be more useful than negative feedback to an IR system? Why might only using one non-relevant document be more effective than using several?

9.1.2 Probabilistic relevance feedback

Rather than reweighting the query in a vector space, if a user has told us some relevant and non-relevant documents, then we can proceed to build a classifier. One way of doing this is with a Naive Bayes probabilistic model. If R is a Boolean indicator variable expressing the relevance of a document, then we can estimate that $P(x_t = 1)$, the probability of a term t appearing in a document, depending on whether it is relevant or not, as:

$$\begin{aligned} \hat{P}(x_t = 1|R = 1) &= |VR_t|/|VR| \\ \hat{P}(x_t = 0|R = 0) &= (n_t - |VR_t|)/(N - |VR|) \end{aligned} \tag{9.4}$$

where N is the total number of documents, n_t is the number that contain t, VR is the set of known relevant documents, and VR_t is the subset of this set containing t. Even though the set of known relevant documents is a perhaps small subset of the true set of relevant documents, if we assume that the set of relevant documents is a small subset of the set of all documents then the estimates given above will be reasonable. This gives a basis for another way of changing the query term weights. We will discuss such probabilistic approaches more in Chapters 11 and 13, and in particular outline

the application to relevance feedback in Section 11.3.4 (page 216). For the moment, observe that using just Equation (9.4) as a basis for term-weighting is likely insufficient. The equations use only collection statistics and information about the term distribution within the documents judged relevant. They preserve no memory of the original query.

9.1.3 When does relevance feedback work?

The success of relevance feedback depends on certain assumptions. Firstly, the user has to have sufficient knowledge to be able to make an initial query which is at least somewhere close to the documents they desire. This is needed anyhow for successful information retrieval in the basic case, but it is important to see the kinds of problems that relevance feedback cannot solve alone. Cases where relevance feedback alone is not sufficient include:

- Misspellings. If the user spells a term in a different way to the way it is spelled in any document in the collection, then relevance feedback is unlikely to be effective. This can be addressed by the spelling correction techniques of Chapter 3.
- Cross-language information retrieval. Documents in another language are not nearby in a vector space based on term distribution. Rather, documents in the same language cluster more closely together.
- Mismatch of searcher's vocabulary versus collection vocabulary. If the user searches for laptop but all the documents use the term notebook computer, then the query will fail, and relevance feedback is again most likely ineffective.

Secondly, the relevance feedback approach requires relevance prototypes to be well-behaved. Ideally, the term distribution in all relevant documents will be similar to that in the documents marked by the users, while the term distribution in all non-relevant documents will be different from those in relevant documents. Things will work well if all relevant documents are tightly clustered around a single prototype, or, at least, if there are different prototypes, if the relevant documents have significant vocabulary overlap, while similarities between relevant and non-relevant documents are small. Implicitly, the Rocchio relevance feedback model treats relevant documents as a single *cluster*, which it models via the centroid of the cluster. This approach does not work as well if the relevant documents are a multimodal class, which consists of several clusters of documents within the vector space. This can happen with:

- Subsets of the documents using different vocabulary, such as Burma vs. Myanmar

- A query for which the answer set is inherently disjunctive, such as Pop stars who once worked at Burger King.
- Instances of a general concept, which often appear as a disjunction of more specific concepts, for example, felines.

Good editorial content in the collection can often provide a solution to this problem. For example, an article on the attitudes of different groups to the situation in Burma could introduce the terminology used by different parties, thus linking the document clusters.

Relevance feedback is not necessarily popular with users. Users are often reluctant to provide explicit feedback, or in general do not wish to prolong the search interaction. Furthermore, it is often harder to understand why a particular document was retrieved after relevance feedback is applied.

Relevance feedback can also have practical problems. The long queries that are generated by straightforward application of relevance feedback techniques are inefficient for a typical IR engine. This results in a high computing cost for the retrieval and potentially long response times for the user. A partial solution to this is to only reweight certain prominent terms in the relevant documents, such as perhaps the top 20 terms by term frequency. Some experimental results have also suggested that using a limited number of terms like this may give better results (Harman 1992) though other work has suggested that using more terms is better in terms of retrieved document quality (Buckley et al. 1994b).

9.1.4 Relevance feedback on the web

Some web search engines offer a similar/related pages feature: the user indicates a document in the results set as exemplary from the standpoint of meeting his information need and requests more documents like it. This can be viewed as a particular simple form of relevance feedback. However, in general relevance feedback has been little used in web search. One exception was the Excite web search engine, which initially provided full relevance feedback. However, the feature was in time dropped, due to lack of use. On the web, few people use advanced search interfaces and most would like to complete their search in a single interaction. But the lack of uptake also probably reflects two other factors: relevance feedback is hard to explain to the average user, and relevance feedback is mainly a recall enhancing strategy, and web search users are only rarely concerned with getting sufficient recall.

Spink et al. (2000) present results from the use of relevance feeback in the Excite engine. Only about 4% of user query sessions used the relevance feedback option, and these were usually exploiting the "More like this" link next to each result. About 70% of users only looked at the first page of results and

did not pursue things any further. For people who used relevance feedback, results were improved about two thirds of the time.

Exercise 9.3

In Rocchio's algorithm, what weight setting for $\alpha/\beta/\gamma$ does a "Find pages like this one" search correspond to?

9.1.5 Evaluation of relevance feedback strategies

Interactive relevance feedback can give very substantial gains in retrieval performance. Empirically, one round of relevance feedback is often very useful. Two rounds is sometimes marginally more useful. Successful use of relevance feedback requires enough judged documents, otherwise the process is unstable in that it may drift away from the user's information need. Accordingly, having at east five judged documents is recommended.

There is some subtlety to evaluating the effectiveness of relevance feedback in a sound and enlightening way. The obvious first strategy is to start with an initial query q_0 and to compute a precision-recall graph. Following one round of feedback from the user, we compute the modified query q_m and again compute a precision-recall graph. Here, in both rounds we assess performance over all documents in the collection, which makes comparisons straightforward. If we do this, we find spectacular gains from relevance feedback: gains on the order of 50% in mean average precision. But unfortunately it is cheating. The gains are partly due to the fact that known relevant documents (judged by the user) are now ranked higher. Fairness demands that we should only evaluate with respect to documents not seen by the user.

A second idea is to use documents in the *residual collection* (the set of documents minus those assessed relevant) for the second round of evaluation. This seems like a more realistic evaluation. Unfortunately, the measured performance can then often be lower than for the original query. This is particularly the case if there are few relevant documents, and so a fair proportion of them have been judged by the user in the first round. The relative performance of variant relevance feedback methods can be validly compared, but it is difficult to validly compare performance with and without relevance feedback because the collection size and the number of relevant documents changes from before the feedback to after it.

Thus neither of these methods is fully satisfactory. A third method is to have two collections, one which is used for the initial query and relevance judgements, and the second that is then used for comparative evaluation. The performance of both q_0 and q_m can be validly compared on the second collection.

Perhaps the best evaluation of the utility of relevance feedback is to do user studies of its effectiveness, in particular by doing a time-based comparison:

	Precision at $k = 50$	
Term weighting	no RF	pseudo RF
lnc.ltc	64.2%	72.7%
Lnu.ltu	74.2%	87.0%

▶ **Figure 9.5** Results showing pseudo relevance feedback greatly improving performance. These results are taken from the Cornell SMART system at TREC 4 (Buckley et al. 1996), and also contrast the use of two different length normalization schemes (L vs. l). Pseudo-relevance feedback consisted of adding 20 terms to each query.

how fast does a user find relevant documents with relevance feedback vs. another strategy (such as query reformulation), or alternatively, how many relevant documents does a user find in a certain amount of time. Such notions of user utility are fairest and closest to real system usage.

9.1.6 Pseudo-relevance feedback

PSEUDO-RELEVANCE FEEDBACK
BLIND RELEVANCE FEEDBACK

Pseudo-relevance feedback, also known as *blind relevance feedback*, provides a method for automatic local analysis. It automates the manual part of relevance feedback, so that the user gets improved retrieval performance without an extended interaction. The method is to do normal retrieval to find an initial set of most relevant documents, to then *assume* that the top k ranked documents are relevant, and finally to do relevance feedback as before under this assumption.

This automatic technique mostly works. Evidence suggests that it tends to work better than global analysis (Section 9.2). It has been found to improve performance in the TREC ad hoc task. See for example the results in Figure 9.5. But it is not without the dangers of an automatic process. For example, if the query is about copper mines and the top several documents are all about mines in Chile, then there may be query drift in the direction of documents on Chile.

9.1.7 Indirect relevance feedback

IMPLICIT RELEVANCE FEEDBACK

We can also use indirect sources of evidence rather than explicit feedback on relevance as the basis for relevance feedback. This is often called *implicit (relevance) feedback*. Implicit feedback is less reliable than explicit feedback, but is more useful than pseudo relevance feedback, which contains no evidence of user judgements. Moreover, while users are often reluctant to provide explicit feedback, it is easy to collect implicit feedback in large quantities for a high volume system, such as a web search engine.

On the web, DirectHit introduced the idea of ranking more highly docu-

ments that users chose to look at more often. In other words, clicks on links were assumed to indicate that the page was likely relevant to the query. This approach makes various assumptions, such as that the document summaries displayed in results lists (on whose basis users choose which documents to click on) are indicative of the relevance of these documents. In the original DirectHit engine, the data about the click rates on pages was gathered globally, rather than being user or query specific. This is one form of the general area of *clickstream mining*. Today, a closely related approach is used in ranking the advertisements that match a web search query (Chapter 19).

CLICKSTREAM MINING

9.1.8 Summary

Relevance feedback has been shown to be very effective at improving relevance of results. Its successful use requires queries for which the set of relevant documents is medium to large. Full relevance feedback is often onerous for the user, and its implementation is not very efficient in most IR systems. In many cases, other types of interactive retrieval may improve relevance by about as much with less work.

Beyond the core ad hoc retrieval scenario, other uses of relevance feedback include:

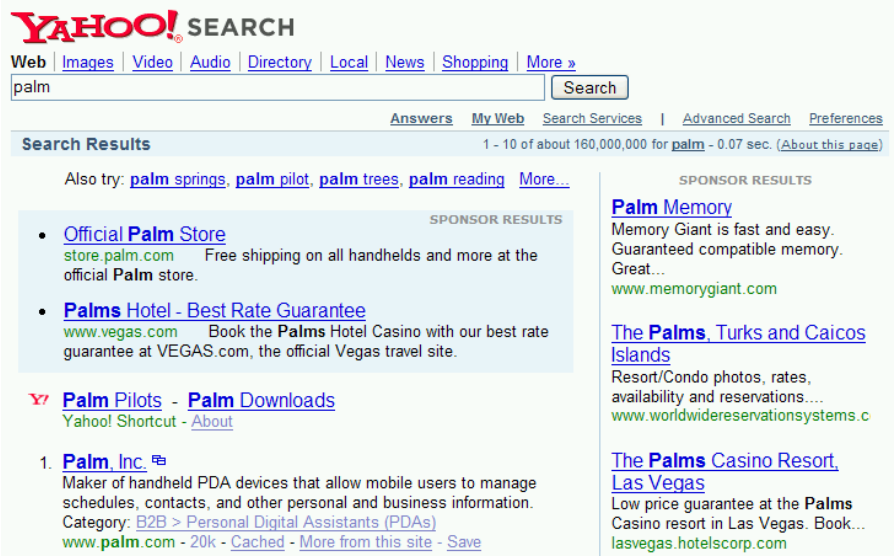
- Following a changing information need (e.g., names of car models of interest change over time)
- Maintaining an information filter (e.g., for a news feed). Such filters are discussed further in Chapter 13.
- Active learning (deciding which examples it is most useful to know the class of to reduce annotation costs).

9.2 Global methods for query reformulation

In this section we more briefly discuss three global methods for expanding a query: by simply aiding the user in doing so, by using a manual thesaurus, and through building a thesaurus automatically.

9.2.1 Vocabulary tools for query reformulation

Various user supports in the search process can help the user see how their searches are or are not working. This includes information about words that were omitted from the query because they were on stop lists, what words were stemmed to, the number of hits on each term or phrase, and whether words were dynamically turned into phrases. The IR system might also suggest search terms by means of a thesaurus or a controlled vocabulary. A user



► **Figure 9.6** An example of query expansion in the interace of the Yahoo! web search engine in 2006. The expanded query suggestions appear just below the "Search Results" bar.

can also be allowed to browse lists of the terms that are in the inverted index, and thus find good terms that appear in the collection.

9.2.2 Query expansion

QUERY EXPANSION

In relevance feedback, users give additional input on documents (by marking documents in the results set as relevant or not), and this input is used to reweight the terms in the query for documents. In *query expansion* on the other hand, users give additional input on query words or phrases, possibly suggesting additional query terms. Some search engines (especially on the web) suggest related queries in response to a query; the users then opt to use one of these alternative query suggestions. Figure 9.6 shows an example of query suggestion options being presented in the Yahoo! web search engine. The central question in this form of query expansion is how to generate alternative or expanded queries for the user. The most common form of query expansion is global analysis, using some form of thesaurus. For each term t in a query, the query can be automatically expanded with synonyms and related words of t from the thesaurus. Use of a thesaurus can be combined with ideas of term weighting: for instance, one might weight added terms

- User query: `cancer`
- PubMed query: ("neoplasms"[TIAB] NOT Medline[SB]) OR "neoplasms"[MeSH Terms] OR cancer[Text Word]
- User query: `skin itch`
- PubMed query: ("skin"[MeSH Terms] OR ("integumentary system"[TIAB] NOT Medline[SB]) OR "integumentary system"[MeSH Terms] OR skin[Text Word]) AND (("pruritus"[TIAB] NOT Medline[SB]) OR "pruritus"[MeSH Terms] OR itch[Text Word])

► **Figure 9.7** Examples of query expansion via the PubMed thesaurus. When a user issues a query on the PubMed interface to Medline at http://www.ncbi.nlm.nih.gov/entrez/, their query is mapped on to the Medline vocabulary as shown.

less than original query terms.

Methods for building a thesaurus for query expansion include:

- Use of a controlled vocabulary that is maintained by human editors. Here, there is a canonical term for each concept. The subject headings of traditional library subject indices, such as the Library of Congress Subject Headings, or the Dewey Decimal system are examples of a controlled vocabulary. Use of a controlled vocabulary is quite common for well-resourced domains. A well-known example is the Unified Medical Language System (UMLS) used with MedLine for querying the biomedical research literature. For example, in Figure 9.7, neoplasms was added to a search for cancer.
- A manual thesaurus. Here, human editors have built up sets of synonymous names for concepts, without designating a canonical term. The UMLS metathesaurus is one example of a thesaurus. Statistics Canada maintains a thesaurus of preferred terms, synonyms, broader terms, and narrower terms for matters on which the government collects statistics, such as goods and services. This thesaurus is also bilingual English and French.
- An automatically derived thesaurus. Here, word co-occurrence statistics over a collection of documents in a domain are used to automatically induce a thesaurus; see Section 9.2.3.
- Query reformulations based on query log mining. Here, we exploit the manual query reformulations of other users to make suggestions to a new

Word	Nearest neighbors
absolutely	absurd, whatsoever, totally, exactly, nothing
bottomed	dip, copper, drops, topped, slide, trimmed
captivating	shimmer, stunningly, superbly, plucky, witty
doghouse	dog, porch, crawling, beside, downstairs
makeup	repellent, lotion, glossy, sunscreen, skin, gel
mediating	reconciliation, negotiate, case, conciliation
keeping	hoping, bring, wiping, could, some, would
lithographs	drawings, Picasso, Dali, sculptures, Gauguin
pathogens	toxins, bacteria, organisms, bacterial, parasite
senses	grasp, psyche, truly, clumsy, naive, innate

► **Figure 9.8** An example of an automatically generated thesaurus. This example is based on the work in Schütze (1998), which employs Latent Semantic Indexing (see Chapter 18).

user. This requires a huge query volume, and is thus particularly appropriate to web search.

Thesaurus-based query expansion has the advantage of not requiring any user input. Use of query expansion generally increases recall and is widely used in many science and engineering fields. As well as such global analysis techniques, it is also possible to do query expansion by local analysis, for instance, by analysing the documents in the result set. User input is now usually required, but a distinction remains as to whether the user is giving feedback on documents or on query terms.

9.2.3 Automatic thesaurus generation

As an alternative to the cost of a manual thesaurus, we could attempt to generate a thesaurus automatically by analyzing a collection of documents. There are two main approaches. One is simply to exploit word cooccurrence. We say that words co-occurring in a document or paragraph are likely to be in some sense similar or related in meaing, and simply count text statistics to find the most similar words. The other approach is to use a shallow grammatical analysis of the text and to exploit grammatical relations or grammatical dependencies. For example, we say that entities that are grown, cooked, eaten, and digested, are more likely to be food items. Simply using word cooccurrence is more robust, but using grammatical relations is more accurate.

The simplest way to compute a co-occurrence thesaurus is based on term-term similarities, which can be derived from a term-document matrix A by calculating $C = AA^T$. If A_{td} has a normalized weighted count w_{td} for term t

and document d, then C_{uv} has a similarity score between terms u and v, with a larger number being better. Figure 9.8 shows an example of a thesaurus derived automatically in this way. While some of the thesaurus terms are good or at least suggestive, others are marginal or bad. The quality of the associations is typically a problem. Term ambiguity easily introduces irrelevant statistically correlated terms. For example, a query for Apple computer may expand to Apple red fruit computer. In general these thesauri suffer from both false positives and false negatives. Moreover, since the terms in the automatic thesaurus are highly correlated in documents anyway (and often the collection used to derive the thesaurus is the same as the one being indexed), this form of query expansion may not retrieve many additional documents.

Query expansion is often effective in increasing recall. However, there is a high cost to manually producing a thesaurus and then updating it for scientific and terminological developments within a field. In general a domain-specific thesaurus is required: general thesauri and dictionaries give far too little coverage of the rich domain-particular vocabularies of most scientific fields. However, it may also significantly decrease precision, particularly when the query contains ambiguous terms. For example, if the user searches for interest rate, expanding the query to interest rate fascinate evaluate is unlikely to be useful. Overall, query expansion is less successful than relevance feedback, though it may be as good as pseudo-relevance feedback. It does, however, have the advantage of being much more understandable to the system user.

Exercise 9.4

If A is simply a Boolean cooccurrence matrix, then what do you get as the entries in C?

9.3 References and further reading

The main initial papers on relevance feedback using vector space models all appear in Salton (1971b), including the presentation of the Rocchio algorithm (Rocchio 1971) and the Ide dec-hi variant along with evaluation of several variants (Ide 1971). Another variant is to regard *all* documents in the collection apart from those judged relevant as non-relevant, rather than only ones that are explicitly judged non-relevant. However, Schütze et al. (1995) and Singhal et al. (1997) show that better results are obtained for routing by using only documents close to the query of interest rather than all documents. Other later work includes Salton and Buckley (1990) and the recent survey paper Ruthven and Lalmas (2003).

The effectiveness of interactive relevance feedback systems is discussed in (Salton 1989, Harman 1992, Buckley et al. 1994b). Koenemann and Belkin (1996) do user studies of the effectiveness of relevance feedback.

Use of clickthrough data on the web to provide indirect relevance feedback is studied in more detail in (Joachims 2002b, Joachims et al. 2005). The very successful use of web link structure (see Chapter 21) can also be viewed as implicit feedback, but provided by page authors rather than readers (though in practice most authors are also readers).

Traditionally Roget's thesaurus has been the best known English language thesaurus Roget (1946). In recent computational work, people almost always use WordNet Fellbaum (1998), not only because it is free, but also because of its rich link structure. It is available at: http://wordnet.princeton.edu.

Qiu and Frei (1993) and Schütze (1998) discuss automatic thesaurus generation. Xu and Croft (1996) explore using both local and global query expansion.

9.4 Exercises

Exercise 9.5

Suppose that a user's initial query is cheap CDs cheap DVDs extremely cheap CDs. The user examines two documents, d_1 and d_2. She judges d_1, with the content *CDs cheap software cheap CDs* relevant and d_2 with content *cheap thrills DVDs* nonrelevant. Assume that we are using direct term frequency (with no scaling and no document frequency). There is no need to length-normalize vectors. Using Rocchio relevance feedback as in Equation (9.3) what would the revised query vector be after relevance feedback? Assume $\alpha = 1, \beta = 0.75, \gamma = 0.25$.

Exercise 9.6 [⋆]

Omar has implemented a relevance feedback web search system, where he is going to do relevance feedback based only on words in the title text returned for a page (for efficiency). The user is going to rank 3 results. The first user, Jinxing, queries for:

banana slug

and the top three titles returned are:

banana slug Ariolimax columbianus
Santa Cruz mountains banana slug
Santa Cruz Campus Mascot

Jinxing judges the first two documents Relevant, and the third Not Relevant. Assume that Omar's search engine uses term frequency but no length normalization nor IDF. Assume that he is using the Rocchio relevance feedback mechanism, with $\alpha = \beta = \gamma = 1$. Show the final revised query that would be run. (Please list the vector elements in alphabetical order.)

Exercise 9.7 [⋆]

Give three reasons why relevance feedback has been little used in web search.

10 *XML retrieval*

Information retrieval systems are often contrasted with relational databases. Traditionally, IR systems have retrieved information from *unstructured text* – by which we mean "raw" text without markup. Databases are designed for searching *relational data*: sets of records that have values for predefined attributes such as employee number, title and salary. There are fundamental differences between information retrieval and database systems in terms of retrieval model, data structures and query language as shown in Table 10.1.[1]

Some highly structured text search problems are best solved with a relational database, for example, if the employee table contains an attribute for short textual job descriptions and I want to find all employees who are involved with invoicing. In this case, the SQL query:

```
select lastname from employees where job_desc like 'invoic%';
```

may be sufficient to satisfy my information need with high precision and recall.

However, as we argued in Example 1.1 (page 13) unranked retrieval models like the Boolean model suffer from low recall for high-precision searches. Most searches over text content require ranked retrieval, which is difficult to reconcile with the relational database model. The same argument applies to structured retrieval, that is, retrieval over strucutured text documents. In most applications, some form of ranked retrieval is necessary. In this chapter, we look at how ranked retrieval for unstructured text can be adapted to for structured text.

The only form of structured text we will look at is XML, the currently most widely used standard for encoding structured documents. We will view an XML document as a tree that has *leaf nodes* containing text and *labeled internal nodes* that define the roles of the leaf nodes in the document. We call this type of text *structured text* and retrieval over it *XML retrieval* or, if we need a more

XML RETRIEVAL

1. In most modern database systems, one can enable full-text search for text columns. This usually means that an inverted index is created and Boolean or vector space search enabled, effectively combining core database with information retrieval technologies.

	RDB search	unstructured retrieval	structured retrieval
objects	record	unstructured document	tree with text at leaves
model	relational calculus	vector space & others	?
main data structure	table	inverted index	?
queries	SQL	text queries	?

► **Table 10.1** RDB (relational data base) search, unstructured retrieval and structured retrieval. There is no consensus yet as to which formal models, query languages and data structures are consistently successful for structured retrieval.

STRUCTURED RETRIEVAL

general term that also applies to other markup standards, *structured retrieval*. In the example in Figure 10.2, some of the leaves shown are Shakespeare, Macbeth, and Macbeth's castle, and the labeled internal nodes encode either the structure of the document (*title*, *act*, and *scene*) or metadata functions (*author*).

There is actually a second type of information retrieval problem that is intermediate between unstructured retrieval and querying a relational database: *parametric search*, which we discussed in Section 6.1 (page 103). In the data model of parametric search, there are text attributes that each take a chunk of unstructured text as value and also relational attributes like *Date* or *File-Size*. The data model is flat, that is, there is no nesting of attributes. Two examples of text attributes in Figure 6.1 (page 104) were *Author* and *Title*. In contrast, XML documents have the more complex tree structure that we see in Figure 10.2, that is, attributes can be nested.

EXTENSIBLE MARKUP LANGUAGE
XML

Structured retrieval has become increasingly important in recent years because of the growing use of *Extensible Markup Language* or *XML*. XML is used for web content, for documents produced by office productivity suites, for the import and export of text content in general, and many other applications. Here, we neglect the specifics that distinguish XML from other standards for marked up data such as HTML and SGML.

After presenting the basic concepts of XML in Section 10.1, this chapter first discusses the challenges we face in XML retrieval (Section 10.2). Next we describe a vector space model for XML retrieval (Section 10.3). Section 10.4 presents INEX, a shared task evaluation that has been held for a number of years and currently is the most important venue for XML retrieval research. Section 10.5 discusses database approaches to XML retrieval and contrasts them with the IR approch that we present in this chapter.

10.1 Basic XML concepts

XML ELEMENT
XML ATTRIBUTE

An XML document is an ordered, labeled tree. Each node of the tree is an *XML element* and is written with an opening and closing *tag*. An element can have one or more *XML attributes*. The *scene* element in the XML document in

```
<play>
<author>Shakespeare</author>
<title>Macbeth</title>
<act number="I">
<scene number="VII">
<title>Macbeth's castle</title>
<verse>Will I with wine and wassail ...</verse>
</scene>
</act>
</play>
```

► **Figure 10.1** An XML document.

Figure 10.1 is enclosed by the two tags `<scene ...>` and `</scene>`. It has an attribute *number* with value *VII* and two child elements, *title* and *verse*.

XML DOM

There is a standard way of accessing and processing XML documents, the XML Document Object Model or *DOM*. The DOM represents elements, attributes and text within elements as nodes in a tree. Figure 10.2 shows the DOM representation of the XML document in Figure 10.1. With a DOM API, it is easy to process an XML document by starting at the root element and then descending down the tree from parents to children.

XPATH

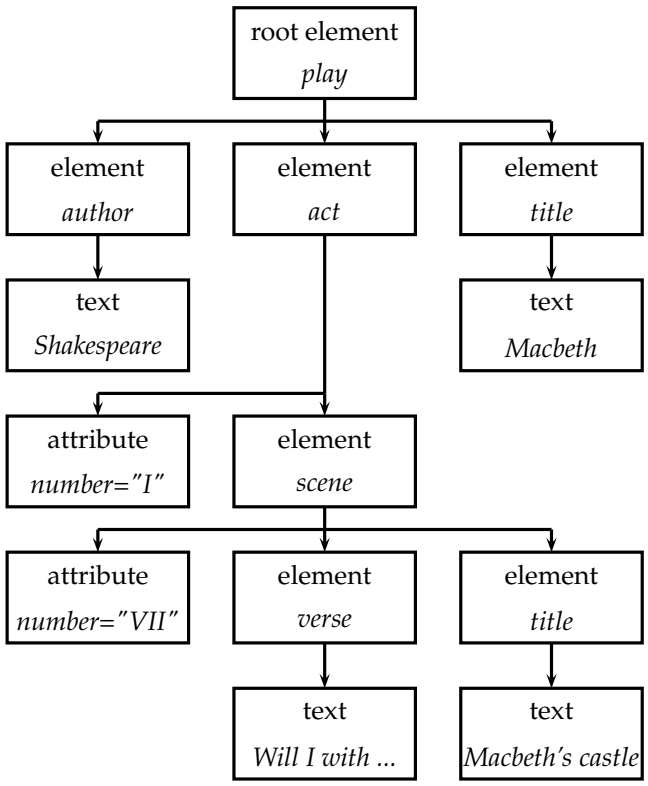
XML CONTEXT

XPath is a standard for enumerating paths in an XML document collection. We will also refer to paths as *XML contexts* in this chapter. Only a small subset of XPath is needed for our purposes. The XPath expression `node` selects all nodes of that name. Successive elements of a path are separated by slashes, so `act/scene` selects all *scene* elements whose parent is an *act* element. Double slashes indicate that an arbitrary number of elements can intervene on a path: `play//scene` selects all *scene* elements occurring in a *play* element. In Figure 10.2 this set consists of a single *scene* element, which is accessible via the path *play*, *act*, *scene* from the top. An initial slash starts the path at the root element. `/play/title` selects the play's title in Figure 10.1, `/play//title` selects a set with two members (the play's title and the scene's title), and `/scene/title` selects no elements. For notational convenience, we allow the final element of a path to be a string, e.g. `title/"Macbeth"` for all titles containing the word Macbeth, even though this does not conform to the XPath standard.

SCHEMA

XML DTD

We also need the concept of *schema* in this chapter. A schema puts constraints on the structure of allowable XML documents for a particular application. A schema for Shakespeare's plays may stipulate that scenes can only occur as children of acts and that only acts and scenes have the *number* attribute. Two standards for schemas for XML documents are *XML DTD*



► **Figure 10.2** The XML document in Figure 10.1 as a DOM object. Parents point to their children.

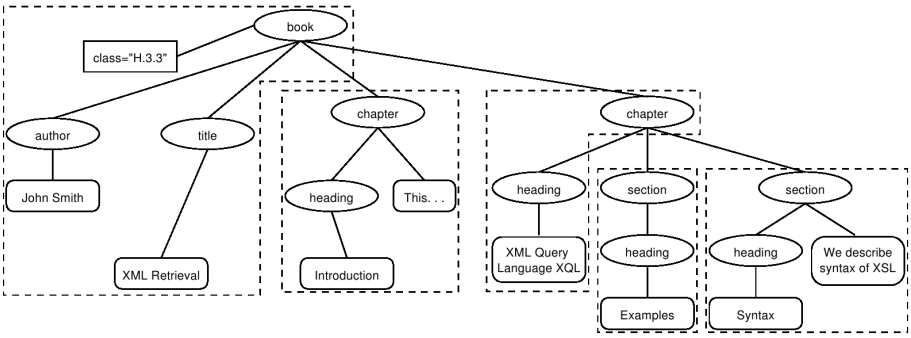
XML SCHEMA

(document type definition) and *XML Schema*. Users can only write structured queries for an XML retrieval system if they have some minimal knowledge about the schema of the underlying collection.

10.2 Challenges in XML retrieval

In Section 2.1.2 (page 20), we discussed the need for a document unit in indexing and retrieval. In unstructured retrieval, it is usually clear what the right document unit is: files on your desktop, email messages, web pages on the web etc. The first challenge in XML retrieval is that we do not have such a natural document unit or *indexing unit*. If we query Shakespeare's plays for Macbeth's castle, should we return the scene, the act or the whole play in Figure 10.2? In this case, the user is probably looking for the scene. On the

INDEXING UNIT



► **Figure 10.3** Partitioning an XML document into non-overlapping indexing units.

other hand, an otherwise unspecified search for Macbeth should return the play of this name, not a subunit.

STRUCTURED DOCUMENT RETRIEVAL PRINCIPLE

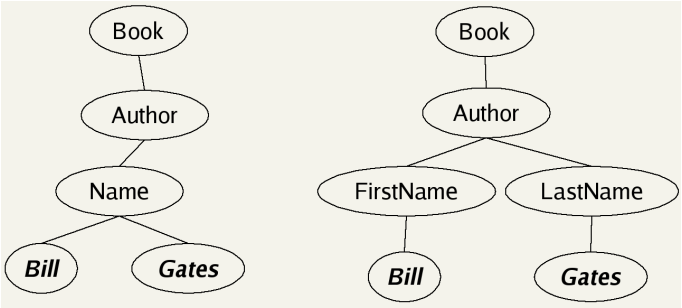
One decision criterion for selecting the most appropriate part of a document is the *structured document retrieval principle*:

> **Structured document retrieval principle.** A system should always retrieve the most specific part of a document answering the query.

This principle motivates a retrieval strategy that returns the smallest unit that contains the information sought, but does not go below this level. However, it can be hard to implement this principle algorithmically. Consider the query `title/"Macbeth"` applied to Figure 10.2. The title of the tragedy, *Macbeth*, and the title of Act 1, Scene 7, *Macbeth's castle*, are both good hits because they contain the matching term Macbeth. But in this case, the title of the tragedy, the higher node, is preferred. Deciding which level of the tree is right for answering a query is difficult.

There are at least three different approaches to defining the indexing unit in XML retrieval. One is to index all elements that are eligible to be returned in a search result. All subtrees in Figure 10.1 meet this criterion, but typographical XML elements as in `<b>definitely</b>` or an ISBN number without context may not. This scheme has the disadvantage that search results will contain overlapping units that have to be filtered out in a postprocessing step to reduce redundancy.

Another approach is to group nodes into non-overlapping pseudodocuments as shown in Figure 10.3. In the example, books, chapters and sections have been designated to be indexing units, but without overlap. For example, the leftmost dashed indexing unit contains only those parts of the tree dominated by book that are not already part of other indexing units. This scheme avoids the overlap problem, but pseudodocuments may not make



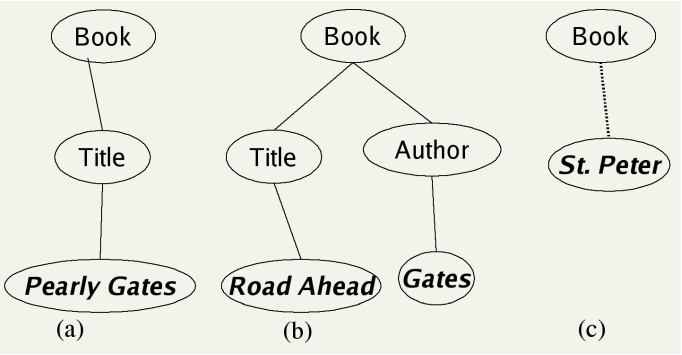
► **Figure 10.4** An example of a schema mismatch between a query (left) and a document (right).

intuitive sense to the user. Also, they have to be fixed at indexing time, leaving no flexibility to answer queries at a more specific or more general level.

The third approach is to designate one XML element as the substitute for the document unit. This is the approach taken by the system in the next section where the document collection is a collection of articles from IEEE journals and each element dominated by an article node is treated as a document. As with the node groups in Figure 10.3, we have the problem that indexing units are fixed. However, we can attempt to extract the most relevant subelement from each hit in a postprocessing step.

A related challenge in XML retrieval is that we may need to distinguish different contexts of a term when we compute term statistics for ranking, in particular inverse document frequency (idf) statistics (Section 6.2.1, page 111). If an XML collection has an element that can serve as a natural indexing unit, then we can compute idf as in unstructured retrieval. This is the case for the INEX IEEE collection that we will describe in Section 10.4 But if there is no such element, then there is no simple way of computing idf. For example, the term Gates under the node Author is unrelated to an occurrence under a content node like Section if used to refer to the plural of gate. For this example, it makes little sense to compute a single document frequency for Gates. One solution is to compute idf for XML-context/term pairs. So we would compute different idf weights for `author/"Gates"` and `section/"Gates"`. Unfortunately, this scheme will run into sparse data problems, a problem we will return to in Section 10.4 when discussing the Merge algorithm.

In many cases, several different XML schemas occur in a collection since the XML documents in an IR application often come from different sources. This presents yet another challenge. Comparable elements may have different names and be represented differently structurally. In Figure 10.4, the node Name in the query (the left tree) corresponds to the two nodes FirstName



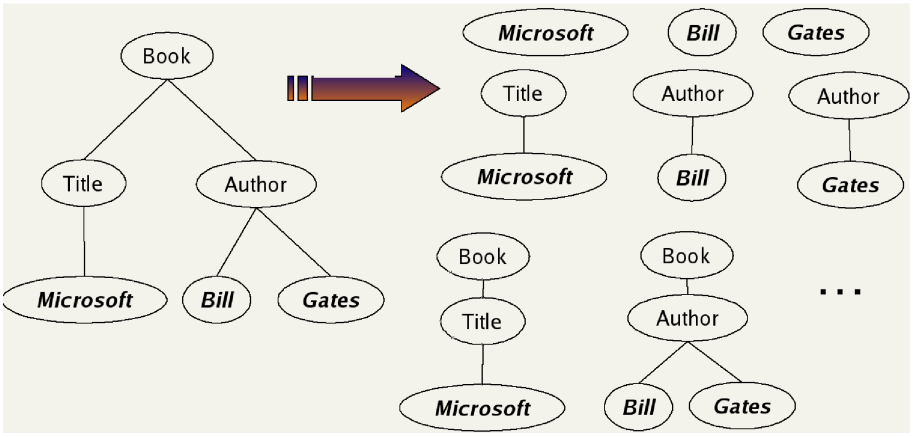
► **Figure 10.5** Simple XML queries can be represented as trees.

and LastName in the document (the right tree). Some form of approximate matching of element names in combination with semi-automatic matching of different document structures can help here. Human editing of correspondences of elements in different schemas will usually do better than automatic methods.

The schema of an XML collection is often a challenge for interface design because users are not familiar with its naming conventions and its structure. Consider the queries in Figure 10.5. These queries search for books with the words Pearly Gates in the title (a); books with titles containing Road Ahead and authors containing Gates (b); and books that contain St. Peter in any subelement (c). Query (c) is an *extended query* because it contains a dashed line representing a descending path of arbitrary length from Book to St. Peter. The pseudo-XPath notation for this query is `book//"St. Peter"`. It is quite common for users to issue such extended queries without specifying the exact structural configuration in which a query term should occur – either because they do not care about the exact configuration or because they do not know enough about the schema of the collection.

EXTENDED QUERY

For query (b) the user has made the assumption that the node referring to the creator of the document is called Author, but it could also be named Writer or Creator (the latter being the choice of the Dublin Core Metadata standard). Query (c) is a search for books that contain St. Peter anywhere. The user interface should expose the tree structure of the collection and allow users to specify the elements they are querying. As a consequence the query interface is more complex than a search box for keyword queries in unstructured retrieval. This is one of the challenges currently being addressed by the research community.



► **Figure 10.6** A mapping of an XML document (left) to a set of "lexicalized" subtrees (right).

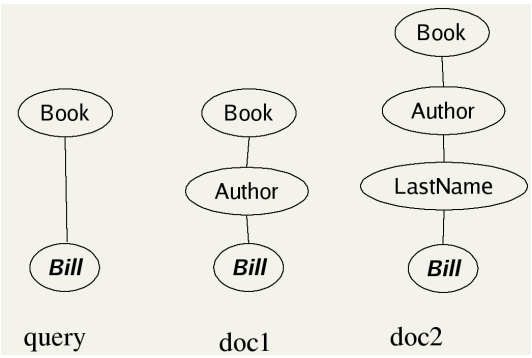
10.3 A vector space model for XML retrieval

In this section, we present a simple vector space model for XML retrieval. It is not intended to be a complete description of a state-of-the-art system. Instead, we want to give the reader a flavor of how documents can be represented and retrieved in XML retrieval.

To take account of structure in retrieval, we want a document authored by Bill Gates to be a match for the second query in Figure 10.5, but not for the first. In unstructured retrieval, there would be a single dimension of the vector space for Gates. In XML retrieval, we must separate the title word Gates from the author name Gates. One way of doing this is to have each dimension encode a word together with its position within the XML tree.

Figure 10.6 illustrates this representation. We first take each text node (which in our setup is always a leaf) and break it into several nodes, one for each word. So the leaf node `Bill Gates` is split into two leaves `Bill` and `Gates`. Next we define the dimensions of the vector space as subtrees of documents that contain at least one vocabulary term. A subset of these possible subtrees is shown in the figure, but there are others – e.g., the subtree corresponding to the whole document with the leaf node Gates removed.

There is a tradeoff between the dimensionality of the space and accuracy of query results. If we trivially restrict dimensions to content words, then we have a standard vector space retrieval system that will retrieve many documents that do not match the structure of the query (e.g., Gates in the title as opposed to the author field). If we create a separate dimension for



► **Figure 10.7** Query-document matching for extended queries.

each subtree occurring in the collection, the dimensionality of the space becomes very large and many dimensions will have little utility since there is only a single document with the corresponding subtree. A compromise is to index all paths that end in a single vocabulary term, in other words, all XML-context/term pairs. We call such an XML-context/term pair a *structural term*. The document in Figure 10.6 has nine structural terms as can be easily verified. Seven are shown (e.g., `"Bill"` and `Author/"Bill"`) and two are not shown: `/Book/Author/"Bill"` and `/Book/Author/"Gates"`. The tree with the leaves Bill and Gates is a subtre that is not a structural term.

STRUCTURAL TERM

We can treat structural terms just like regular terms in ordinary vector space retrieval. For instance, we can compute term frequency weights and perform stemming and case folding for the vocabulary term. However, to compute idf weights for structural terms, we need to define a document unit. We will assume here that there is such a unit, for example, the article element in a collection of journal articles. We can then compute idf in the standard way (see Section 6.2.1, page 111).

We also want to weight XML contexts in the query. Users often care more about some parts of the query than others. In query (b) in Figure 10.5, the user may want to give more weight to the author because she is not sure whether she remembers the title correctly. This weighting can either be done in the user interface as part of query input; or by the system designer in cases where the importance of different parts of the query is likely to be the same across users.

One of the results of the INEX evaluation we will discuss in the next section is that users are very bad at remembering details about the schema and at constructing queries that comply with the schema. It is therefore a good idea to interpret the structural constraints of the query liberally. We will

do this here by viewing queries as extended queries. Each parent-child link in the query will be interpreted as a descendant link in the document, that is, there can be an arbitrary number of intervening nodes in the document. But we still prefer documents that match the query structure closely by inserting fewer additional nodes. We ensure that retrieval results respect this preference by computing a weight for each match. A simple measure of the similarity of two paths is the following *context resemblance* function cr:

CONTEXT RESEMBLANCE

$$\text{cr}(q,d) = \frac{1+|q|}{1+|d|}$$

where $|q|$ and $|d|$ are the number of nodes in the query path and document path, respectively. The context resemblance function returns 0 if the query path cannot be extended to match the document path. Its value is 1.0 if q and d are identical. The context resemblance values for the two examples in Figure 10.7 are $\text{cr}(q,d_1) = 3/4 = 0.75$ and $\text{cr}(q,d_2) = 3/5 = 0.6$.

The final score for a document is computed as a variant of the cosine measure (Equation (6.14), page 118), the *context resemblance similarity*. It is defined as follows:

CONTEXT RESEMBLANCE SIMILARITY

$$\text{sim-cr}(q,d) = \sum_{c_k \in C} \text{weight}(q,t,c_k) \cdot \text{cr}(c_k,c_l) \cdot \sum_{c_l \in C} \sum_{t \in V} \frac{\text{weight}(d,t,c_l)}{\sqrt{\sum_{c \in C, t \in V} \text{weight}^2(d,t,c)}} \tag{10.1}$$

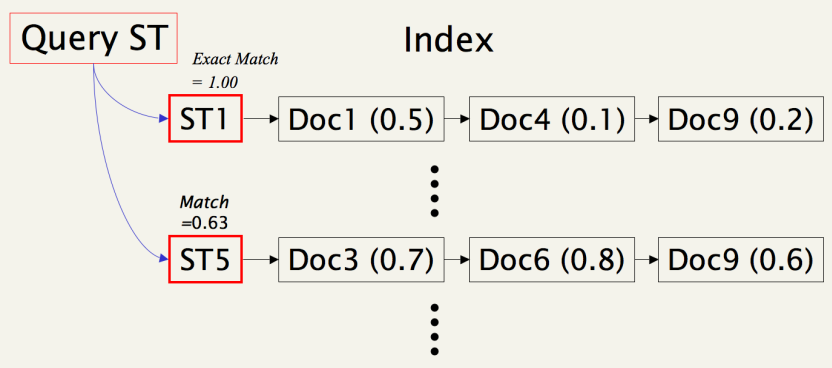
where V is the vocabulary of non-structural terms; C is the set of all XML paths; and $\text{weight}(d,t,c_k)$ is the weight of term t in XML context c_k in document d using one of the weightings from Chapter 6, e.g., $\text{idf}_t \cdot \text{wf}_{t,d}$. idf_t depends on which elements we compute df_t over and that the components of $\vec{q}$ and $\vec{d}$ are the weights $\text{weight}(q,t,c)$ and $\text{weight}(d,t,c)$, respectively. $\text{sim-cr}(q,d)$ is not a true cosine measure since its values can be larger than 1.0 (Exercise 10.10).

An example of an inverted index search in extended query matching is given in Figure 10.8. The structural term ST in the query occurs as ST1 in the index. The match value $\text{cr}(\text{ST}, \text{ST1})$ is 0.63 and the match value $\text{cr}(\text{ST}, \text{ST5})$ is 1.0. In this example, the highest ranking document is Doc9 with a similarity of $1.0 \times 0.2 + 0.63 \times 0.6 = 0.578$. Query weights are assumed to be 1.0.

Figure 10.9 summarizes the indexing and query processing algorithms.

Idf weights for the retrieval algorithm just introduced are computed separately for each structural term. We call this method *NoMerge* since XML contexts of different structural terms are not merged. An alternative is a *Merge* method that computes statistics for term (t,c) by collapsing all XML contexts c' that have a non-zero context resemblance with c. For instance, for computing the document frequency of the structural term `/atl/"recognition"`, we also count occurrences of recognition in XML contexts `fm/atl`, `article//atl`

NOMERGE MERGE



► **Figure 10.8** Inverted index search for extended queries.

Indexing
For each indexing unit i:
  Compute structural terms for i
Construct index
Search
Compute structural terms for query
For each structural term t:
  Find matching structural terms in dictionary
  For each matching structural term t':
    Compute matching weight $\text{cr}(t, t')$
Search inverted index with computed terms and weights
Return ranked list

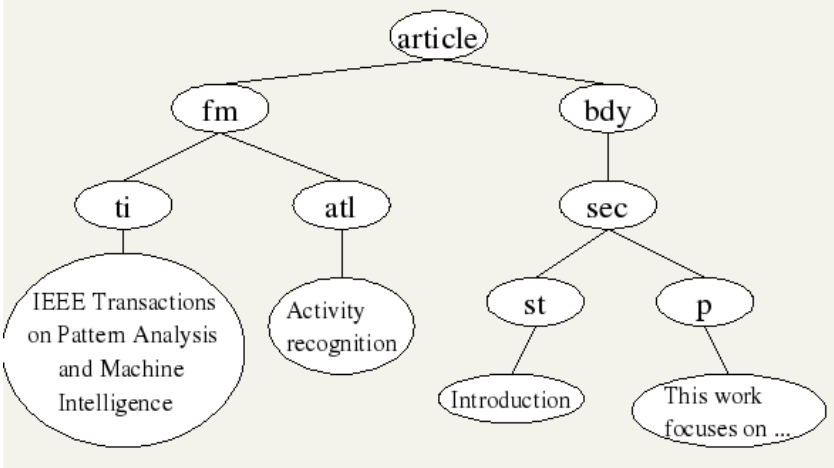
► **Figure 10.9** Indexing and search in vector space XML retrieval.

etc. This scheme addresses the sparse data problems that occur when computing idf weights for structural terms. The Merge method also extends this merging of structural terms to computing the similarity between query and document. Equation (10.1) is modified such that, for a given structural term (t, c) in the query, all structural terms in the document with a context c' that has a non-zero match with c are merged. For example, the contexts `/play/act/scene/title` and `/play/title` will be merged when matching against the query term `/play/title/"Macbeth"`.

A final modification concerns the context resemblance function. In Merge, we replace it by $\text{qc}(c) = |c| + 1$. So weight is a linear function of the path length or specificity of the XML context. This weighting function captures the intuition that a term occurring in a specific XML context (e.g., in a `/play/act/scene`

12,107	number of documents
494 MB	size
1995–2002	time of publication of articles
1,532	average number of XML nodes per document
6.9	average depth of a node
30	number of CAS topics
30	number of CO topics

► **Table 10.2** INEX 2002 collection statistics. There are two types of topics: content only (CO) and content and structure (CAS). An example of a CAS topic is given in Figure 10.11.



► **Figure 10.10** Simplified schema of the documents in the INEX collection. The selected element tags shown here are **f**ront **m**atter (fm), **ti**tle (ti), **a**rticle **titl**e (atl), **bo**d**y** (bdy), **sec**tion (sec), **s**ection **t**itle (st) and **p**aragraph (p).

element) should be weighted higher than one occurring in a non-specific context (e.g., in a `/play` element).

We evaluate Merge and NoMerge in the next section.

10.4 Evaluation of XML Retrieval

INEX

The premier venue for research on XML retrieval is the *INEX* (**IN***itiative for the* **E***valuation of* **X***ML retrieval*) program, a collaborative effort that has produced reference collections, sets of queries, and relevance judgments. A yearly INEX meeting is held to present and discuss research results. The

```
<te>article</te>
<cw>non-monotonic reasoning</cw>   <ce>bdy/sec</ce>
<cw>1999 2000</cw>                 <ce>hdr//yr</ce>
<cw>-calendar</cw>                 <ce>tig/atl</ce>
```

▶ **Figure 10.11** An INEX CAS topic. *tig* is the tag for **ti**tle **g**roup.

INEX 2002 collection consists of about 12,000 articles from IEEE journals. We give collection statistics in Table 10.2 and show the structure of the documents in Figure 10.10.

TOPICS
CO TOPICS
CAS TOPICS

Two types of information needs or *topics* in INEX are content-only or CO topics and content-and-structure or CAS topics. *CO topics* are regular keyword queries as in unstructured information retrieval. *CAS topics* have structural constraints in addition to keywords. The CAS topic in Figure 10.11 is a search for articles on non-monotonic reasoning from 1999 or 2000 that are not calendars of events. The first line specifies that retrieved elements should be articles (te = target element). The other three lines are pairs of content word (cw) and content element (ce) conditions, indicating the content words that should occur (non-monotonic reasoning, 1999, 2000) or should not occur (calendar) in a particular XML context.

Since CAS queries have both structural and content criteria, relevance assessments are more complicated than in unstructured retrieval. INEX 2002 defined *component coverage* and *topical relevance* as orthogonal dimensions of relevance. The component coverage dimension evaluates whether the element retrieved is "structurally" correct, i.e., neither too low nor too high in the tree. We distinguish four cases:

COMPONENT COVERAGE
TOPICAL RELEVANCE

- Exact coverage (E). The information sought is the main topic of the component and the component is a meaningful unit of information.
- Too small (S). The information sought is the main topic of the component, but the component is not a meaningful (self-contained) unit of information.
- Too large (L). The information sought is present in the component, but is not the main topic.
- No coverage (N). The information sought is not a topic of the component.

The topical relevance dimension also has four levels: highly relevant (3), fairly relevant (2), marginally relevant (1) and nonrelevant (0). Components are judged on both dimensions and the judgments are then combined into a digit-letter code. 2S is a fairly relevant component that is too small and 3E is a highly relevant component that has exact coverage. In theory, there

are 16 combinations of coverage and relevance, but many cannot occur. For example, a non-relevant component cannot have exact coverage, so the combination 3N is not possible.

The relevance-coverage combinations are then quantized as follows:

$$\mathbf{Q}(rel, cov) = \begin{cases} 1.00 & \text{if} \quad (rel, cov) = 3\text{E} \\ 0.75 & \text{if} \quad (rel, cov) \in \{2\text{E}, 3\text{L}\} \\ 0.50 & \text{if} \quad (rel, cov) \in \{1\text{E}, 2\text{L}, 2\text{S}\} \\ 0.25 & \text{if} \quad (rel, cov) \in \{1\text{S}, 1\text{L}\} \\ 0.00 & \text{if} \quad (rel, cov) = 0\text{N} \end{cases}$$

This evaluation scheme takes account of the fact that binary relevance judgments, which are standard in unstructured information retrieval (Section 8.5.1, page 157), are not appropriate for XML retrieval. A 2S component provides incomplete information and may be difficult to interpret without more context, but it does answer the query partially. The quantization function $\mathbf{Q}$ does not impose a binary choice relevant/nonrelevant and instead allows us to grade the component as partially relevant.

The number of relevant components in a retrieved set C of components can then be computed as:

$$\#(\text{relevant items retrieved}) = \sum_{c \in C} \mathbf{q}(rel(c), cov(c))$$

As an approximation, the standard definitions of precision, recall and F from Chapter 8 can be applied to this modified definition of relevant items retrieved, with some subtleties because we sum graded as opposed to binary relevance assessments. See the references on focused retrieval in Section 10.6 for further discussion.

One flaw of measuring relevance this way is that overlap is not accounted for. We discussed the concept of marginal relevance in the context of unstructured retrieval in Section 8.5.1. This problem is worse in XML retrieval because the same element can occur multiple times in a ranking as part of different higher-level elements. The play, act, scene and title elements on the path between the root node and Macbeth's castle in Figure 10.1 can all be returned as *nested elements* in a result set. The leaf node would then occur four times. Much of the recent focus at INEX has been on developing algorithms and evaluation measures that return non-redundant result lists and evaluate them properly. See Section 10.6.

NESTED ELEMENTS

Table 10.3 shows two INEX 2002 runs of JuruXML, the vector space system we described in Section 10.3. The better run is the Merge run, which incorporates few structural constraints and mostly relies on keyword matching. Merge's median average precision (where the median is with respect to average precision numbers over topics) is 0.147. About 50% of the first 10 hits

algorithm	mean average precision
Merge	0.271
NoMerge	0.242

► **Table 10.3** INEX 2002 results of the vector space model in Section 10.3 for content-and-structure (CAS) queries and the quantization function **Q**.

measure	content-only	full-structure	improvement
precision at 0.05	0.2000	0.3265	63.3%
precision at 0.10	0.1820	0.2531	39.1%
precision at 0.20	0.1700	0.1796	5.6%
precision at 0.30	0.1527	0.1531	0.3%

► **Table 10.4** A comparison of content-only and full-structure search in INEX 2003/2004.

were partially relevant on average. Effectiveness numbers in XML retrieval when evaluated as described here can be lower than those in unstructured retrieval on a standard evaluation because graded judgments lower measured performance. Consider a system that returns a document with graded relevance 0.6 and binary relevance 1 at the top of the retrieved list. Then, interpolated precision at 0.00 recall is 1.0 on a binary evaluation, but can be as low as 0.6 on a graded evaluation.

Table 10.3 gives us a sense of the typical performance of XML retrieval, but it does not directly compare structured with unstructured retrieval. The results in Table 10.4 directly show the effect of using structure in retrieval. The results are for a language-model-based system (cf. Chapter 12) that is evaluated on a subset of CAS topics from INEX 2003 and 2004. The evaluation metric is precision at k as defined in Chapter 8 (page 154). The discretization function used for the evaluation maps 3E to 1 and all other values to 0. So only the most specific and most relevant items are viewed as relevant. The content-only system treats queries and documents as unstructured bags of words. The full-structure model ranks elements that satisfy structural constraints higher than elements that do not. For instance, for the query in Figure 10.11 a document that contains non-monotonic reasoning in a section element will be rated higher than one that contains it in a front matter element.

The table shows that structure helps increase precision at the top of the result list. There is a large increase of precision at 0.05 and at 0.1. There is almost no improvement at 0.3 recall. This is to be expected since structure imposes additional constraints on what to return. Documents that pass this structural filter are more likely to be relevant, but recall may suffer at high levels of recall because some relevant documents will be filtered out.

10.5 Content-centric vs. structure-centric XML retrieval

CONTENT-CENTRIC XML RETRIEVAL

In vector space XML retrieval, XML structure serves as a framework within which conventional text matching is performed. This exemplifies the *content-centric* approach to XML retrieval. While both structure and text are important, we give higher priority to text matching. We adapt unstructured retrieval methods to handle additional structural constraints.

STRUCTURE-CENTRIC XML RETRIEVAL

In contrast, *structure-centric XML retrieval* puts the emphasis on the structural aspects of a user query. A clear example is: "chapters of books that have the same title as the book". This query has no text component. It is purely structural.

Content-centric approaches are appropriate for data that are essentially text documents, marked up as XML to capture document structure. This is becoming a de facto standard for publishing text databases since most text documents have some form of interesting structure – paragraphs, sections, footnotes etc. Examples include assembly manuals, issues of journals, Shakespeare's collected works and newswire articles.

Structure-centric approaches are commonly used for data collections with complex structures that contain text as well as non-text data. A content-centric retrieval engine will have a hard time with proteomic data that may be part of a biomedical publication – or with the representation of a street map that (together with street names and other textual descriptions) forms a navigational database.

We have treated XML retrieval here as an extension of conventional text retrieval, which is characterized by (i) long text fields (e.g., sections of a document), (ii) inexact matches of paths and words, and (iii) relevance-ranked results. Relational databases do not deal well with this use case.

We have concentrated on applications where XML is used for encoding a tree structure with semantically typed nodes. For this type of application, content-centric approaches suffice. But XML is a much richer representation formalism. In particular, schemas that contain many attributes and values usually have more of a database flavor and are best handled by a relational database or by parametric search.

Two other types of queries that cannot be handled in a vector space model are joins and ordering constraints. The following query requires a join:

> Find figures that decribe the Corba architecture and the paragraphs that refer to those figures.

This query imposes an ordering constraint:

> Retrieve the chapter of the book Introduction to algorithms that follows the chapter Binomial heaps.

The Corba query requires a join of paragraphs and figures. The Binomial heap

query relies on the ordering of elements in XML – in this case the ordering of chapter elements underneath the book node. There are powerful query languages for XML that can handle attributes, joins and ordering constraints. The best known of these is XQuery, a language proposed for standardization by the W3C. It is designed to be broadly applicable in all areas where XML is used. At the time of this writing, little research has been done on testing the ability of XQuery to satisfy the demands of typical information retrieval settings, in particular ranked retrieval. Efficiency is a major concern in this regard. Due to its complexity, it is challenging to implement an XQuery-based information retrieval system with the performance characteristics that users have come to expect in information retrieval.

Relational databases are better equipped to handle many structural constraints, particularly joins. But ordering is also difficult in a database framework – the tuples of a relation in the relational calculus are not ordered. Still, many structure-centric XML retrieval systems are extensions of relational databases. If text fields are short, exact matches for paths and text are desired and retrieval results in form of unordered sets are desired, then using a relational database for XML retrieval is appropriate.

10.6 References and further reading

There are many good introductions to XML, including (Harold and Means 2004). Section 10.4 follows the overview of INEX 2002 by Gövert and Kazai (2003), published in the proceedings of the meeting (Fuhr et al. 2003a). The proceedings of the four following INEX meetings were published as Fuhr et al. (2003b), Fuhr et al. (2005), Fuhr et al. (2006), and Fuhr et al. (2007). An uptodate overview article is Fuhr and Lalmas (2007). The results in Table 10.4 are from Kamps et al. (2006).

The structured document retrieval principle is due to Fuhr and Großjohann (2004) and Figure 10.3 is also from this article. The vector-space based XML retrieval method in Section 10.3 is essentially IBM Haifa's JuruXML system as presented in (Mass et al. 2003, Carmel et al. 2003). Schlieder and Meuss (2002) and Grabs and Schek (2002) also represent XML documents in the vector space model. Carmel et al. propose to represent queries as *XML fragments*. The trees that represent XML queries in this chapter are all XML fragments, but XML fragments also permit the operators $+$, $-$ and *phrase* on content nodes.

XML FRAGMENT

We chose to present the vector space model for XML retrieval because it is simple and a natural extension of the unstructured vector space model in Chapter 6. But many other unstructured retrieval methods have been applied to XML retrieval with at least as much success as the vector space model. These methods include language models (cf. Chapter 12, e.g., Kamps

et al. (2004), List et al. (2005), Ogilvie and Callan (2005)), systems like TopX that use a relational database as a backend (Theobald et al. 2005; 2007), probabilistic weighting (Lu et al. 2007), and fusion (Larson 2005). There is currently no consensus as to what the best approach to XML retrieval is.

FOCUSED RETRIEVAL

One of the most active current areas of XML retrieval research is *focused retrieval* (Trotman et al. 2007), which aims to avoid returning nested elements that share one or more common subelements (cf. discussion in Section 10.2, page 200). Focused retrieval requires evaluation measures that penalize redundant result lists (Kazai and Lalmas 2006, Lalmas et al. 2007). Trotman and Geva (2006) argue that XML retrieval is a form of *passage retrieval* Salton et al. (1993), Zobel et al. (1995), Hearst (1997), Kaszkiel and Zobel (1997). In passage retrieval, the retrieval system returns short passages instead of documents in response to a user query. While element boundaries in XML documents are cues for identifying good segment boundaries between passages, the most relevant passage often does not conincide with an XML element.

PASSAGE RETRIEVAL

NEXI

In the last several years, the query format at INEX has been *NEXI* (Narrowed Extended XPath I) (Trotman and Sigurbjörnsson 2004). NEXI queries are similar to XML fragments, but allow users to specify the context in which a target element should occur (e.g., a section in an article that also contains an abstract) among other differences. O'Keefe and Trotman (2004) give evidence that users cannot reliably distinguish the child and descendant axes. This justifies only permitting descendant axes in XML fragments and NEXI. These structural constraints were only treated as "hints" in recent INEXes. Assessors can judge an element highly relevent even though it violates one of the structural constraints specified in a NEXI query. An alternative approach to NEXI is a more sophisticated user interface for query formulation van Zwol et al. (2006), Tannier and Geva (2005).

A broad overview of XML search that covers database as well as IR approaches is (Amer-Yahia and Lalmas 2006). (Grossman and Frieder 2004, ch. 6) is a good introduction to structured text retrieval from a database perspective. The proposed standard for XQuery can be found at http://www.w3.org/TR/xquery/. Rahm and Bernstein (2001) give a survey of automatic schema matching that is also applicable to XML.

10.7 Exercises

Exercise 10.1

Find a reasonably sized XML document collection (or a collection using a markup language different from XML like HTML) on the web and download it. The first 10,000 documents of the Wikipedia are a good choice. Create three CAS topics of the type shown in Figure 10.11 that you would expect to do better than analogous CO topics. Make plausible that an XML retrieval system would be able to exploit the XML structure of the documents to achieve better retrieval results than an unstructured retrieval system.

Exercise 10.2

For the collection and the topics in Exercise 10.1, (i) are there pairs of elements e_1 and e_2, with e_2 a subelement of e_1 such that both answer one of the topics? Find a case where (ii) e_1 (iii) e_2 is the better answer to the query.

Exercise 10.3

Implement the (i) Merge (ii) NoMerge algorithm in Section 10.3 and run it for the collection and the topics in Exercise 10.1. (iii) Evaluate the results by assigning binary relevance judgments to the first five documents of the three retrieved lists for each algorithm. Which algorithm performs better?

Exercise 10.4

Write down all the structural terms occurring in the XML document in Figure 10.6.

Exercise 10.5

Are all of the elements in Exercise 10.1 appropriate to be returned as hits to a user or are there elements (as in the example `<b>definitely</b>` above, page 191) that you would exclude?

Exercise 10.6

We discussed the tradeoff between accuracy of results and dimensionality of the vector space on page 194. If we only index structural terms (as opposed to subtrees in general), what type of query can we not answer correctly?

Exercise 10.7

How many structural terms does the document in Figure 10.1 yield?

Exercise 10.8

If we index all structural terms, what is the size of the index as a function of text size?

Exercise 10.9

If we index all subtrees that contain at least one vocabulary term, what is the size of the index as a function of text size?

Exercise 10.10

Give an example of a query-document pair for which sim-cr(q, d) is larger than 1.0.

Exercise 10.11

Consider computing df for a structural term as the number of times that the structural term occurs under a particular parent node. If the structural term `Title//"Microsoft"` occurs twice as the child of the node `Book`, then its idf weight is $\log 1000/2$ in this scheme assuming that there are 1000 `Book` nodes in the collection. (i) Implement this weighting method and apply it to the collection in Exercise 10.1. (ii) Does the method give intuitive results for parent nodes that are rare? Consider the case of a structural term that occurs once under a parent node that occurs only a few times in the collection.

11 *Probabilistic information retrieval*

During the discussion of relevance feedback in Section 9.1.2, we observed that if we have some known relevant and non-relevant documents, then we can straightforwardly start to estimate the probability of a term t appearing in a relevant document $P(t|R = 1)$, and that this could be the basis of a classifier that decides whether documents are relevant or not. In this chapter, we more systematically introduce this probabilistic approach to IR, which provides a different formal basis for a retrieval model and results in different techniques for setting term weights.

Users start with *information needs*, which they translate into *query representations*. Similarly, there are *documents*, which are converted into *document representations* (the latter differing at least by how text is tokenized, but perhaps containing fundamentally less information, as when a non-positional index is used). Based on these two representations, a system tries to determine how well documents satisfy information needs. In the Boolean or vector space models of IR, matching is done in a formally defined but semantically imprecise calculus of index terms. Given only a query, an IR system has an uncertain understanding of the information need. Given the query and document representations, a system has an uncertain guess of whether a document has content relevant to the information need. Probability theory provides a principled foundation for such reasoning under uncertainty. This chapter provides one answer as to how to exploit this foundation to estimate how likely it is that a document is relevant to an information need.

There is more than one possible retrieval model which has a probabilistic basis. Here, we will introduce probability theory and the Probability Ranking Principle (Sections 11.1–11.2), and then concentrate on the *Binary Independence Model* (Section 11.3), which is the original and still most influential probabilistic retrieval model. Finally, we will introduce related but extended methods which use term counts, including the empirically successful Okapi BM25 weighting scheme, and Bayesian Network models for IR (Section 11.4). In Chapter 12, we then present the alternate probabilistic language model-

ing approach to IR, which has been developed with considerable success in recent years.

11.1 Review of basic probability theory

We hope that the reader has seen a little basic probability theory previously. We will give a very quick review; some references for further reading appear at the end of the chapter. A variable A represents an event (a subset of the space of possible outcomes). Equivalently, we can represent the subset via a RANDOM VARIABLE *random variable*, which is a function from outcomes to numbers; the subset is the domain over which the random variable A has a particular value. Often we will not know with certainty whether an event is true in the world. We can ask the probability of the event $0 \leq P(A) \leq 1$. For two events A and B, there is the concept of a joint event where both are true, with probability $P(A, B)$, and a conditional probability, such as $P(A|B)$, the probability of event A given that event B is true. The fundamental relationship between CHAIN RULE joint and conditional probabilities is given by the *chain rule*:

$$P(A, B) = P(A \cap B) = P(A|B)P(B) = P(B|A)P(A) \tag{11.1}$$

Without assumptions, the probability of a joint event equals the probability of one of the events multiplied by the probability of the other event conditioned on knowing the first event happened.

Writing $P(\overline{A})$ for the complement of an event, we similarly have:

$$P(\overline{A}, B) = P(B|\overline{A})P(\overline{A}) \tag{11.2}$$

PARTITION RULE Probability theory also has a *partition rule*, which says that if an event B can be divided into an exhaustive set of subcases, then the probability of B is the sum of the probabilities of the subcases. A special case of this rule gives that:

$$P(B) = P(A, B) + P(\overline{A}, B) \tag{11.3}$$

BAYES' RULE From these we can derive *Bayes' Rule* for inverting conditional probabilities:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \left[\frac{P(B|A)}{\sum_{X \in \{A, \overline{A}\}} P(B|X)P(X)}\right] P(A) \tag{11.4}$$

This equation can also be thought of as a way of updating probabilities. We start off with an initial estimate of how likely the event A is when we do PRIOR PROBABILITY not have any other information; this is the *prior probability* $P(A)$. Bayes' rule POSTERIOR PROBABILITY lets us derive a *posterior probability* $P(A|B)$ after having seen the evidence B, based on the likelihood of B occurring in the two cases that A does or does not hold.

ODDS

Finally, it is often useful to talk about the *odds* of an event, which provide a kind of multiplier for how probabilities change:

$$\text{Odds:} \quad O(A) = \frac{P(A)}{P(\overline{A})} = \frac{P(A)}{1 - P(A)} \tag{11.5}$$

11.2 The Probability Ranking Principle

11.2.1 The 1/0 loss case

We assume a ranked retrieval setup as in Chapter 7, where there is a collection of documents, the user issues a query, and an ordered list of documents is returned, and we continue to work with a binary notion of relevance. For a query q and a document d in the collection, let $R_{d,q}$ be an indicator random variable which says whether d is relevant with respect to a given query q. That is, it takes on a value of 1 when the document is relevant and 0 otherwise. In context we will often write just R for $R_{d,q}$.

Using a probabilistic model, the obvious order in which to present documents to the user is to rank documents by their estimated probability of relevance with respect to the information need: $P(R = 1|d, q)$. This is the basis of the *Probability Ranking Principle* (PRP) (van Rijsbergen 1979, 113–114):

PROBABILITY RANKING PRINCIPLE

> "If a reference retrieval system's response to each request is a ranking of the documents in the collection in order of decreasing probability of relevance to the user who submitted the request, where the probabilities are estimated as accurately as possible on the basis of whatever data have been made available to the system for this purpose, the overall effectiveness of the system to its user will be the best that is obtainable on the basis of those data."

In the simplest case of the PRP, there are no retrieval costs or other utility concerns that would differentially weight actions or errors. You lose a point for either returning an irrelevant document or failing to return a relevant document (such a binary situation where you are evaluated on your *accuracy* is called *1/0 loss*). The goal is to return the best possible results as the top k documents, for any value of k the user chooses to examine. The PRP then says to simply rank all documents by $P(R = 1|d, q)$. If a set of retrieval results is to be returned, rather than an ordering, the Bayes Optimal Decision Rule is to use a simple even odds threshold:

1/0 LOSS

$$d \text{ is relevant iff } P(R = 1|d, q) > P(R = 0|d, q) \tag{11.6}$$

Theorem 11.1. *Using the PRP is optimal, in the sense that it minimizes the expected loss (also known as the* Bayes risk*) under 1/0 loss.*

BAYES RISK

The proof can be found in Ripley (1996). However, it requires that all probabilities are known correctly. This is never the case in practice. Nevertheless, the PRP still provides a very useful foundation for developing models of IR.

11.2.2 The PRP with retrieval costs

Suppose instead that we assume a model of retrieval costs. Let C_1 be the cost of retrieval of a relevant document and C_0 the cost of retrieval of a non-relevant document. Then the Probability Ranking Principle says that if for a specific document d and for all documents d' not yet retrieved

$$C_1 \cdot P(R = 1|d) + C_0 \cdot P(R = 0|d) \leq C_1 \cdot P(R = 1|d') + C_0 \cdot P(R = 0|d') \tag{11.7}$$

then d is the next document to be retrieved. Such a model gives a formal framework where we can model differential costs of false positives and false negatives and even system performance issues at the modeling stage, rather than simply at the evaluation stage, as we did in Section 8.6 (page 159). However, we will not further consider loss/utility models in this chapter.

11.3 The Binary Independence Model

BINARY INDEPENDENCE MODEL

The *Binary Independence Model* (BIM) we present in this section is the model that has traditionally been used with the PRP. It introduces some simple assumptions, which make estimating the probability function $P(R|d, q)$ practical. Here, "binary" is equivalent to Boolean: documents and queries are both represented as binary term incidence vectors. That is, a document d is represented by the vector $\vec{x} = (x_1, \ldots, x_M)$ where $x_t = 1$ if term t is present in document d and $x_t = 0$ if t is not present in d. With this representation, many possible documents have the same vector representation. Similarly, we represent q by the incidence vector $\vec{q}$ (the distinction between q and $\vec{q}$ is less central since commonly q is in the form of a set of words). "Independence" means that terms are modeled as occurring in documents independently. The model recognizes no association between terms. This assumption is far from correct, but it nevertheless often gives satisfactory results in practice; it is the "naive" assumption of Naive Bayes models, discussed further in Section 13.4 (page 248). Indeed, the Binary Independence Model is exactly the same as the multivariate Bernoulli Naive Bayes model presented in Section 13.3 (page 246). In a sense this assumption is equivalent to an assumption of the vector space model, where each term is a dimension that is orthogonal to all other terms.

We will first present a model which assumes that the user has a single step information need. As discussed in Chapter 9, seeing a range of results might let the user refine their information need. Fortunately, as mentioned

there, it is straightforward to extend the Binary Independence Model so as to provide a framework for relevance feedback, and we present this model in Section 11.3.4.

To make a probabilistic retrieval strategy precise, we need to estimate how terms in documents contribute to relevance, specifically, we wish to know how term frequency, document frequency, document length, and other statistics we can compute influence judgements about document relevance, and how they can be reasonably combined to estimate the probability of document relevance. We then order documents by decreasing estimated probability of relevance.

We assume here that the relevance of each document is independent of the relevance of other documents. As we noted in Section 8.5.1 (page 157), this is incorrect: the assumption is especially harmful in practice if it allows a system to return duplicate or near duplicate documents. Under the BIM, we model the probability $P(R|d,q)$ that a document is relevant via the probability in terms of term incidence vectors $P(R|\vec{x},\vec{q})$. Then, using Bayes rule, we have:

$$P(R=1|\vec{x},\vec{q}) = \frac{P(\vec{x}|R=1,\vec{q})P(R=1|\vec{q})}{P(\vec{x}|\vec{q})} \tag{11.8}$$

$$P(R=0|\vec{x},\vec{q}) = \frac{P(\vec{x}|R=0,\vec{q})P(R=0|\vec{q})}{P(\vec{x}|\vec{q})}$$

Here, $P(\vec{x}|R=1,\vec{q})$ and $P(\vec{x}|R=0,\vec{q})$ are the probability that if a relevant or non-relevant, respectively, document is retrieved, then that document's representation is $\vec{x}$. You should think of this quantity as defined with respect to a space of possible documents in a domain. How do we compute all these probabilities? We never know the exact probabilities, and so we have to use estimates: Statistics about the actual document collection are used to estimate these probabilities. $P(R=1|\vec{q})$ and $P(R=0|\vec{q})$ indicate the prior probability of retrieving a relevant or non-relevant document respectively for a query $\vec{q}$. Again, if we knew the percentage of relevant documents in the collection, then we could use this number to estimate $P(R=1|\vec{q})$ and $P(R=0|\vec{q})$. Since a document is either relevant or non-relevant to a query, we must have that:

$$P(R=1|\vec{x},\vec{q}) + P(R=0|\vec{x},\vec{q}) = 1 \tag{11.9}$$

11.3.1 Deriving a ranking function for query terms

Given a query q, we wish to order returned documents by descending $P(R=1|d,q)$. Under the BIM, this is modeled as ordering by $P(R=1|\vec{x},\vec{q})$. Rather than estimating this probability directly, as we are interested only in the ranking of documents, we work with some other quantities which are easier to

compute and which give the same ordering of documents. In particular, we can rank documents by their odds of relevance (as the odds of relevance is monotonic with the probability of relevance). This makes things easier, because we can ignore the common denominator in (11.8), giving:

$$O(R|\vec{x},\vec{q}) = \frac{P(R=1|\vec{x},\vec{q})}{P(R=0|\vec{x},\vec{q})} = \frac{\frac{P(R=1|\vec{q})P(\vec{x}|R=1,\vec{q})}{P(\vec{x}|\vec{q})}}{\frac{P(R=0|\vec{q})P(\vec{x}|R=0,\vec{q})}{P(\vec{x}|\vec{q})}} = \frac{P(R=1|\vec{q})}{P(R=0|\vec{q})} \cdot \frac{P(\vec{x}|R=1,\vec{q})}{P(\vec{x}|R=0,\vec{q})} \tag{11.10}$$

The left term in the rightmost expression of Equation (11.10) is a constant for a given query. Since we are only ranking documents, there is thus no need for us to estimate it. The right-hand term does, however, require estimation, and this initially appears to be difficult: How can we accurately estimate the probability of an entire term incidence vector occurring? It is at this point that we make the *Naive Bayes conditional independence assumption* that the presence or absence of a word in a document is independent of the presence or absence of any other word (given the query):

NAIVE BAYES ASSUMPTION

$$\frac{P(\vec{x}|R=1,\vec{q})}{P(\vec{x}|R=0,\vec{q})} = \prod_{t=1}^{M} \frac{P(x_t|R=1,\vec{q})}{P(x_t|R=0,\vec{q})} \tag{11.11}$$

So:

$$O(R|\vec{x},\vec{q}) = O(R|\vec{q}) \cdot \prod_{t=1}^{M} \frac{P(x_t|R=1,\vec{q})}{P(x_t|R=0,\vec{q})} \tag{11.12}$$

Since each x_t is either 0 or 1, we can separate the terms to give:

$$O(R|\vec{x},\vec{q}) = O(R|\vec{q}) \cdot \prod_{t:x_t=1} \frac{P(x_t=1|R=1,\vec{q})}{P(x_t=1|R=0,\vec{q})} \cdot \prod_{t:x_t=0} \frac{P(x_t=0|R=1,\vec{q})}{P(x_t=0|R=0,\vec{q})} \tag{11.13}$$

Henceforth, let $p_t = P(x_t = 1|R = 1, \vec{q})$ be the probability of a term appearing in a document relevant to the query, and $u_t = P(x_t = 1|R = 0, \vec{q})$ be the probability of a term appearing in a non-relevant document. These quantities can be visualized in the following contingency table where the columns add to 1:

(11.14)

	Document	Relevant ($R = 1$)	Non-relevant ($R = 0$)
Term present	$x_t = 1$	p_t	u_t
Term absent	$x_t = 0$	$1 - p_t$	$1 - u_t$

Let us make an additional simplifying assumption that terms not occurring in the query are equally likely to occur in relevant and non-relevant documents: that is, if $q_t = 0$ then $p_t = u_t$. (This assumption can be changed,

as when doing relevance feedback in Section 11.3.4.) Then we need only consider terms in the products that appear in the query, and so,

$$O(R|\vec{q},\vec{x}) = O(R|\vec{q}) \cdot \prod_{t:x_t=q_t=1} \frac{p_t}{u_t} \cdot \prod_{t:x_t=0,q_t=1} \frac{1-p_t}{1-u_t} \tag{11.15}$$

The left product is over query terms found in the document and the right product is over query terms not found in the document.

We can manipulate this expression by including the query terms found in the document into the right product, but simultaneously dividing through by them in the left product, so the value is unchanged. Then we have:

$$O(R|\vec{q},\vec{x}) = O(R|\vec{q}) \cdot \prod_{t:x_t=q_t=1} \frac{p_t(1-u_t)}{u_t(1-p_t)} \cdot \prod_{t:q_t=1} \frac{1-p_t}{1-u_t} \tag{11.16}$$

The left product is still over query terms found in the document, but the right product is now over all query terms. That means that this right product is a constant for a particular query, just like the odds $O(R|\vec{q})$. So the only quantity that needs to be estimated to rank documents for relevance to a query is the left product. We can equally rank documents by the log of this term, since log is also a monotonic function. The resulting quantity used for ranking is called the *Retrieval Status Value* (RSV) in this model:

RETRIEVAL STATUS VALUE

$$RSV_d = \log \prod_{t:x_t=q_t=1} \frac{p_t(1-u_t)}{u_t(1-p_t)} = \sum_{t:x_t=q_t=1} \log \frac{p_t(1-u_t)}{u_t(1-p_t)} \tag{11.17}$$

So everything comes down to computing the RSV. Define c_t:

$$c_t = \log \frac{p_t(1-u_t)}{u_t(1-p_t)} = \log \frac{p_t}{(1-p_t)} + \log \frac{1-u_t}{u_t} \tag{11.18}$$

The c_t terms are log odds ratios for the terms in the query. We have the odds of the term appearing if the document is relevant ($p_t/(1-p_t)$) and the odds of the term appearing if the document is not relevant ($u_t/(1-u_t)$). The *odds ratio* is the ratio of two such odds, and then we finally take the log of that quantity. The value will be 0 if a term has equal odds of appearing in relevant and non-relevant documents, and positive if it is more likely to appear in relevant documents. The c_t quantities function as term weights in the model, and the document score for a query is $RSV_d = \sum_{x_t=q_t=1} c_t$. Operationally, we sum them in accumulators for query terms appearing in documents, just as for the vector space model calculations discussed in Section 7.1 (page 127). We now turn to how we estimate these c_t quantities for a particular collection and query.

ODDS RATIO

11.3.2 Probability estimates in theory

For each term t, what would these c_t numbers look like for the whole collection? (11.19) gives a contingency table of counts of documents in the collection, where df_t is the number of documents that contain term t:

(11.19)

	Documents	Relevant	Non-relevant	Total
Term present	$x_t = 1$	s	$\mathrm{df}_t - s$	df_t
Term absent	$x_t = 0$	$S - s$	$(N - \mathrm{df}_t) - (S - s)$	$N - \mathrm{df}_t$
	Total	S	$N - S$	N

Using this, $p_t = s/S$ and $u_t = (\mathrm{df}_t - s)/(N - S)$ and

$$c_t = K(N, \mathrm{df}_t, S, s) = \log \frac{s/(S-s)}{(\mathrm{df}_t - s)/((N - \mathrm{df}_t) - (S - s))} \tag{11.20}$$

To avoid the possibility of zeroes (such as if every or no relevant document has a particular term) it is fairly standard to add $\frac{1}{2}$ to each of the quantities in the center 4 terms of (11.19), and then to adjust the marginal counts (the totals) accordingly (so, the bottom right cell totals $N + 2$). Then we have:

$$\hat{c}_t = K(N, \mathrm{df}_t, S, s) = \log \frac{(s + \frac{1}{2})/(S - s + \frac{1}{2})}{(\mathrm{df}_t - s + \frac{1}{2})/(N - \mathrm{df}_t - S + s + \frac{1}{2})} \tag{11.21}$$

SMOOTHING

Adding $\frac{1}{2}$ in this way is a simple form of *smoothing*. One way to estimate the probability of an event from data is simply to count the number of times an event occurred divided by the total number of observed events. This is referred to as the the *relative frequency* of the event. For trials with categorical outcomes (such as noting the presence or absence of a term), estimating the probability as the relative frequency is the *maximum likelihood estimate* (or *MLE*), because this value makes the observed data maximally likely. However, if we simply use the MLE, then the probability given to events we happened to see is usually slightly too high, whereas other events may be completely unseen and giving them as a probability estimate their relative frequency of 0 is both an underestimate, and normally breaks our models, since anything multiplied by 0 is 0. Simultaneously decreasing the estimated probability of seen events and increasing the probability of unseen events is referred to as *smoothing*. One simple way of smoothing is to add a number α to each of the observed counts. These *pseudocounts* correspond to the use of a *Bayesian prior*, following Equation (11.4). We initially assume a uniform distribution over events, where the size of α denotes the strength of our belief in uniformity, and we then update the probability based on observed events. Since our belief in uniformity is weak, we use $\alpha = \frac{1}{2}$. This is a form

RELATIVE FREQUENCY

MAXIMUM LIKELIHOOD ESTIMATE MLE

SMOOTHING PSEUDOCOUNTS BAYESIAN PRIOR

MAXIMUM A POSTERIORI MAP

of *maximum a posteriori* (*MAP*) estimation, where we choose the most likely point value for probabilities based on the prior and the observed evidence, following Equation (11.4). We will further discuss methods of smoothing estimated counts to give probability models in Section 12.1.2 (page 229); the simple method of adding $\frac{1}{2}$ to each observed count will do for now.

11.3.3 Probability estimates in practice

Under the assumption that relevant documents are a very small percentage of the collection, it is plausible to approximate statistics for non-relevant documents by statistics from the whole collection. Under this assumption, u_t (the probability of term occurrence in non-relevant documents for a query) is df_t/N and

$$\log[(1-u_t)/u_t] = \log[(N-\mathrm{df}_t)/\mathrm{df}_t] \approx \log N/\mathrm{df}_t \tag{11.22}$$

In other words, we can provide a theoretical justification for the most frequently used form of idf weighting, which we saw in Section 6.2.1.

The approximation technique in Equation (11.22) cannot easily be extended to relevant documents. The quantity p_t can be estimated in various ways:

1. We can use the frequency of term occurrence in known relevant documents (if we know some). This is the basis of probabilistic approaches to relevance feedback weighting in a feedback loop, discussed in the next subsection.

2. Croft and Harper (1979) proposed using a constant in their combination match model. For instance, we might assume that p_t is constant over all terms x_t in the query and that $p_t = 0.5$. This means that each term has even odds of appearing in a relevant document, and so the p_t and $(1-p_t)$ factors cancel out in the expression for RSV. Such an estimate is weak, but doesn't violently disagree with our hopes for the search terms appearing in many but not all relevant documents. Combining this method with our earlier approximation for u_t, the document ranking is determined simply by which query terms occur in documents scaled by their idf weighting. For short documents (titles or abstracts) in situations in which iterative searching is undesirable, using this weighting term alone can be quite satisfactory, although in many other circumstances we would like to do better.

3. Greiff (1998) argues that the constant estimate of p_t in the Croft and Harper (1979) model is theoretically problematic and not observed empirically, and argues that a much better estimate is found by simply estimating p_t from collection level statistics about the occurrence of t. That is, using $p_t = \mathrm{df}_t/N$.

Iterative methods of estimation, which combine some of the above ideas, are discussed in the next subsection.

11.3.4 Probabilistic approaches to relevance feedback

We can use (pseudo-)relevance feedback, perhaps in an iterative process of estimation, to get a more accurate estimate of p_t. The probabilistic approach to relevance feedback works as follows:

1. Guess initial estimates of p_t and u_t. This can be done using the probability estimates of the previous section. For instance, we can assume that p_t is constant over all x_t in the query, in particular, perhaps taking $p_t = \frac{1}{2}$.

2. Use the current estimates of p_t and u_t to determine a best guess at the set of relevant documents $R = \{d : R_{d,q} = 1\}$. Use this model to retrieve a set of candidate relevant documents, which we present to the user.

3. We interact with the user to refine the model of R. We do this by learning from the user relevance judgements for some subset of documents V. Based on relevance judgements, V is partitioned into two subsets: $VR = \{d \in V, R_{d,q} = 1\} \subset R$ and $VNR = \{d \in V, R_{d,q} = 0\}$, which is disjoint from R.

4. We reestimate p_t and u_t on the basis of known relevant and irrelevant documents. If the sets VR and VNR are large enough, we may be able to estimate these quantities directly from these documents as maximum likelihood estimates:

$$p_t = |VR_t|/|VR| \tag{11.23}$$

(where VR_t is the set of documents in VR containing x_t). In practice, we usually need to smooth these estimates. We can do this by adding $\frac{1}{2}$ to both the count $|VR_t|$ and to the number of relevant documents not containing the term, giving:

$$p_t = \frac{|VR_t| + \frac{1}{2}}{|VR| + 1} \tag{11.24}$$

However, the set of documents judged by the user (V) is usually very small, and so the resulting statistical estimate is quite unreliable (noisy), even if the estimate is smoothed. So it is often better to combine the new information with the original guess in a process of Bayesian updating. In this case we have:

$$p_t^{(k+1)} = \frac{|VR_t| + \kappa p_t^{(k)}}{|VR| + \kappa} \tag{11.25}$$

Here $p_t^{(k)}$ is the k^{th} estimate for p_t in an iterative updating process and κ is the weight given to the Bayesian prior. Relating this equation back to Equation (11.4) requires a bit more probability theory than we have presented here (we need to use a beta distribution prior, conjugate to the Bernoulli random variable X_t). But the form of the resulting equation is quite straightforward: rather than uniformly distributing pseudocounts, we now distribute a total of κ pseudocounts according to the previous estimate, which acts as the prior distribution. In the absence of other evidence (and assuming that the user is perhaps indicating roughly 5 relevant or non-relevant documents) then a value of around $\kappa = 5$ is perhaps appropriate. That is, the prior is strongly weighted so that the estimate does not change too much from the evidence provided by a very small number of documents.

5. Repeat the above process from step 2, generating a succession of approximations to R and hence p_t, until the user is satisfied.

It is also straightforward to derive a pseudo-relevance feedback version of this algorithm, where we simply pretend that $VR = V$. More briefly:

1. Assume initial estimates for p_t and u_t as above.

2. Determine a guess for the size of the relevant document set. If unsure, a conservative (too small) guess is likely to be best. This motivates use of a fixed size set V of highest ranked documents.

3. Improve our guesses for p_t and u_t. We choose from the methods of Equations (11.23) and (11.25) for re-estimating p_t, except now based on the set V instead of VR. If we let V_t be the subset of documents in V containing x_t and use add $\frac{1}{2}$ smoothing, we get:

$$p_t = \frac{|V_t| + \frac{1}{2}}{|V| + 1} \tag{11.26}$$

and if we assume that documents that are not retrieved are not relevant then we can update our u_t estimates as:

$$u_t = \frac{\mathrm{df}_t - |V_t| + \frac{1}{2}}{N - |V| + 1} \tag{11.27}$$

4. Go to step 2 until the ranking of the returned results converges.

Once we have a real estimate for p_t then the c_t weights used in the RSV value look almost like a tf-idf value. For instance, using Equation (11.18),

Equation (11.22), and Equation (11.26), we have:

$$c_t = \log\left[\frac{p_t}{1-p_t}\cdot\frac{1-u_t}{u_t}\right] \approx \log\left[\frac{|V_t|+\frac{1}{2}}{|V|-|V_t|+1}\cdot\frac{N}{\mathrm{df}_t}\right] \tag{11.28}$$

But things aren't quite the same: $p_t/(1-p_t)$ measures the (estimated) proportion of relevant documents that the term t occurs in, not term frequency. Moreover, if we apply log identities:

$$c_t = \log\frac{|V_t|+\frac{1}{2}}{|V|-|V_t|+1} + \log\frac{N}{\mathrm{df}_t} \tag{11.29}$$

we see that we are now *adding* the two log scaled components rather than multiplying them.

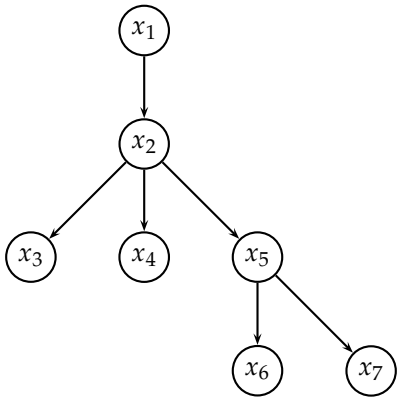
11.3.5 The assumptions of the Binary Independence Model

Getting reasonable approximations of the needed probabilities for a probabilistic IR model is possible, but it requires some major assumptions. In the BIM these are:

- a Boolean representation of documents/queries/relevance
- term independence
- terms not in the query don't affect the outcome
- document relevance values are independent

A general problem seems to be that probabilistic models either require partial relevance information or else only allow for deriving apparently inferior term weighting models.

However, some of these assumptions can be removed. For example, we can remove the assumption that terms are independent. This assumption is very far from true in practice. A case that particularly violates this assumption is term pairs like Hong and Kong, which are strongly dependent. But dependencies can occur in various complex configurations, such as between the set of terms New, York, England, City, Stock, Exchange, and University. van Rijsbergen (1979) proposed a simple, plausible model which allowed a tree structure of term dependencies, as in Figure 11.1. In this model each term can be directly dependent on only one other, giving a tree structure of dependencies. When it was invented in the 1970s, estimation problems held back the practical success of this model, but the idea was reinvented as the Tree Augmented Naive Bayes model by Friedman and Goldszmidt (1996), who used it with some success on various machine learning data sets. In the



► **Figure 11.1** A tree of dependencies between terms. In this graphical model representation, a term x_i is directly dependent on a term x_k if there is an arrow $x_k \rightarrow x_i$.

next section we consider more nuanced probabilistic term weighting models and the prospect of using much more elaborate probabilistic models in the style of Figure 11.1 for IR.

11.4 An appraisal and some extensions

11.4.1 An appraisal of probabilistic models

Probabilistic methods are one of the oldest formal models in IR. Already in the 1970s they were held out as an opportunity to place IR on a firmer theoretical footing, and with the resurgence of probabilistic methods in computational linguistics in the 1990s, that hope has returned, and probabilistic methods are again one of the currently hottest topics in IR. Traditionally, probabilistic IR has had neat ideas but the methods have never won on performance. That started to change in the 1990s when the BM25 weighting scheme, which we discuss in the next section, showed very good performance, and started to be adopted as a term weighting scheme by many groups. The difference between "vector space" and "probabilistic" IR systems is not that great: in either case, you build an information retrieval scheme in the exact same way that we discussed in Chapter 7. For a probabilistic IR system, it's just that, at the end, you score queries not by cosine similarity and tf-idf in a vector space, but by a slightly different formula motivated by probability theory. Indeed, sometimes people have changed an

existing vector-space IR system into an effectively probabilistic system simply by adopted term weighting formulas from probabilistic models. Here we briefly present two influential extensions of the traditional probabilistic model, and in the next chapter, we look at the somewhat different probabilistic language modeling approach to IR.

11.4.2 Okapi BM25: a non-binary model

BM25 WEIGHTS
OKAPI WEIGHTING

The BIM was originally designed for short catalog records and abstracts of fairly consistent length, and it works reasonably in these contexts, but for modern full-text search collections, it seems clear that a model should pay attention to term frequency and document length, as in Chapter 6. The *BM25 weighting scheme*, often called *Okapi weighting*, after the system in which it was first implemented, was developed as a way of building a probabilistic model sensitive to these quantities while not introducing too many additional parameters into the model (Spärck Jones et al. 2000). We will not develop the full theory behind the model here, but just present a series of forms that build up to the standard form now used for document scoring. The simplest score for document d is just idf weighting of the query terms present, as in Equation (11.22):

$$RSV_d = \sum_{t \in q} \log \frac{N}{\mathrm{df}_t} \tag{11.30}$$

Sometimes, an alternative version of idf is used. If we start with the formula in Equation (11.21) but in the absence of relevance feedback information we estimate that $S = s = 0$, then we get an alternative idf formulation as follows:

$$RSV_d = \sum_{t \in q} \log \frac{N - \mathrm{df}_t + \frac{1}{2}}{\mathrm{df}_t + \frac{1}{2}} \tag{11.31}$$

This variant behaves slightly strangely: if a term occurs in over half the documents in the collection then this model gives a negative term weight, which is presumably undesirable. But, assuming the use of a stop list, this normally doesn't happen, and the value for each summand can be given a floor of 0.

We can improve on Equation (11.30) by factoring in the frequency of each term and document length:

$$RSV_d = \sum_{t \in q} \log \left[\frac{N}{\mathrm{df}_t} \right] \cdot \frac{(k_1 + 1)\mathrm{tf}_{td}}{k_1((1 - b) + b \times (L_d / L_{\mathrm{ave}})) + \mathrm{tf}_{td}} \tag{11.32}$$

Here, tf_{td} is the frequency of term t in document d, and L_d and L_{ave} are the length of document d and the average document length for the whole collection. The variable k_1 is a positive tuning parameter that calibrates the

document term frequency scaling. A k_1 value of 0 corresponds to a binary model (no term frequency), and a large value corresponds to using raw term frequency. b is another tuning parameter ($0 \leq b \leq 1$) which determines the scaling by document length: $b = 1$ corresponds to fully scaling the term weight by the document length, while $b = 0$ corresponds to no length normalization.

If the query is long, then we might also use similar weighting for query terms. This is appropriate if the queries are paragraph long information needs, but unnecessary for short queries.

$$RSV_d = \sum_{t \in q} \left[\log \frac{N}{\mathrm{df}_t} \right] \cdot \frac{(k_1 + 1)\mathrm{tf}_{td}}{k_1((1-b) + b \times (L_d / L_{\mathrm{ave}})) + \mathrm{tf}_{td}} \cdot \frac{(k_3 + 1)\mathrm{tf}_{tq}}{k_3 + \mathrm{tf}_{tq}} \tag{11.33}$$

with tf_{tq} being the frequency of term t in the query q, and k_3 being another positive tuning parameter that this time calibrates term frequency scaling of the query. In the equation presented, there is no length normalization of queries (it is as if $b = 0$ here). Length normalization of the query is unnecessary because retrieval is being done with respect to a single fixed query. The tuning parameters of these formulas should ideally be set to optimize performance on a development query collection. In the absence of such optimization, experiments have shown reasonable values are to set k_1 and k_3 to a value between 1.2 and 2 and $b = 0.75$.

If we have relevance judgements available, then we can use the full form of (11.21) in place of the approximation $\log(N/\mathrm{df}_t)$ introduced in (11.22):

$$\begin{aligned} RSV_d &= \sum_{t \in q} \log \left[\frac{(|VR_t| + \frac{1}{2})/(|VNR_t| + \frac{1}{2})}{(\mathrm{df}_t - |VR_t| + \frac{1}{2})/(N - \mathrm{df}_t - |VR| + |VR_t| + \frac{1}{2})} \right] \\ &\quad \times \frac{(k_1 + 1)\mathrm{tf}_{td}}{k_1((1-b) + b(L_d / L_{\mathrm{ave}})) + \mathrm{tf}_{td}} \times \frac{(k_3 + 1)\mathrm{tf}_{tq}}{k_3 + \mathrm{tf}_{tq}} \end{aligned} \tag{11.34}$$

Here, VR_t, NVR_t, and VR are used as in Section 11.3.4. The first part of the expression reflects relevance feedback (or just idf weighting if no relevance information is available), the second implements document term frequency and document length scaling, and the third considers term frequency in the query.

Rather than just providing a term weighting method for terms in a user's query, relevance feedback can also involve augmenting the query (automatically or with manual review) with some (say, 10–20) of the top terms in the known-relevant documents as ordered by the relevance factor $\hat{c}_t$ from Equation (11.21), and the above formula can then be used with such an augmented query vector $\vec{q}$.

The BM25 term weighting formulas have been used quite widely and quite successfully across a range of corpora and search tasks. Especially in the

TREC evaluations, they performed well and were widely adopted by many groups. See Spärck Jones et al. (2000) for extensive motivation and discussion of experimental results.

11.4.3 Bayesian network approaches to IR

BAYESIAN NETWORKS

Turtle and Croft (1989; 1991) introduced into information retrieval the use of *Bayesian networks* (Jensen and Jensen 2001), a form of probabilistic graphical model. We skip the details because fully introducing the formalism of Bayesian networks would require much too much space, but conceptually, Bayesian networks use directed graphs to show probabilistic dependencies between variables, as in Figure 11.1, and have led to the development of sophisticated algorithms for propagating influence so as to allow learning and inference with arbitrary knowledge within arbitrary directed acyclic graphs. Turtle and Croft used a sophisticated network to better model the complex dependencies between a document and a user's information need.

The model decomposes into two parts: a document collection network and a query network. The document collection network is large, but can be precomputed: it maps from documents to terms to concepts. The concepts are a thesaurus-based expansion of the terms appearing in the document. The query network is relatively small but a new network needs to be built each time a query comes in, and then attached to the document network. The query network maps from query terms, to query subexpressions (built using probabilistic or "noisy" versions of AND and OR operators), to the user's information need.

The result is a flexible probabilistic network which can generalize various simpler Boolean and probabilistic models. The system allowed efficient large-scale retrieval, and was the basis of the InQuery text retrieval system, used at the University of Massachusetts, and for a time sold commercially. On the other hand, the model still used various approximations and independence assumptions to make parameter estimation and computation possible. There has not been much follow-on work along these lines, but we would note that this model was actually built very early on in the modern era of using Bayesian networks, and there have been many subsequent developments in the theory, and the time is perhaps right for a new generation of Bayesian network-based information retrieval systems.

11.5 References and further reading

Longer introductions to the needed probability theory can be found in most introductory probability and statistics books, such as Grinstead and Snell

(1997), Rice (2006), Ross (2006). An introduction to Bayesian utility theory can be found in (Ripley 1996).

The probabilistic approach to IR originated in the UK in the 1950s. The first major presentation of a probabilistic model is Maron and Kuhns (1960). Robertson and Spärck Jones (1976b) introduce the main foundations of the BIM and van Rijsbergen (1979) presents in detail the classic BIM probabilistic model. The idea of the PRP is variously attributed to Stephen Robertson, M. E. Maron and William Cooper (the term "Probabilistic Ordering Principle" is used in Robertson and Spärck Jones (1976b), but PRP dominates in later work). Fuhr (1992) is a more recent presentation of probabilistic IR, which includes coverage of other approaches such as probabilistic logics and Bayesian networks. Crestani et al. (1998) is another survey. Spärck Jones et al. (2000) is the definitive presentation of probabilistic IR experiments by the "London school", and Robertson (2005) presents a retrospective on the group's participation in TREC evaluations, including detailed discussion of the Okapi BM25 model and its development.

11.6 Exercises

Exercise 11.1

Work through the derivation of Equation (11.20) from Equations (11.18) and (11.19).

Exercise 11.2

What are the differences between standard vector space tf-idf weighting and the BIM probabilistic retrieval model (in the case where no document relevance information is available)?

Exercise 11.3 [⋆⋆]

Let X_t be a random variable indicating whether the term t appears in a document. Suppose we have $|R|$ relevant documents in the document collection and that $X_t = 1$ in s of the documents. Take the observed data to be just these observations of X_t for each document in R. Show that the MLE for the parameter $p_t = P(X_t = 1|R = 1, \vec{q})$, that is, the value for p_t which maximizes the probability of the observed data, is $p_t = s/|R|$.

Exercise 11.4

Describe the differences between vector space relevance feedback and probabilistic relevance feedback.

12 *Language models for information retrieval*

In the traditional probabilistic approach to IR, the user has an information need, and determines a query q which is run against documents d, and we try to determine the probability of relevance $P(R|q,d)$. The original language modeling approach bypasses overtly modeling the concept of relevance. It instead builds a probabilistic language model M_d from each document d, and ranks documents based on the probability of the model generating the query: $P(q|M_d)$.

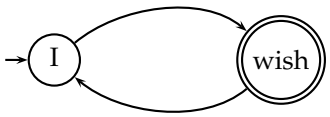
A common suggestion to users for coming up with good queries is to think of words that would likely appear in a relevant document, and to use those words as your query. The language modeling approach to IR directly models that idea: a document is a good match to a query if the document model is likely to generate the query, which will in turn happen if the document contains the query words often.

GENERATIVE MODEL

What do we mean by a document model generating a query? A traditional *generative model* of language of the kind familiar from formal language theory can be used either to recognize or to generate strings. For example, the finite automaton shown in Figure 12.1 can generate strings that include the examples shown. The full set of strings that can be generated is called the language of the automaton.

LANGUAGE MODEL

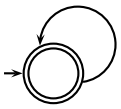
If instead each node has a probability distribution over generating different words, we have a language model. A (stochastic or probabilistic) *language model* is a function that puts a probability measure over strings drawn from some vocabulary. One simple kind of language model is equivalent to a probabilistic finite automaton consisting of just a single node with a single probability distribution of producing different words, as shown in Figure 12.2, coupled with a probability of stopping when in a finish state. Such a model places a probability distribution over any sequence of words. By construction, it also provides a model for generating text according to its distribution. To find the probability of a word sequence, we just multiply the probabilities



I wish
I wish I wish
I wish I wish I wish
I wish I wish I wish I wish I wish I wish
...

*wish I wish

► **Figure 12.1** A simple finite automaton and some of the strings in the language that it generates. → shows the start state of the automaton and a double circle indicates a (possible) finishing state.



the	0.2
a	0.1
frog	0.01
toad	0.01
said	0.03
likes	0.02
that	0.04

► **Figure 12.2** A one-state finite automaton that acts as a unigram language model. We show a partial specification of the state emission probabilities.

which it gives to each word in the sequence. For example,

$$P(\text{frog said that toad likes frog}) = 0.01 \times 0.03 \times 0.04 \times 0.02 \times 0.01 = 0.0000000024 \quad (12.1)$$

Here we omit the probability of stopping after *frog*. An explicit stop probability is needed for the finite automaton to generate and give probabilities to finite strings, but we will in general omit mention of it, since, if fixed, it does not alter the ranking of documents.

Suppose, now, that we have two language models M_1 and M_2, shown partially in Figure 12.3. Each gives a probability estimate to a sequence of words, as shown in the example. The language model that gives the higher probability to the sequence of words is more likely to have generated the word sequence. For the sequence shown, we get:

Model M_1		Model M_2	
the	0.2	the	0.15
a	0.1	a	0.12
frog	0.01	frog	0.0002
toad	0.01	toad	0.0001
said	0.03	said	0.03
likes	0.02	likes	0.04
that	0.04	that	0.04
dog	0.005	dog	0.01
cat	0.003	cat	0.015
monkey	0.001	monkey	0.002
...	...	...	...

► **Figure 12.3** Partial specification of two unigram language models.

(12.2)

s	frog	said	that	toad	likes	that	dog
M_1	0.01	0.03	0.04	0.01	0.02	0.04	0.005
M_2	0.0002	0.03	0.04	0.0001	0.04	0.04	0.01

$$P(s|M_1) = 0.00000000000048$$
$$P(s|M_2) = 0.000000000000000384$$

and we see that $P(s|M_1) > P(s|M_2)$.

How do people build probabilities over word sequences? We can always use the chain rule to decompose the probability of a sequence of events into the probability of each successive events conditioned on earlier events:

$$P(w_1w_2w_3w_4) = P(w_1)P(w_2|w_1)P(w_3|w_1w_2)P(w_4|w_1w_2w_3)$$

UNIGRAM LANGUAGE MODEL

The simplest form of language model simply throws away all conditioning context, and estimates each word independently. Such a model is called a *unigram language model*:

$$P_{\text{uni}}(w_1w_2w_3w_4) = P(w_1)P(w_2)P(w_3)P(w_4)$$

Under this model the order of words is irrelevant, and so such models are sometimes called "bag of words" models as discussed in Chapter 6 (page 110). There are many more complex kinds of language models, such as bigram language models, which condition on the previous word,

$$P_{\text{bi}}(w_1w_2w_3w_4) = P(w_1)P(w_2|w_1)P(w_3|w_2)P(w_4|w_3)$$

and even more complex grammar-based language models such as probabilistic context-free grammars. However, most language-modeling work in IR

has used unigram language models, and IR is probably not the most productive place to try using complex language models, since IR does not directly depend on the structure of sentences to the extent that other tasks like speech recognition do. Moreover, since, as we shall see, IR language models are frequently estimated from a single document, there is often not enough training data and losses from sparseness outweigh any gains from richer models.

The fundamental problem in designing language models is that we generally do not know what exactly we should use as the model M_d. However, we do generally have a sample of text that is representative of that model. This problem makes a lot of sense in the original, primary uses of language models. For example, in speech recognition, we have a training sample of text, but we have to expect that in the future, users will use different words and in different sequences, which we have never observed before, and so the model has to generalize beyond the observed data to allow unknown words and sequences. This interpretation is not so clear in the IR case, where a document is finite and usually fixed. However, we pretend that the document d is only a representative sample of text drawn from a model distribution, we estimate a language model from this sample, use that model to calculate the probability of observing any word sequence, and finally rank documents according to their probability of generating the query.

12.1 The query likelihood model

12.1.1 Using query likelihood language models in IR

QUERY LIKELIHOOD MODEL

Language modeling is a quite general formal approach to IR, with many variant realizations. The original and basic method for using language models in IR is the *query likelihood model*. In it, we construct from each document d in the collection a language model M_d. Our goal is to rank documents by $P(d|q)$, where the probability of a document is interpreted as the likelihood that it is relevant to the query. Using Bayes rule, we have:

$$P(d|q) = P(q|d)P(d)/P(q)$$

$P(q)$ is the same for all documents, and so can be ignored. The prior $P(d)$ is often treated as uniform across all d and so it can also be ignored, but we could implement a genuine prior which could include criteria like authority, length, genre, newness, and number of previous people who have read the document. But, given these simplifications, we return results ranked by simply $P(q|d)$, the probability of the query q given by the language model derived from d. The Language Modeling approach thus attempts to model the query generation process: Documents are ranked by the probability that a query would be observed as a random sample from the respective document model.

The most common way to do this is using the multinomial unigram language model, which is equivalent to a multinomial Naive Bayes model (page 246), where the documents are the classes, each treated in the estimation as a separate "language". Under this model, we have that:

$$P(q|M_d) = \prod_{w \in V} P(w|M_d)^{\text{tf}_w} \tag{12.3}$$

Usually a unigram estimate of words is used in IR. There is some work on bigrams, paralleling the discussion of van Rijsbergen in Chapter 11 (page 218), but it hasn't been found very necessary. While modeling term cooccurrence should improve estimates somewhat, IR is different to tasks like speech recognition: word order and sentence structure are not very necessary to modeling the topical content of documents.

For retrieval based on a probabilistic language model, we treat the generation of queries as a random process. The approach is to

1. Infer a language model for each document.
2. Estimate the probability of generating the query according to each of these models.
3. Rank the documents according to these probabilities.

The intuition is that the user has a prototype document in mind, and generates a query based on words that appear in this document. Often, users have a reasonable idea of terms that are likely to occur in documents of interest and they will choose query terms that distinguish these documents from others in the collection. Collection statistics are an integral part of the language model, rather than being used heuristically as in many other approaches.

12.1.2 Estimating the query generation probability

In this section we describe how to estimate $P(q|M_d)$. The probability of producing the query given the language model M_d of document d using maximum likelihood estimation (MLE) and given the unigram assumption is:

$$\hat{P}(q|M_d) = \prod_{t \in q} \hat{P}_{\text{mle}}(t|M_d) = \prod_{t \in q} \frac{\text{tf}_{t,d}}{dl_d} \tag{12.4}$$

where M_d is the language model of document d, $\text{tf}_{t,d}$ is the (raw) term frequency of term t in document d, and dl_d is the number of tokens in document d.

The classic problem with such models is one of estimation (the $\hat{}$ is used above to stress that the model is estimated). In particular, some words will

not have appeared in the document at all, but are possible words for the information need, which the user may have used in the query. If we estimate $\hat{P}(t|M_d) = 0$ for a term missing from a document d, then we get a strict conjunctive semantics: documents will only give a query non-zero probability if all of the query terms appear in the document. This may or may not be undesirable: it is partly a human-computer interface issue: vector space systems have generally preferred more lenient matching, though recent web search developments have tended more in the direction of doing searches with such conjunctive semantics. But regardless of one's approach here, there is a more general problem of estimation: occurring words are also badly estimated; in particular, the probability of words occurring once in the document is normally overestimated, since there one occurrence was partly by chance.

This problem of insufficient data and a zero probability preventing any non-zero match score for a document can spell disaster. We need to smooth probabilities: to discount non-zero probabilities and to give some probability mass to unseen things. There's a wide space of approaches to smoothing probability distributions to deal with this problem, such as adding a number (1, 1/2, or a small ϵ) to counts and renormalizing, discounting, Dirichlet priors and interpolation methods. A simple idea that works well in practice is to use a mixture between the document multinomial and the collection multinomial distribution.

The general approach is that a non-occurring term is possible in a query, but no more likely than would be expected by chance from the whole collection. That is, if $\text{tf}_{t,d} = 0$ then

$$\hat{P}(t|M_d) \leq cf_t/T$$

where cf_t is the raw count of the term in the collection, and T is the raw size (number of tokens) of the entire collection. We can guarantee this by mixing together a document-specific model with a whole collection model:

$$\hat{P}(w|d) = \lambda \hat{P}_{\text{mle}}(w|M_d) + (1-\lambda)\hat{P}_{\text{mle}}(w|M_c) \tag{12.5}$$

where $0 < \lambda < 1$ and M_c is a language model built from the entire document collection. This mixes the probability from the document with the general collection frequency of the word. Correctly setting λ is important to the good performance of this model. A high value of lambda makes the search "conjunctive-like" – suitable for short queries. A low value is more suitable for long queries. One can tune λ to optimize performance, including not having it be constant but a function of document size.

So, the retrieval ranking for a query q under the basic LM for IR is given by:

$$P(d|q) \propto P(d) \prod_{t \in q} ((1-\lambda)P(t|M_c) + \lambda P(t|M_d)) \tag{12.6}$$

The equation captures the probability that the document that the user had in mind was in fact this one.

✎ **Example 12.1:** Suppose the document collection contains two documents:

- d_1: Xyz reports a profit but revenue is down
- d_2: Qrs narrows quarter loss but revenue decreases further

The model will be MLE unigram models from the documents and collection, mixed with $\lambda = 1/2$.

Suppose the query is *revenue down*. Then:

(12.7)
$$\begin{aligned} P(q|d_1) &= [(1/8 + 2/16)/2] \times [(1/8 + 1/16)/2] \\ &= 1/8 \times 3/32 = 3/256 \\ P(q|d_2) &= [(1/8 + 2/16)/2] \times [(0/8 + 1/16)/2] \\ &= 1/8 \times 1/32 = 1/256 \end{aligned}$$

So, the ranking is $d_1 > d_2$.

12.2 Ponte and Croft's Experiments

Ponte and Croft (1998) present the first experiments on the language modeling approach to information retrieval. Their basic approach where each document defines a language model is the model that we have presented until now. However, we have presented an approach where the language model is a mixture of two multinomials, much as in Miller et al. (1999), Hiemstra (2000) rather than Ponte and Croft's multivariate Bernoulli model. The use of multinomials has been standard in most subsequent work in the LM approach and evidence from text categorization (see Chapter 13) suggests that it is superior. Ponte and Croft argued strongly for the effectiveness of the term weights that come from the language modeling approach over traditional tf-idf weights. We present a subset of their results in Figure 12.4 where they compare tf-idf to language modeling by evaluating TREC topics 202–250 evaluated on TREC disks 2 and 3. The queries are sentence length natural language queries. The language modeling approach yields significantly better results than their baseline tf-idf based term weighting approach. And indeed the gains shown here have been extended in subsequent work.

12.3 Language modeling versus other approaches in IR

The language modeling approach provides a novel way of looking at the problem of text retrieval, which links it with a lot of recent work in speech and language processing. As Ponte and Croft (1998) emphasize, the language modeling approach to IR provides a different form of scoring matches

	Precision			
Rec.	tf-idf	LM	%chg	
0.0	0.7439	0.7590	+2.0	
0.1	0.4521	0.4910	+8.6	
0.2	0.3514	0.4045	+15.1	*
0.3	0.2761	0.3342	+21.0	*
0.4	0.2093	0.2572	+22.9	*
0.5	0.1558	0.2061	+32.3	*
0.6	0.1024	0.1405	+37.1	*
0.7	0.0451	0.0760	+68.7	*
0.8	0.0160	0.0432	+169.6	*
0.9	0.0033	0.0063	+89.3	
1.0	0.0028	0.0050	+76.9	
Ave	0.1868	0.2233	+19.55	*

► **Figure 12.4** Results of a comparison of tf-idf to language modeling (LM) term weighting by Ponte and Croft (1998). The version of tf-idf from the INQUERY IR system includes length normalization of tf. The table gives an evaluation according to 11-point average precision with significance marked with a * according to Wilcoxon signed rank test. While the language modeling approach always does better in these experiments, note that where the approach shows significant gains is at higher levels of recall.

between queries and documents, and the hope is that the probabilistic language modeling foundation improves the weights that are used, and hence the performance of the model. The major issue is estimation of the document model, such as choices of how to smooth it effectively. It has achieved very good retrieval results. Compared to other probabilistic approaches, such as BIM from Chapter 11, the main difference is that the LM approach attempts to do away with explicitly modeling relevance (whereas this is the central variable evaluated in the BIM approach). The LM approach assumes that documents and expressions of information problems are objects of the same type, and assesses their match by importing the tools and methods of language modeling from speech and natural language processing. The resulting model is mathematically precise, conceptually simple, computationally tractable, and intuitively appealing.

On the other hand, like all IR models, one can also raise objections to the model. The assumption of equivalence between document and information problem representation is unrealistic. Current LM approaches use very simple models of language, usually unigram models. Without an explicit notion of relevance, relevance feedback is difficult to integrate into the model, as are user preferences or priors over document relevance. It also isn't easy to

see how to accommodate notions of phrasal matching or passage matching or Boolean retrieval operators. Subsequent work in the LM approach has looked at addressing some of these concerns, including putting relevance back into the model and allowing a language mismatch between the query language and the document language.

The model has some relation to traditional tf-idf models. Term frequency is directly in tf-idf models, and much recent work has recognized the importance of document length normalization. The effect of doing a mixture of document generation probability with collection generation probability is a little like idf: terms rare in the general collection but common in some documents will have a greater influence on the ranking of documents. In most concrete realizations, the models share treating terms as if they were independent. On the other hand, the intuitions are probabilistic rather than geometric, the mathematical models are more principled rather than heuristic, and the details of how statistics like term frequency and document length are used differ. If one is concerned mainly with performance numbers, while the LM approach has been proven quite effective in retrieval experiments, there is little evidence that its performance exceeds a well-tuned traditional ranked retrieval system.

12.4 Extended language modeling approaches

In this section we briefly note some of the work that has taken place that extends the basic language modeling approach.

There are other ways that one could think of using the language modeling idea in IR settings, and many of them have been tried in subsequent work. Rather than looking at the probability of a document language model generating the query, you can look at the probability of a query language model generating the document. The main reason that doing things in this direction is less appealing is that there is much less text available to estimate a query language model, and so the model will be worse estimated, and will have to depend more on being smoothed with some other language model. On the other hand, it is easy to see how to incorporate relevance feedback into such a model: one can expand the query with terms taken from relevant documents in the usual way and hence update the query language model (Zhai and Lafferty 2001a). Indeed, with appropriate modeling choices, this approach leads to the BIR model of Chapter 11.

Rather than directly generating in either direction, one can make a language model from both the document and query, and then ask how different these two language models are from each other. Lafferty and Zhai (2001) lay out these three ways of thinking about things, which we show in Figure 12.5 and develop a general risk minimization approach for document retrieval.

► **Figure 12.5** Three ways of developing the language modeling approach: query likelihood, document likelihood and model comparison.

KULLBACK-LEIBLER DIVERGENCE

For instance, one way to model the risk of returning a document d as relevant to a query q is to use the *Kullback-Leibler divergence* between their respective language models:

$$R(d;q) = KL(d\|q) = \sum_w P(w|M_q) \log \frac{P(w|M_q)}{P(w|M_d)}$$

This asymmetric divergence measure coming from information theory shows how bad the probability distribution M_q is at modeling M_d. Lafferty and Zhai (2001) present results suggesting that a model comparison approach outperforms both query-likelihood and document-likelihood approaches.

Basic LMs do not address issues of alternate expression, that is, synonymy, or any deviation in use of language between queries and documents. Berger and Lafferty (1999) introduce translation models to bridge this query-document gap. A translation model lets you generate query words not in a document by translation to alternate terms with similar meaning. This also provides a basis for performing cross-lingual IR. Assuming a probabilistic dictionary D which gives information on synonymy or translation pairs, the nature of the translation query generation model is:

$$P(q|M_d) = \prod_{w \in q} \sum_{v \in D} P(v|M_d) T(w|v)$$

The left term on the right hand side is the basic document language model, and the right term performs translation. This model is clearly more computationally intensive and one needs to build a translation model, usually using

separate resources (such as a traditional bilingual dictionary or a statistical machine translation system's translation dictionary).

12.5 References and further reading

For more details on the basic concepts and smoothing methods for probabilistic language models, see either Manning and Schütze (1999, Ch. 6) or Jurafsky and Martin (2000, Ch. 6).

The important initial papers that originated the language modeling approach to IR are: (Ponte and Croft 1998, Hiemstra 1998, Berger and Lafferty 1999, Miller et al. 1999). Other relevant papers can be found in the next several years of SIGIR proceedings. Croft and Lafferty (2003) contains a collection of papers from a workshop on language modeling approaches and Hiemstra and Kraaij (2005) reviews one prominent thread of work on using language modeling approaches for TREC tasks. System implementers should consult Zhai and Lafferty (2001b), Zaragoza et al. (2003) for detailed empirical comparisons of different smoothing methods for language models in IR. Additionally, recent work has achieved some gains by going beyond the unigram model, providing the higher order models are smoothed with lower order models Gao et al. (2004), Cao et al. (2005). For a critical viewpoint on the rationale for the language modeling approach, see Spärck Jones (2004).

13 *Text classification and Naive Bayes*

Thus far, this book has mainly discussed the process of *ad hoc retrieval* where a user has a transient information need, which they try to address by posing one or more queries to a search engine. However, many users have ongoing information needs. For example, because of my job in the computer industry, I might need to track developments in *multicore computer chips*. One way of doing this is for me to issue the query multicore AND computer AND chip against an index of recent newswire articles each morning. In this and the following two chapters we examine the question: how can this repetitive task be automated? To this end, many systems support *standing queries*. A standing query is like any other query except that it is periodically executed on a collection to which new documents are incrementally added over time.

STANDING QUERY

If my standing query is just multicore AND computer AND chip, I will tend to miss many relevant new articles which use other terms such as *multicore processors*. To achieve good recall, standing queries thus have to be refined over time and can gradually become quite complex. In this example, using a Boolean search engine with stemming, I might end up with a query like (multicore OR multi-core) AND (chip OR processor OR microprocessor).

To capture the generality and scope of the problem space to which standing queries belong, we now introduce the general notion of a *classification* problem. Given a set of *classes*, we seek to determine which class(es) a given document belongs to. In the example, the standing query serves to divide new newswire articles into the two classes: *documents about multicore computer chips* and *documents* not *about multicore computer chips*. We refer to this as *two-class classification*. Classification using standing queries is also called *routing* or *filtering*.

CLASSIFICATION

ROUTING
FILTERING

A class need not be as narrowly focused as the standing query *multicore computer chips*. Often, a class is a more general subject area like *China* or *coffee*. Such more general classes are usually referred to as *topics*, and the classification task is then called *text classification*, *text categorization*, *topic classification* or *topic spotting*. An example for *China* appears in Figure 13.1. Standing queries and topics differ in their degree of specificity, but the methods for solving

TEXT CLASSIFICATION

routing, filtering and text classification are essentially the same. We therefore include routing and filtering under the rubric of text classification in this and the following chapters.

The notion of classification is very general and has many applications within and beyond information retrieval. For instance in computer vision, a classifier may be used to divide images into three classes: landscape, portrait and neither. We focus here on examples from information retrieval such as:

- Several of the preprocessing steps necessary for indexing as discussed in Chapter 2: detecting a document's encoding (ASCII, Unicode UTF-8 etc; page 19); word segmentation (Is the gap between two letters a word boundary or not? page 25); truecasing (page 30); and identifying the language of a document (page 42)
- The automatic detection of spam pages (which then are not included in the search engine index)
- The automatic detection of sexually explicit content (which is included in search results only if the user turns an option such as SafeSearch off)
- VERTICAL SEARCH ENGINE Topic-specific or *vertical* search. *Vertical search engines* restrict searches to a particular topic. For example, the query computer science on a vertical search engine for the topic *China* will return a list of Chinese computer science departments with higher precision and recall than the query computer science China on a general purpose search engine. This is because the vertical search engine does not include web pages in its index that contain the word china in a different sense (e.g., referring to a hard white ceramic), but does include relevant pages even if they don't explicitly mention the term China.

While the classification task we will use as an example in this book is text classification, this list shows the general importance of classification in information retrieval. Most retrieval systems today contain multiple components that use some form of classifier.

A computer is not essential for classification. Many classification tasks have traditionally been solved manually. Books in a library are assigned library of congress categories by a librarian. But manual classification is expensive to scale. The *multicore computer chips* example illustrates one alternative approach: classification by the use of standing queries – which can be thought of as *rules* – most commonly written by hand. As in our example (multicore OR multi-core) AND (chip OR processor OR microprocessor), rules are sometimes equivalent to Boolean expressions.

RULES

A rule captures a certain combination of keywords that indicates a class. Hand-coded rules have good scaling properties, but creating and maintaining them over time is labor-intensive. A technically skilled person (e.g., a

domain expert who is good at writing regular expressions) can create rule sets that will rival or exceed the accuracy of the automatically generated classifiers we will discuss shortly. But it can be hard to find someone with this specialized skill.

Apart from manual classification and hand-crafted rules, there is a third approach to text classification, machine learning-based text classification. It is the approach that we focus on in this book. In machine learning, the set of rules or, more generally, the decision criterion of the text classifier is learned automatically from training data. This approach is also called *statistical text classification* if the learning method is statistical. In statistical text classification, we require a number of good example documents (or training documents) for each class. The need for manual classification is not eliminated since the training documents come from a person who has labeled them – *labeling* refers to the process of annotating each document with its class. But labeling is arguably an easier task than writing rules. Almost anybody can look at a document and decide whether or not it is about the geographic region China. Sometimes such labeling is already implicitly part of an existing workflow. For instance, I may go through the news articles returned by a standing query each morning and put the relevant ones in a special folder.

STATISTICAL TEXT CLASSIFICATION

LABELING

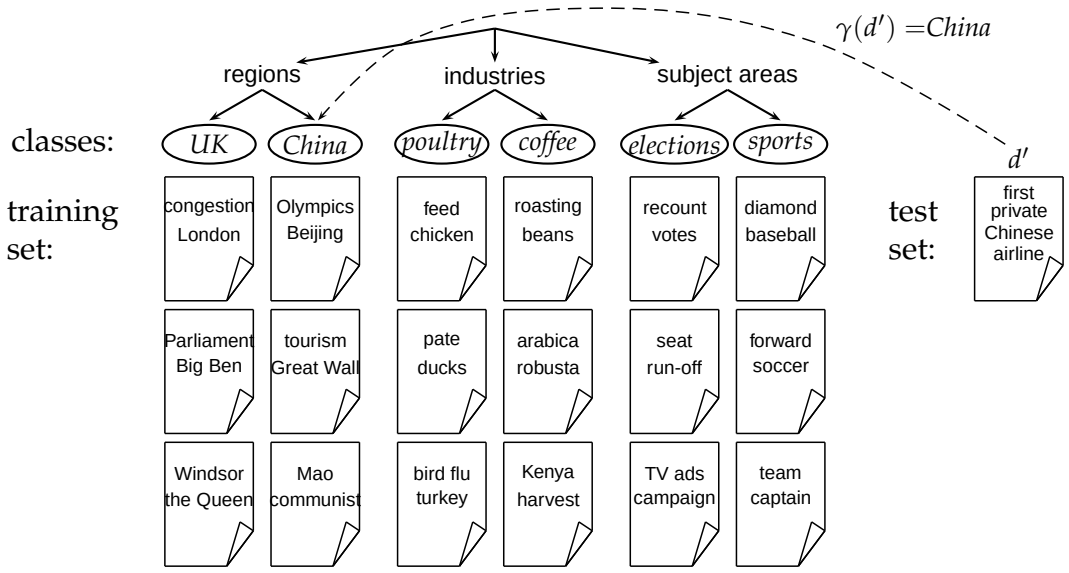
We begin this chapter with a general introduction to the text classification problem including a formal definition (Section 13.1); we then cover Naive Bayes, a particularly simple and effective classification method (Sections 13.2–13.4). All of the classification algorithms we study view documents as vectors in high-dimensional spaces. To improve the efficiency of these algorithms, it is generally desirable to reduce the dimensionality of these spaces; to this end, a technique known as *feature selection* is commonly applied in text classification as discussed in Section 13.5. Section 13.6 covers evaluation of text classification. In the following chapters, Chapters 14 and 15, we look at two other families of classification methods, vector space classifiers and support vector machines.

13.1 The text classification problem

In text classification, we are given a description $d \in \mathbb{X}$ of a document, where $\mathbb{X}$ is the *document space*; and a fixed set of *classes* $\mathbb{C} = \{c_1, c_2, \ldots, c_J\}$. Classes are also called *categories* or *labels*. Typically, the document space is some type of high-dimensional space, and the classes are human-defined for the needs of an application, as in the examples *China* and *documents that talk about multicore computer chips* above. We are given a *training set D* of labeled documents

DOCUMENT SPACE
CLASS
CATEGORY
LABEL

TRAINING SET



► **Figure 13.1** Classes, training set and test set in text classification.

$\langle d, c\rangle$,[1] where $\langle d, c\rangle \in \mathbb{X} \times \mathbb{C}$. For example:

$$\langle d, c\rangle = \langle \text{Beijing joins the World Trade Organization}, \textit{China}\rangle$$

for the one-sentence document *Beijing joins the World Trade Organization* and the class *China*.

LEARNING METHOD
CLASSIFIER

Using a *learning method* or *learning algorithm*, we then wish to learn a *classifier* or *classification function* γ that maps documents to classes:

$$\gamma : \mathbb{X} \to \mathbb{C} \tag{13.1}$$

SUPERVISED LEARNING

This type of learning is called *supervised learning* since a "supervisor" (the human who defines the classes and labels training documents) serves as a teacher directing the learning process. We denote the supervised learning method by Γ and write $\Gamma(D) = \gamma$. The learning method Γ takes the labeled training set D as input and returns the learned classification function γ.

Unfortunately, most names for learning methods Γ are also used for classifiers γ. We talk about the Naive Bayes *learning method* Γ when we say that

1. Note that D denotes a *labeled* set of documents in the text classification chapters. Document sets D in the other chapters are not labeled.

"Naive Bayes is robust", meaning that it can be applied to many different learning problems and is unlikely to produce classifiers that fail catastrophically. But when we say that "Naive Bayes had an error rate of 20%", we are describing an experiment in which a particular Naive Bayes *classifier* γ (which was produced by the Naive Bayes learning method) had a 20% error rate in an application.

Figure 13.1 shows an example of text classification from the Reuters-RCV1 collection, introduced in Section 4.2, page 63. There are six classes (*UK*, *China*, ..., *sports*), each with three training documents. We show a few mnemonic words for each document's content. The training set provides some typical examples for each class, so that we can learn the classification function γ.

TEST SET

Once we have learned γ, we can apply it to the *test set* (or *test data*), for example the new document *first private Chinese airline* whose class is unknown. In Figure 13.1, the classification function assigns the new document to class $\gamma(d) = \textit{China}$, which is the correct assignment.

The classes in text classification often have some interesting structure such as the hierarchy in Figure 13.1. There are two instances each of region categories, industry categories and subject area categories. A hierarchy can be an important aid in solving a classification problem. See Section 13.7 for references on *hierarchical classification*. We will make the simplifying assumption in the three classification chapters (Chapter 13 – 15) that the classes form a set with no subset relationships between them.

HIERARCHICAL CLASSIFICATION

Definition (13.1) stipulates that a document is member of exactly one class. This is not the most appropriate model for the hierarchy in Figure 13.1. For instance, a document about the 2008 Olympics should be a member of two classes: the *China* class and the *sports* class. This type of classification problem is referred to as an *any-of* problem and we will return to it in Section 14.4 (page 283). For the time being, we only consider *one-of* problems where a document is a member of exactly one class.

Our goal in text classification is high accuracy on test data or *new data* – for example, the newswire articles that we will encounter tomorrow morning in the multicore chip example. It is easy to achieve high accuracy on the training set (e.g., we can simply memorize the labels). But high accuracy on the training set in general does not mean that the classifier will work well on new data in an application.

When we use the training set to learn a classifier for test data, we make the assumption that training data and test data are similar or from *the same distribution*. We defer a precise definition of this notion to Section 14.5 (page 286).

13.2 Naive Bayes text classification

MULTINOMIAL NAIVE BAYES

The first supervised learning method is the *multinomial Naive Bayes* model, a

probabilistic learning method. The probability of a document d being in class c is computed as

$$P(c|d) \propto P(c) \prod_{1 \leq k \leq n_d} P(w_k|c) \tag{13.2}$$

where $P(w_k|c)$ is the conditional probability of word[2] w_k occurring in a document of class c, $P(c)$ is the prior probability of class c, and $\langle w_1, w_2, \ldots, w_{n_d} \rangle$ are the tokens in d that are part of the vocabulary we use for classification. For example, $\langle w_1, w_2, \ldots, w_{n_d} \rangle$ for the one-sentence document *Beijing and Taipei join the WTO* might be $\langle$Beijing, Taipei, join, WTO$\rangle$, with $n_d = 4$, if and is treated as a stop word.

MAXIMUM A-POSTERIORI

In text classification, our goal is to find the "best" class for the document. The best class in NB classification is the most likely or *maximum a-posteriori* (MAP) class c_{map}:

$$c_{\text{map}} = \arg\max_{c_j \in \mathbb{C}} P(c_j|d) = \arg\max_{c_j \in \mathbb{C}} \hat{P}(c_j) \prod_{1 \leq k \leq n_d} \hat{P}(w_k|c_j) \tag{13.3}$$

We write $\hat{P}$ for P since we do not know the true values of the parameters $P(c_j)$ and $P(w_k|c_j)$, but estimate them from the training set as we will see in a moment.

In Equation (13.3), many conditional probabilities are multiplied, one for each position $1 \leq k \leq n_d$. This can result in a floating point underflow. It is therefore better to perform the computation by adding logarithms of probabilities instead of multiplying probabilities. The class with the highest log probability score is still the most probable since $\log(xy) = \log(x) + \log(y)$ and the logarithm function is monotonic. Hence, the maximization that is actually done in most implementations of Naive Bayes is:

$$c_{\text{map}} = \arg\max_{c_j \in \mathbb{C}} [\log \hat{P}(c_j) + \sum_{1 \leq k \leq n_d} \log \hat{P}(w_k|c_j)] \tag{13.4}$$

Equation (13.4) has a simple interpretation. Each conditional parameter $\log \hat{P}(w_k|c_j)$ is a weight that indicates how good an indicator w_k is for c_j. Similarly, the prior $\log \hat{P}(c_j)$ is a weight that indicates the relative frequency of c_j. More frequent classes are more likely to be the correct class than infrequent classes. Equation (13.4) selects the class with the largest sum of log prior and word weights.

2. It would be more accurate to talk about terms, not words since text classification systems often preprocess text using the same term normalization procedures as indexers (such as downcasing and stemming). We follow convention in Chapters 13–15 and use the terms word and term interchangeably.

We will initially work this intuitive interpretation of the multinomial NB model and defer a derivation to Section 13.4. The model is formally identical to the multinomial unigram language model (Section 12.1.1, page 228).

How do we estimate the parameters $\hat{P}(c_j)$ and $\hat{P}(w_k|c_j)$? We first try the maximum likelihood estimate (MLE), which is simply the relative frequency and corresponds to the most likely value of each parameter given the training data. For the priors this estimate is:

$$\hat{P}(c_j) = \frac{N_j}{N} \tag{13.5}$$

where N_j is the number of documents in class c_j and N is the total number of documents.

We estimate the conditional probability $\hat{P}(w_k|c_j)$ as the relative frequency of w_k in c_j documents:

$$\hat{P}(w_k|c_j) = \frac{T_{jk}}{\sum_k T_{jk}}$$

where T_{jk} is the number of occurrences (or tokens) of w_k in training documents from class c_j, including multiple occurrences of a term in a document.

The problem with the MLE estimate is that it is zero for a word-class combination that did not occur in the training data. If occurrences of the word WTO in the training data only occurred in *China* documents, then the MLE estimates for the other classes, for example *UK*, will be zero:

$$\hat{P}(\text{WTO}|UK) = 0$$

Now the one-sentence document *Britain is a member of the WTO* will get a conditional probability of zero for *UK* since we're multiplying the conditional probabilities for all words in Equation (13.2). (Or, equivalently, it will get a value of negative infinity in Equation (13.4).) Clearly, the model should assign a high probability to the *UK* class since the word Britain occurs. The problem is that the zero probability for WTO cannot be "conditioned away," no matter how strong the evidence for the class *UK* from other features. The estimate is 0 because of *sparseness*: The training data is never large enough to represent the frequency of rare events adequately, for example, the probability that WTO occurs in *UK* documents.

SPARSENESS

ADD-ONE SMOOTHING
LAPLACE SMOOTHING

To eliminate zeros, we use *add-one* or *Laplace* smoothing, which simply adds one to each count:

$$\hat{P}(w_k|c_j) = \frac{T_{jk}+1}{\sum_k(T_{jk}+1)} = \frac{T_{jk}+1}{(\sum_k T_{jk})+B} \tag{13.6}$$

where $B = |V|$ is the number of distinct terms w_k in the vocabulary. Laplace smoothing can be interpreted as a uniform prior (each word occurs once for

TRAINMULTINOMIALNBCLASSIFIER($\mathbb{C}, D$)
1 $V \leftarrow$ EXTRACTVOCABULARY(D)
2 $N \leftarrow$ COUNTDOCS(D)
3 **for** each class $c_j \in \mathbb{C}$
4 **do** $N_j \leftarrow$ COUNTDOCSINCLASS(D, c_j)
5 $prior[c_j] \leftarrow N_j/N$
6 $text_j \leftarrow$ CONCATENATETEXTOFALLDOCSINCLASS(D, c_j)
7 **for** each word $w_i \in V$
8 **do** $T_{ji} \leftarrow$ COUNTTOKENSOFWORD($text_j, w_i$)
9 **for** each word $w_i \in V$
10 **do** $condprob[w_i][c_j] \leftarrow \frac{T_{ji}+1}{\sum_i (T_{ji}+1)}$
11 **return** $V, prior, condprob$

APPLYMULTINOMIALNBCLASSIFIER($\mathbb{C}, V, prior, condprob, d$)
1 $W \leftarrow$ EXTRACTTOKENSFROMDOC(V, d)
2 **for** each class $c_j \in \mathbb{C}$
3 **do** $score[c_j] \leftarrow \log prior[c_j]$
4 **for** each word $w_k \in W$
5 **do** $score[c_j] += \log condprob[w_k][c_j]$
6 **return** $\arg\max_c score[c]$

► **Figure 13.2** Naive Bayes algorithm (multinomial model): Training and testing.

	docID	words in document	in c = *China*?
training set	1	Chinese Beijing Chinese	yes
	2	Chinese Chinese Shanghai	yes
	3	Chinese Macao	yes
	4	Tokyo Japan Chinese	no
test set	5	Japan Chinese Chinese Chinese Tokyo	?

► **Table 13.1** Data for parameter estimation examples.

each class) that is then updated as evidence from the training data comes in. Note that this is a prior probability for the occurrence of a *word* as opposed to the prior probability of a *class* which we estimate in Equation (13.5) on the document level.

We have now introduced all the elements we need for training and applying an NB classifier. The complete algorithm is described in Figure 13.2.

mode	time complexity
training	$\Theta(\|D\|L_{\text{ave}} + \|\mathbb{C}\||V|)$
testing	$\Theta(\|\mathbb{C}\|L_{\text{ave}})$

► **Table 13.2** Training and test times for Naive Bayes. L_{ave} is the average number of tokens in a document. M_{ave} is the average number of distinct terms in the document.

✎ **Example 13.1:** For the example in Table 13.1, the multinomial parameters we need to classify the test document are the priors $\hat{P}(c) = 3/4$ and $\hat{P}(\overline{c}) = 1/4$ and the conditional probabilities are:

$$\begin{aligned}
\hat{P}(\textsf{Chinese}|c) &= (5+1)/(8+6) = 6/14 = 3/7 \\
\hat{P}(\textsf{Tokyo}|c) = \hat{P}(\textsf{Japan}|c) &= (0+1)/(8+6) = 1/14 \\
\hat{P}(\textsf{Chinese}|\overline{c}) &= (1+1)/(3+6) = 2/9 \\
\hat{P}(\textsf{Tokyo}|\overline{c}) = \hat{P}(\textsf{Japan}|\overline{c}) &= (1+1)/(3+6) = 2/9
\end{aligned}$$

The denominators are $(8+6)$ and $(3+6)$ because the lengths of $text_c$ and $text_{\overline{c}}$ are 8 and 3, respectively, and because the constant B in Equation (13.6) is 6 as the vocabulary consists of six words. We then get:

$$\begin{aligned}
\hat{P}(c|d) &\propto 3/4 \cdot (3/7)^3 \cdot 1/14 \cdot 1/14 \approx 0.0003 \\
\hat{P}(\overline{c}|d) &\propto 1/4 \cdot (2/9)^3 \cdot 2/9 \cdot 2/9 \approx 0.0001
\end{aligned}$$

Thus, the classifier assigns the test document to c = *China*. The reason for this classification decision is that the three occurrences of the positive indicator Chinese in d_5 outweigh the occurrences of the two negative indicators Japan and Tokyo.

What is the time complexity of Naive Bayes? The complexity of computing the parameters is $\Theta(|\mathbb{C}||V|)$ since the set of parameters consists of $|\mathbb{C}||V|$ conditional probabilities and $|\mathbb{C}|$ priors. The preprocessing necessary for computing the parameters (extracting the vocabulary, counting words etc.) can be done in one pass through the training data. The time complexity of this component is therefore $\Theta(|D|L_{\text{ave}})$ where $|D|$ is the number of documents and L_{ave} is the average length of a document. The time complexity of classifying a document is $\Theta(|\mathbb{C}|L_{\text{ave}})$ as can be observed from Figure 13.2.

Table 13.2 summarizes the time complexities. In general, we have $|\mathbb{C}||V| < |D|L_{\text{ave}}$, so both training and testing complexity is linear in the time it takes to scan the data. Since we have to look at the data at least once, Naive Bayes can be said to have optimal time complexity. Its efficiency is one reason why Naive Bayes is a popular text classification method.

13.2.1 Relation to multinomial unigram language model

Equation (13.2) is equivalent to Equation (12.6) from page 229, which we repeat here for $\lambda = 1$:

$$P(q|d) \propto P(d) \prod_{t \in q} P(t|M_d) \tag{13.7}$$

The document d in text classification (Equation (13.2)) takes the role of the query in language modeling (Equation (13.7)) and the classes c in text classification take the role of the documents d in language modeling. We used Equation (13.7) to rank documents according to the probablity that they would generate the query q. In NB classification, we are usually only interested in the top-ranked class.

We also used MLE estimates in Section 12.1.2 (page 229) and encountered the problem of zero estimates due to sparse data (page 229); but instead of add-one smoothing, we used a mixture of two distributions to address the problem there. Add-one smoothing is closely related to add-$\frac{1}{2}$ smoothing in Section 11.3.4 (page 216).

13.3 The Bernoulli model

MULTINOMIAL MODEL

There are two different ways we can set up an NB classifier. The model we have worked with so far is the *multinomial model*. It generates one word from the vocabulary in each position of the document, where we assume that documents are produced by a generative model that, for a particular set of values for its parameters, defines a random generation process as discussed on page 225. In Section 13.4, we will describe in more detail the generative models that Naive Bayes classification is based on.

BERNOULLI MODEL

An alternative to the Bernoulli model is the *multivariate binomial model* or *multivariate Bernoulli model* – or simply: *Bernoulli model*. It is equivalent to the BIM of Section 11.3 (page 210), which generates an indicator for each word of the vocabulary, either 0 indicating absence or 1 indicating presence of the word in the document. Figure 13.3 presents training and testing algorithms for the Bernoulli model. The Bernoulli model has the same time complexity as the multinomial model.

The different generation models imply different estimation strategies for the parameters. The Bernoulli model estimates $\hat{P}(w|c_j)$ as the *fraction of documents* of class c_j that contain word w (Figure 13.3, TRAINBERNOULLINB-CLASSIFIER, line 8). In contrast, the multinomial model estimates $\hat{P}(w|c_j)$ as the *fraction of tokens* or *fraction of positions* in documents of class c_j that contain word w (Equation (13.6)). When classifying a test document, the Bernoulli model uses binary occurrence information, ignoring the number of occurrences, whereas the multinomial model keeps track of multiple occurrences.

```
TRAINBERNOULLINBCLASSIFIER(ℂ, D)
1  V ← EXTRACTVOCABULARY(D)
2  N ← COUNTDOCS(D)
3  for each class c ∈ ℂ
4  do N_c ← COUNTDOCSINCLASS(D, c)
5     prior[c] ← N_c / N
6     for each word w ∈ V
7     do N_cw ← COUNTDOCSINCLASSCONTAININGWORD(D, c, w)
8        condprob[w][c] ← (N_cw + 1) / (N_c + 2)
9  return V, prior, condprob

APPLYBERNOULLINBCLASSIFIER(ℂ, V, prior, condprob, d)
1  V_d ← EXTRACTWORDTYPESFROMDOC(V, d)
2  for each class c ∈ ℂ
3  do score[c] ← log prior[c]
4     for each word w ∈ V
5     do if w ∈ V_d
6           then score[c] += log condprob[w][c]
7           else score[c] += log(1 − condprob[w][c])
8  return arg max_c score[c]
```

► **Figure 13.3** Naive Bayes algorithm (Bernoulli model): Training and testing. The add-one smoothing in line 8 (top) is in analogy to Equation (13.6).

As a result, the Bernoulli model typically makes many mistakes when classifying long documents. For example, it may assign an entire book to the class *China* because of a single occurrence of the word China.

The models also differ in how non-occurring words are used in classification. They do not affect the classification decision in the multinomial model; but in the binomial model the probability of non-occurrence is factored in when computing $P(c|d)$ (Figure 13.3, APPLYBERNOULLINBCLASSIFIER, line 7).

✎ **Example 13.2:** Applying the Bernoulli model to the example in Table 13.1, we have the same estimates for the priors as before: $\hat{P}(c) = 3/4$, $\hat{P}(\overline{c}) = 1/4$. The conditional probabilities are:

$$\begin{aligned}
\hat{P}(\text{Chinese}|c) &= (3+1)/(3+2) = 4/5 \\
\hat{P}(\text{Japan}|c) = \hat{P}(\text{Tokyo}|c) &= (0+1)/(3+2) = 1/5 \\
\hat{P}(\text{Beijing}|c) = \hat{P}(\text{Macao}|c) = \hat{P}(\text{Shanghai}|c) &= (1+1)/(3+2) = 2/5
\end{aligned}$$

$$\begin{aligned}
\hat{P}(\textsf{Chinese}|\overline{c}) &= (1+1)/(1+2) = 2/3 \\
\hat{P}(\textsf{Japan}|\overline{c}) = \hat{P}(\textsf{Tokyo}|\overline{c}) &= (1+1)/(1+2) = 2/3 \\
\hat{P}(\textsf{Beijing}|\overline{c}) = \hat{P}(\textsf{Macao}|\overline{c}) = \hat{P}(\textsf{Shanghai}|\overline{c}) &= (0+1)/(1+2) = 1/3
\end{aligned}$$

The denominators are $(3+2)$ and $(1+2)$ because there are 3 documents in c and 1 document in $\overline{c}$ and because the constant B in Equation (13.6) is 2 – there are two cases to consider for each word, occurrence and non-occurrence.

The scores of the test document for the two classes are

$$\begin{aligned}
\hat{P}(c|d) &\propto \hat{P}(c) \cdot \hat{P}(\textsf{Chinese}|c) \cdot \hat{P}(\textsf{Japan}|c) \cdot \hat{P}(\textsf{Tokyo}|c) \\
&\quad \cdot (1-\hat{P}(\textsf{Beijing}|c)) \cdot (1-\hat{P}(\textsf{Shanghai}|c)) \cdot (1-\hat{P}(\textsf{Macao}|c)) \\
&= 3/4 \cdot 4/5 \cdot 1/5 \cdot 1/5 \cdot (1-2/5) \cdot (1-2/5) \cdot (1-2/5) \\
&\approx 0.005
\end{aligned}$$

and, analogously,

$$\begin{aligned}
\hat{P}(\overline{c}|d) &\propto 1/4 \cdot 2/3 \cdot 2/3 \cdot 2/3 \cdot (1-1/3) \cdot (1-1/3) \cdot (1-1/3) \\
&\approx 0.022
\end{aligned}$$

Thus, the classifier assigns the test document to $\overline{c} =$ *not-China*. When looking only at binary occurrence and not at term frequency, Japan and Tokyo are indicators for $\overline{c}$ $(2/3 > 1/5)$ whereas the conditional probabilities of Chinese are not different enough $(4/5$ vs. $2/3)$ to affect the classification decision.

13.4 Properties of Naive Bayes

To gain a better understanding of the two models and the assumptions they make, let us go back and examine how we derived their classification rules in Chapters 11 and 12. We decide class membership of a document by assigning it to the class with the *maximum a-posteriori* or *MAP* probability (cf. (Section 11.3.2, page 214)), which we compute as follows:

MAXIMUM A-POSTERIORI MAP

$$\begin{aligned}
c_{\text{map}} &= \arg\max_{c_j \in \mathbb{C}} P(c_j|d) \\
&= \arg\max_{c_j \in \mathbb{C}} \frac{P(d|c_j)P(c_j)}{P(d)} \qquad (13.8) \\
&= \arg\max_{c_j \in \mathbb{C}} P(d|c_j)P(c_j) \qquad (13.9)
\end{aligned}$$

where Bayes' Rule (Equation (11.4), page 208) is applied in 13.8 and we drop the denominator in the last step since $P(d)$ is the same for all classes and does not affect the argmax.

We can interpret Equation (13.9) as a description of the generative process we assume in Bayesian text classification. To generate a document, we first

choose class c_j with probability $P(c_j)$ (top nodes in Figures 13.4 and 13.5). The two models differ in the formalization of the second step, the generation of the document given the class, corresponding to the conditional distribution $P(d|c_j)$:

$$\textbf{Multinomial} \quad P(d|c_j) = P(< w_1, \ldots, w_{n_d} > |c_j) \tag{13.10}$$

$$\textbf{Bernoulli} \quad P(d|c_j) = P(< e_1, e_2, \ldots, e_M > |c_j) \tag{13.11}$$

where $< w_1, \ldots, w_{n_d} >$ is the sequence of words as it occurs in d (minus words that were excluded from the vocabulary) and $< e_1, e_2, \ldots, e_M >$ is a binary vector of dimensionality M that indicates for each word whether it occurs in d or not.

It should now be clearer why we defined the classification problem as a mapping γ from a document space $\mathbb{X}$ to the set of classes $\mathbb{C}$, as opposed to just saying that we classify documents. A critical step in setting up a text classifier is to choose the document representation. $< w_1, \ldots, w_{n_d} >$ and $< e_1, e_2, \ldots, e_M >$ are two different representations of the same document. In the first case, $\mathbb{X}$ is set of all word sequences. In the second case, $\mathbb{X}$ is $\{0, 1\}^M$.

We cannot use Equations (13.10) and (13.11) for text classification directly. For the Bernoulli model, we would have to estimate $2^M|\mathbb{C}|$ different parameters, one for each possible combination of M attribute values and a class. The number of parameters in the multinomial case has the same order of magnitude. This being a very large quantity, estimating these parameters reliably is infeasible unless our training collection is astronomical in size.

CONDITIONAL INDEPENDENCE ASSUMPTION

To reduce the number of parameters, we make the Naive Bayes *conditional independence assumption*. We assume that attributes are independent of each other given the class:

$$\textbf{Multinomial} \quad P(d|c_j) = P(< w_1, \ldots, w_{n_d} > |c_j) = \prod_{1 \leq k \leq n_d} P(X_k = w_k|c_j) \tag{13.12}$$

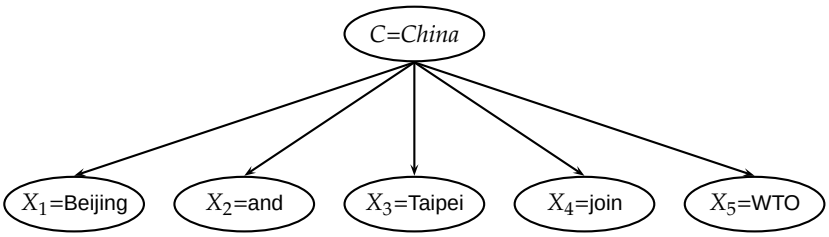
$$\textbf{Bernoulli} \quad P(d|c_j) = P(< e_1, e_2, \ldots, e_M > |c_j) = \prod_{1 \leq i \leq M} P(U_i = e_i|c) \tag{13.13}$$

RANDOM VARIABLE X

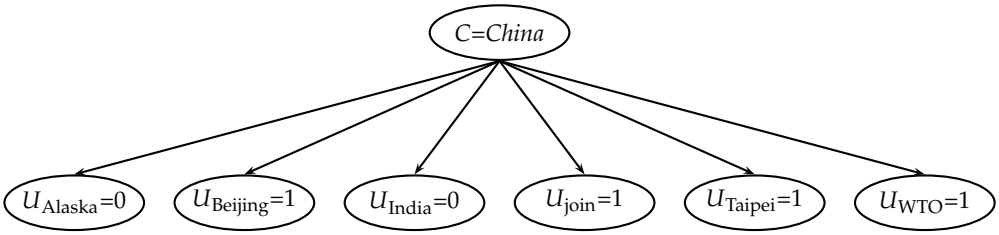
RANDOM VARIABLE U

We have introduced two random variables here to make the two different generative models explicit. X_k is the random variable for position k in the document and takes as values words from the vocabulary. $P(X_k = w|c_j)$ is the probability that in a document of class c_j the word w will occur in position k. U_i is the random variable for vocabulary word i and takes as values 0 (absence) and 1 (presence). $\hat{P}(U_i = 1|c_j)$ is the probability that in a document of class c_j the word w_i will occur – in any position and possibly multiple times.

We illustrate the conditional independence assumption in Figures 13.4 and 13.5. The class *China* generates each of the five word attributes (multinomial) or



► **Figure 13.4** The multinomial Naive Bayes model.



► **Figure 13.5** The Bernoulli Naive Bayes model.

six binary attributes (Bernoulli) with a certain probability, independently of the values of the other attributes. The fact that a document in the class *China* contains the word Taipei does not make it more likely or less likely that it also contains Beijing.

In reality, the conditional independence assumption does not hold for text data. Words *are* conditionally dependent on each other. But as we will discuss below, NB models perform well despite the conditional independence assumption.

Even when assuming conditional independence, we still have too many parameters for the multinomial model if we assume a different probability distribution for each position k in the document. The position of a word in a document by itself does not carry information about the class. While there is a difference between *China sues France* and *France sues China*, the occurrence of China in position 1 vs. position 3 of the document is not useful in Naive Bayes classification since we look at each word separately. The conditional independence assumption commits us to this way of processing the evidence.

Also, if we assumed different word distributions for each position k, we would have to estimate a different set of parameters for each k. The probabil-

ity of bean appearing as the first word of a *coffee* document could be different from it appearing as the second word etc. This would again cause problems in estimation due to data sparseness.

POSITIONAL INDEPENDENCE

For these reasons, we make a second independence assumption for the multinomial model, *positional independence*: The conditional probabilities for a word are the same independent of position in the document.

$$P(X_{k_1} = w|c_j) = P(X_{k_2} = w|c_j)$$

for all positions k_1, k_2, words w and classes c_j. Thus, we have a single multinomial distribution of words that is valid for all positions k_i and we can use X as its symbol. We could call the multinomial model with positional independence univariate multinomial Naive Bayes if we wanted to contrast it with the multiple random variables U_i needed for the multivariate Bernoulli Naive Bayes. Positional independence is equivalent to adopting the bag of words model, which we introduced in the context of ad hoc retrieval in Chapter 6 (page 110).

With conditional and positional independence assumptions, we only need to estimate $\Theta(M|\mathbb{C}|)$ parameters $P(w_k|c_j)$ (multinomial model) or $P(e_i|c_j)$ (Bernoulli model), one for each word-class combination, rather than a number that is exponential in M, the size of the vocabulary. The independence assumptions reduce the number of parameters to be estimated by several orders of magnitude.

RANDOM VARIABLE C

To summarize, we generate a document in the multinomial model (Figure 13.4) by first picking a class $C = c_j$ with $P(c_j)$ where C is a random variable taking values from $\mathbb{C}$ as values. Next we generate word w_k in position k with $P(X_k = w_k|c_j)$ for each of the n_d positions of the document. The X_k all have the same multinomial word distribution for a given c_j. In the example in Figure 13.4, we show the generation of $< w_1, w_2, w_3, w_4, w_5 >$ $= <$ Beijing, and, Taipei, join, WTO $>$, corresponding to the one-sentence document *Beijing and Taipei join WTO*.

For a completely specified document generation model, we would also have to define a distribution $P(n_d|c_j)$ over lengths. Without it, the multionomial model is a token generation model rather than a document generation model.

We generate a document in the Bernoulli model (Figure 13.5) by first picking a class $C = c_j$ with $P(c_j)$ and then generating a binary indicator e_i for each word w_i of the vocabulary ($1 \leq i \leq M$). In the example in Figure 13.5, we show the generation of $< e_1, e_2, e_3, e_4, e_5, e_6 > = < 0, 1, 0, 1, 1, 1 >$, corresponding, again, to the one-sentence document *Beijing and Taipei join WTO* where we have assumed that and is a stop word.

We compare the two models in Table 13.3, including estimation equations and decision rules.

	multinomial model	Bernoulli model
event model	generation of token	generation of document
random variable(s)	$X = w$ iff w occurs at given pos	$U_w = 1$ iff w occurs in doc
document representation	$d =< w_1, w_2, \ldots, w_{n_d} >, w_k \in V$	$d =< e_1, e_2, \ldots, e_M >, e_i \in \{0, 1\}$
parameter estimation	$\hat{P}(X = w\|c_j)$	$\hat{P}(U_i = e\|c_j)$
decision rule: maximize	$\hat{P}(c_j) \prod_{1 \leq k \leq n_d} \hat{P}(X = w_k\|c_j)$	$\hat{P}(c_j) \prod_{w_i \in V} \hat{P}(U_i = e_i\|c_j)$
multiple occurrences	taken into account	ignored
length of docs	can handle longer docs	works best for short docs
# features	can handle more	works best with fewer
estimate for term the	$\hat{P}(X = \text{the}\|c_j) \approx 0.05$	$\hat{P}(U_{\text{the}} = 1\|c_j) \approx 1.0$

► **Table 13.3** Multinomial vs. Bernoulli model.

	$P(c_1\|d)$	$P(c_2\|d)$	class selected
actual probability	0.6	0.4	c_1
Naive Bayes estimate	0.009	0.001	c_1
$\sim$, normalized	0.9	0.1	c_1

► **Table 13.4** Correct estimation implies accurate prediction, but accurate prediction does not imply correct estimation.

Naive Bayes is so called because the independence assumptions we have just made are indeed very naive for a model of natural language. The conditional independence assumption states that features are independent of each other given the class. This is hardly ever true for words in documents. In many cases, the opposite is true. The pairs hong and kong or london and english in Figure 13.7 are examples of highly dependent words. In addition, the multinomial model makes an assumption of positional independence. The Bernoulli model ignores positions in documents altogether since it only cares about absence or presence. This bag of words model discards all information that is communicated by the order of words in natural language sentences. These independence assumptions are so sweeping that Naive Bayes is sometimes called Idiot Bayes. How can Naive Bayes be a good text classifier when its model of natural language is so oversimplified?

The answer lies in a paradox. Even though the *probability estimates* of Naive Bayes are of low quality, its *classification decisions* are surprisingly good. Unless they are normalized to sum to 1 (in the sense of "normalized" defined on page 230), NB probability estimates tend to be close to 0 since multiplying large numbers of conditional probabilities produces numbers close to 0. The winning class usually has a much larger probability than the other classes, so after normalization its probability will be close to 1. In either case, the normalized NB probability is seldom a good estimate of the actual probability.

But the classification decision is based on which class gets the highest score. It does not matter how accurate the probabilities are. An example is shown in Table 13.4. Even though Naive Bayes fails to correctly estimate the actual probabilities, it assigns a higher probability to c_1 and therefore assigns d to the correct class. *Correct estimation implies accurate prediction, but accurate prediction does not imply correct estimation.* Naive Bayes classifiers estimate badly, but classify well.

Even if it is not the method with the highest accuracy for text, Naive Bayes has many virtues that make it a strong contender for text classification. It excels if there are many equally important features that jointly contribute to the classification decision. It is also somewhat robust to noise features (as defined in the next section) and *concept drift* – the gradual change over time of the concept underlying a class like *US president* from Bill Clinton to George W. Bush (see Section 13.7). Its main strength is its efficiency: Training and classification can be accomplished with one pass over the data. Because it combines efficiency with good accuracy it is often used as a baseline in text classification research. It is often the method of choice if: (i) squeezing out a few extra percentage points of accuracy is not worth the trouble in a text classification application, (ii) a very large amount of training data is available and there is more to be gained from training on a lot of data than using a better classifier on a smaller training set, or (iii) if its robustness to concept drift can be exploited.

CONCEPT DRIFT

In this book, we discuss Naive Bayes as a classifier for text. The independence assumptions do not hold for text. However, it can be shown that Naive Bayes is an *optimal classifier* (in the sense of minimal error rate on new data) in domains where the independence assumptions do hold.

OPTIMAL CLASSIFIER

13.5 Feature selection

Feature selection in text classification serves two main purposes. First, it makes training and applying a classifier more efficient by decreasing the size of the effective vocabulary. This is of particular importance for classifiers that, unlike Naive Bayes, are expensive to train. Secondly, feature selection often increases classification accuracy by eliminating noise features. A *noise feature* is one that, when added to the document representation, increases the classification error on new data. Suppose a rare word, say arachnocentric, has no information about a class, say *China*, but all instances of arachnocentric in our training set happen to occur in *China* documents. Then the learning method might produce a classifier that misassigns test documents with arachnocentric to *China*. Such an incorrect generalization from an accidental property of the training set is called *overfitting*. Feature selection often increases accuracy by eliminating noise features and thus avoiding overfitting.

NOISE FEATURE

OVERFITTING

SELECTFEATURES(D, c, k)
1 $V \leftarrow$ EXTRACTVOCABULARY(D)
2 $L \leftarrow []$
3 **for** each word $w \in V$
4 **do** $A(w, c) \leftarrow$ COMPUTEFEATUREUTILITY(D, c, w)
5 APPEND($L, < A(w, c), w >$)
6 **return** LARGESTVALUES(L, k)

► **Figure 13.6** Basic feature selection algorithm for selecting the k best features.

FEATURE SELECTION

The basic *feature selection* algorithm is shown in Figure 13.6. For a given class c, we compute a utility measure $A(w, c)$ for each word of the vocabulary and select the k words of the vocabulary that have the highest values of $A(w, c)$. All other words are discarded and not used in classification. We will introduce three different utility measures in this section: mutual information, $A(w, c) = I(U_w; C_c)$; the χ^2 test, $A(w, c) = X^2(U_w, C_c)$; and frequency, $A(w, c) = N(w, c)$.

Of the two NB models, the Bernoulli model is particularly sensitive to noise features. A Bernoulli NB classifier requires some form of feature selection or else its accuracy will be low.[3]

This section addresses feature selection for two-class classification tasks like *China* vs. *not-China*. Section 13.5.4 briefly discusses optimizations for systems with more than two classes.

13.5.1 Mutual information

MUTUAL INFORMATION

A common feature selection method is to compute $A(w, c)$ as the expected *mutual information* (MI) of word w and class c.[4] MI measures how much information the presence/absence of a word contributes to making the correct classification decision on c. Formally:

$$I(U; C) = \sum_{e_w \in \{1,0\}} \sum_{e_c \in \{1,0\}} P(U = e_w, C = e_c) \log_2 \frac{P(U = e_w, C = e_c)}{P(U = e_w) P(C = e_c)} \tag{13.14}$$

3. Feature selection corresponds to two different formal processes in the two NB models. In the Bernoulli model, the dimensionality of the underlying document representation is reduced. In the multinomial model, the sample space of the multinomial random variable is reduced – it has fewer possible outcomes after feature selection. As is customary, we call both of these processes feature selection here.

4. Take care not to confuse expected mutual information with *pointwise mutual information*, which is defined as $\log N_{11}/E_{11}$ where N_{11} and E_{11} are defined as below. The two measures have very different properties. See Section 13.7.

where U is a random variable that takes values $e_w = 1$ (the document contains word w) and $e_w = 0$ (the document does not contain w), as defined on page 249, and C is a random variable that takes values $e_c = 1$ (the document is in class c) and $e_c = 0$ (the document is not in class c). We write U_w and C_c if it is not clear from context which word w and class c we are referring to.

If we use maximum-likelihood estimates, e.g., $P(U = 1, C = 1) = N_{11}/N$, then Equation (13.14) is equivalent to Equation (13.15):

$$I(U;C) = \frac{N_{11}}{N}\log_2\frac{NN_{11}}{N_{1.}N_{.1}} + \frac{N_{01}}{N}\log_2\frac{NN_{01}}{N_{0.}N_{.1}} + \frac{N_{10}}{N}\log_2\frac{NN_{10}}{N_{1.}N_{.0}} + \frac{N_{00}}{N}\log_2\frac{NN_{00}}{N_{0.}N_{.0}} \tag{13.15}$$

where the N's are counts of documents that have the values of e_w and e_c that are indicated by the two subscripts. For example, N_{10} is the number of documents that contain w ($e_w = 1$) and are not in c ($e_c = 0$). $N_{1.} = N_{10} + N_{11}$ is the number of documents that contain w ($e_w = 1$) and we count documents independent of class membership ($e_c \in \{0, 1\}$). $N = N_{11} + N_{01} + N_{10} + N_{11}$ is the total number of documents.

✎ **Example 13.3:** Consider the class *poultry* and the word export in Reuters-RCV1. The counts of the number of documents with the four possible combinations of indicator values are as follows:

	$e_w = e_{\text{export}} = 1$	$e_w = e_{\text{export}} = 0$
$e_c = e_{\text{poultry}} = 1$	$N_{11} = 49$	$N_{01} = 141$
$e_c = e_{\text{poultry}} = 0$	$N_{10} = 27{,}652$	$N_{00} = 774{,}106$

After plugging these values into Equation (13.15) we get:

$$\begin{aligned} & I(U;C) \\ = \; & \frac{49}{801{,}948}\log_2\frac{801{,}948 \cdot 49}{(49+27{,}652)(49+141)} + \frac{141}{801{,}948}\log_2\frac{801{,}948 \cdot 141}{(141+774{,}106)(49+141)} \\ + \; & \frac{27{,}652}{801{,}948}\log_2\frac{801{,}948 \cdot 27{,}652}{(49+27{,}652)(27{,}652+774{,}106)} + \frac{774{,}106}{801{,}948}\log_2\frac{801{,}948 \cdot 774{,}106}{(141+774{,}106)(27{,}652+774{,}106)} \\ \approx \; & 0.000105 \end{aligned}$$

To select k words $w_1, \ldots, w_k$ for a given class, we use the feature selection algorithm in Figure 13.6: We compute the utility measure as $A(w, c) = I(U_w, C_c)$ and select the k words with the largest values.

Mutual information measures how much information – in the information-theoretic sense – a word contains about the class. If a word's distribution is the same in the class as it is in the collection as a whole, then $I(U;C) = 0$. MI reaches its maximum value if the word is a perfect indicator for class

UK	
london	0.1925
uk	0.0755
british	0.0596
stg	0.0555
britain	0.0469
plc	0.0357
england	0.0238
pence	0.0212
pounds	0.0149
english	0.0126

China	
china	0.0997
chinese	0.0523
beijing	0.0444
yuan	0.0344
shanghai	0.0292
hong	0.0198
kong	0.0195
xinhua	0.0155
province	0.0117
taiwan	0.0108

poultry	
poultry	0.0013
meat	0.0008
chicken	0.0006
agriculture	0.0005
avian	0.0004
broiler	0.0003
veterinary	0.0003
birds	0.0003
inspection	0.0003
pathogenic	0.0003

coffee	
coffee	0.0111
bags	0.0042
growers	0.0025
kg	0.0019
colombia	0.0018
brazil	0.0016
export	0.0014
exporters	0.0013
exports	0.0013
crop	0.0012

elections	
election	0.0519
elections	0.0342
polls	0.0339
voters	0.0315
party	0.0303
vote	0.0299
poll	0.0225
candidate	0.0202
campaign	0.0202
democratic	0.0198

sports	
soccer	0.0681
cup	0.0515
match	0.0441
matches	0.0408
played	0.0388
league	0.0386
beat	0.0301
game	0.0299
games	0.0284
team	0.0264

► **Figure 13.7** Features with high mutual information scores for six Reuters-RCV1 classes.

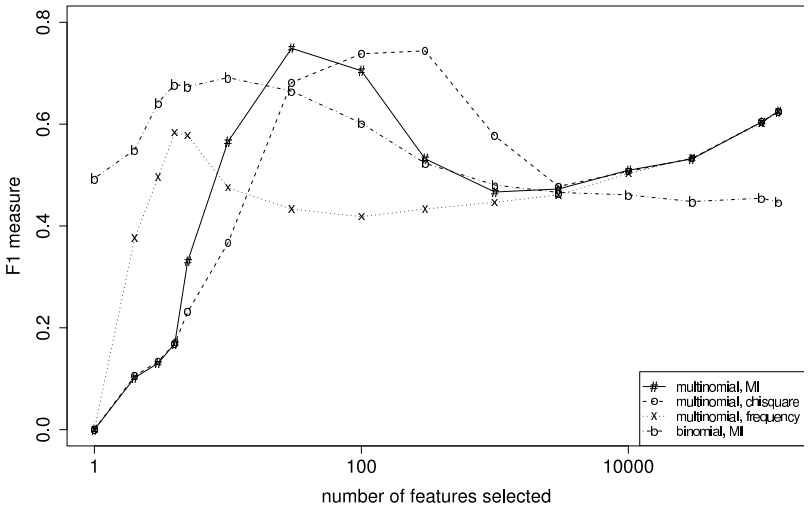
membership, that is, if the word is present in a document if and only if the document is in the class.

Figure 13.7 shows words with high mutual information scores for the six classes in Figure 13.1.[5] The selected words (e.g., london, uk, british for the class *UK*) are of obvious utility for making classification decisions for their respective classes. At the bottom of the list for *UK* we find words like peripherals and tonight (not shown in the figure) that are clearly not helpful in deciding whether the document is in the class. As you might expect, keeping the informative terms and throwing away the non-informative ones tends to reduce noise and improve the classifier's accuracy.

Such an accuracy increase can be observed in Figure 13.8, which shows F_1 as a function of vocabulary size after feature selection for RCV1.[6] Com-

5. Feature scores were computed on the first 100,000 documents, except for poultry, a rare class, for which 800,000 documents were used. We have omitted numbers and other special words from the top 10 lists.

6. We trained the classifiers on the first 100,000 documents and computed F_1 on the next 100,000.



► **Figure 13.8** Effect of feature set size on accuracy for multinomial and Bernoulli models.

paring F_1 at 132,776 features (corresponding to selection of all features) and at 50 features, we see that MI feature selection increases F_1 by about 0.1 for the multinomial model and by more than 0.2 for the Bernoulli model. For the Bernoulli model, F_1 peaks early, at 10 features selected. At that point, the Bernoulli model is better than the multinomial model. When basing a classification decision on only a few features, it is more robust to consider binary occurrence only. For the multinomial model, the peak occurs later at 30 features and its effectiveness recovers somewhat at the end when we use all features. The reason is that the multinomial takes the number of occurrences into account in parameter estimation and classification and therefore better exploits a larger number of features than the Bernoulli model. Regardless of the differences between the two methods, using a carefully selected subset of all features results in better effectiveness than using all features.

13.5.2 χ^2 feature selection

χ^2 FEATURE SELECTION

Another popular feature selection method is χ^2 (pronounced chi-square with chi as in kiting). In statistics, the χ^2 test is applied to test the independence

The graphs are averages over 5 classes.

p	χ^2 critical value
0.1	2.71
0.05	3.84
0.01	6.63
0.005	7.88
0.001	10.83

► **Table 13.5** Critical values of the χ^2 distribution with one degree of freedom. For example, if U and C are independent, then $\Pr(X^2 > 6.63) < 0.01$. So for $X^2 > 6.63$ the assumption of independence can be rejected with 99% confidence.

of two random variables. In feature selection, these two variables are occurrence of the word (U) and occurrence of the class (C), defined as above. We then rank words with respect to the following quantity:

$$X^2(D, w, c) = \sum_{e_w \in \{0,1\}} \sum_{e_c \in \{0,1\}} \frac{(N_{e_w e_c} - E_{e_w e_c})^2}{E_{e_w e_c}} \tag{13.16}$$

where e_w and e_c are defined as above. N is the *observed* frequency in D and E the *expected* frequency. For example, E_{11} is the *expected* frequency of w and c occurring together in a document assuming that word and class are independent.

✎ **Example 13.4:** We first compute compute E_{11} for the data in Example 13.3:

$$\begin{aligned} E_{11} &= N \times P(w) \times P(c) = N \times \frac{N_{11} + N_{01}}{N} \times \frac{N_{11} + N_{10}}{N} \\ &= N \times \frac{49 + 141}{N} \times \frac{49 + 27652}{N} \approx 6.6 \end{aligned}$$

where N is the total number of documents as before.

We compute the other $E_{e_w e_c}$ in the same way:

	$e_{\text{export}} = 1$		$e_{\text{export}} = 0$	
$e_{\text{poultry}} = 1$	$N_{11} = 49$	$E_{11} \approx 6.6$	$N_{10} = 141$	$E_{10} \approx 183.4$
$e_{\text{poultry}} = 0$	$N_{01} = 27{,}652$	$E_{01} \approx 27{,}694.4$	$N_{00} = 774{,}106$	$E_{00} \approx 774{,}063.6$

Plugging these values into Equation (13.16), we get a X^2 value of 284:

$$X^2(D, w, c) = \sum_{e_w \in \{0,1\}} \sum_{e_c \in \{0,1\}} \frac{(N_{e_w e_c} - E_{e_w e_c})^2}{E_{e_w e_c}} \approx 284$$

X^2 is a measure of how much expected counts E and observed counts N deviate from each other. A high value of X^2 indicates that the hypothesis of

independence, which implies that expected and observed counts are similar, is incorrect. In our example, $X^2 \approx 284 > 10.83$. Based on Table 13.5, we can reject the hypothesis that *poultry* and export are independent with only a 0.001 chance of being wrong.[7] Equivalently, we say that the outcome $X^2 \approx 284 > 10.83$ is *statistically significant* at the 0.001 level. If the two events are dependent, then the occurrence of the word makes the occurrence of the class more likely (or less likely), so it should be helpful as a feature. This is the rationale of χ^2 feature selection.

STATISTICAL SIGNIFICANCE

An arithmetically simpler way of computing X^2 is the following:

$$X^2(D, w, c) = \frac{(N_{11} + N_{10} + N_{01} + N_{00}) \times (N_{11}N_{00} - N_{10}N_{01})^2}{(N_{11} + N_{01}) \times (N_{11} + N_{10}) \times (N_{10} + N_{00}) \times (N_{01} + N_{00})} \tag{13.17}$$

This is equivalent to Equation 13.16 (Exercise 13.12).

Assessing χ^2 as a feature selection method

From a statistical point of view, χ^2 feature selection is problematic. For a test with one degree of freedom, the so-called Yates correction should be used (see Section 13.7), which makes it harder to reach statistical significance. Also, whenever a statistical test is used multiple times, then the probability of getting at least one error increases. If 1000 hypotheses are rejected, each with 0.05 error probability, then $0.05 \times 1000 = 50$ calls of the test will be wrong on average. However, in text classification it rarely matters whether a few additional terms are added to the feature set or removed from it. Rather, the *relative* importance of features is important. As long as χ^2 feature selection only ranks features with respect to their usefulness and is not used to make statements about statistical dependence or independence of variables, we need not be overly concerned that it does not adhere strictly to statistical theory.

13.5.3 Frequency-based feature selection

A third feature selection method is *frequency-based feature selection*, i.e., selecting the words that are most common in the class. Frequency can be either defined as the number of documents in the class c that contain the word w or as the number of tokens of w that occur in documents in c. The former is more appropriate for the Bernoulli model, the latter for the multinomial model.

This method will select some frequent words that have no specific information about the class, for example, the days of the week (Monday, Tuesday, ...),

7. We can make this inference because, if U and C are independent, then $X^2 \sim \chi^2$, where χ^2 is the χ^2 distribution. See, for example, Rice (2006).

which are frequent across classes in newswire text. When many thousands of features are selected, then frequency-based feature selection often does very well. If somewhat suboptimal accuracy is acceptable, then frequency-based feature selection is often a good alternative to more complex methods. However, in Figure 13.8, frequency-based feature selection performs a lot worse than MI and χ^2. This application is an example for a case where it should not be used.

13.5.4 Comparison of feature selection methods

Mutual information and χ^2 represent rather different feature selection methods. The independence of term w and class c can sometimes be rejected with high confidence even if w carries little information about membership in c. This is particularly true for rare terms. If a word occurs once in a large collection and that one occurrence is in the *poultry* class, then this is statistically significant. But a single occurrence is not very informative according to the information-theoretic definition of information. Because its criterion is significance, χ^2 selects more rare terms (which are often less reliable indicators) than mutual information. But the selection criterion of mutual information also does not necessarily select the terms that maximize classification accuracy.

Despite the differences between the two methods, the classification accuracy of feature sets selected with χ^2 and MI does not seem to differ systematically. In most text classification problems there are a few strong indicators and many weak indicators. As long as all strong indicators and a large number of weak indicators are selected, accuracy is expected to be good. Both methods do this.

Figure 13.8 compares MI and χ^2 feature selection for the multinomial model. Peak effectiveness is virtually the same for both methods. χ^2 reaches this peak later, at 300 features, probably because the rare, but highly significant features it selects initially do not cover all documents in the class. However, features selected later (in the range 100–300) are of better quality than those selected by MI.

GREEDY FEATURE SELECTION

All three methods – MI, χ^2 and frequency-based – are *greedy* methods. They may select features that contribute no incremental information over previously selected features. In Figure 13.7, kong is selected as the seventh word even though it is highly correlated with previously selected hong and therefore redundant. Although such redundancy can negatively impact accuracy, non-greedy methods (see Section 13.7 for references) are rarely used in text classification due to their computational cost.

In an operational system with a large number of classifiers, it is desirable to select a single set of features instead of a different one for each classifier. One way of doing this is to compute the X^2 statistic for an $n \times 2$ table where

```
<REUTERS TOPICS=''YES'' LEWISSPLIT=''TRAIN''
CGISPLIT=''TRAINING-SET'' OLDID=''12981'' NEWID=''798''>
<DATE> 2-MAR-1987 16:51:43.42</DATE>
<TOPICS><D>livestock</D><D>hog</D></TOPICS>
<TITLE>AMERICAN PORK CONGRESS KICKS OFF TOMORROW</TITLE>
<DATELINE> CHICAGO, March 2 - </DATELINE><BODY>The American Pork
Congress kicks off tomorrow, March 3, in Indianapolis with 160
of the nations pork producers from 44 member states determining
industry positions on a number of issues, according to the
National Pork Producers Council, NPPC.
Delegates to the three day Congress will be considering 26
resolutions concerning various issues, including the future
direction of farm policy and the tax law as it applies to the
agriculture sector. The delegates will also debate whether to
endorse concepts of a national PRV (pseudorabies virus) control
and eradication program, the NPPC said. A large
trade show, in conjunction with the congress, will feature
the latest in technology in all areas of the industry, the NPPC
added. Reuter
&#3;</BODY></TEXT></REUTERS>
```

► **Figure 13.9** A sample document from the Reuters-21578 collection.

the columns are occurrence and non-occurrence of the word and each row corresponds to one of the classes. We can then select the k words with the highest X^2 statistic as before.

More commonly, feature selection statistics are first computed separately for each class on the binary classification task c vs. $\overline{c}$; and then combined (for example, by averaging) into a single figure of merit. Classification accuracy often decreases when selecting k common features for a system with n classifiers as opposed to n different sets of size k. But even if it does, the gain in efficiency due to a common document representation may be worth the loss in accuracy.

13.6 Evaluation of text classification

Historically, the classic Reuters-21578 collection was the main benchmark for text classification evaluation. This is a collection of 21,578 newswire articles, originally collected and labeled by Carnegie Group, Inc. and Reuters, Ltd. in the course of developing the CONSTRUE text categorization system. It is much smaller than and predates the Reuters-RCV1 collection discussed

class	# train	# test	class	# train	# test
earn	2877	1087	*trade*	369	119
acquisitions	1650	179	*interest*	347	131
money-fx	538	179	*ship*	197	89
grain	433	149	*wheat*	212	71
crude	389	189	*corn*	182	56

► **Table 13.6** The ten largest classes in the Reuters-21578 collection with number of documents in training and test sets.

in Chapter 4 (page 63). The articles are assigned classes from a set of 118 topic categories. A document may be assigned several classes or none, but the commonest case is single assignment (documents with at least one class received an average of 1.24 classes). The standard approach to this *any-of* problem (Chapter 14, page 283) is to learn 118 binary classifiers, one for each class, where the *binary classifier* for class c_j is the classifier for the two classes c_j and its complement $\overline{c_j}$.

BINARY CLASSIFIER

For each of these classifiers, we can measure recall, precision, and accuracy. In recent work, people almost invariably use the *ModApte split* which includes only documents with at least one class, and comprises 90 classes, 9603 training documents and 3299 test documents. The distribution of documents in classes is very uneven, and some work evaluates systems on only documents in the 10 largest classes. They are listed in Table 13.6. A typical document with topics is shown in Figure 13.9.

MODAPTE SPLIT

In Section 13.1 we stated as our goal in text classification the minimization of classification error on test data. Classification error is 1.0 minus classification accuracy, the proportion of correct decisions, a measure we introduced in Section 8.3 (page 149). This measure is appropriate if the population rate of the class is high, perhaps 10–20% and higher. But as was discussed in Section 8.3, accuracy is not a good measure for "small" classes since always saying no, a strategy that defeats the purpose of building a classifier, will achieve high accuracy. The always-no classifier is 99% accurate for a class with relative frequency 1%. For small classes, precision, recall and F_1 are better measures. We will use *effectiveness* as a generic term for measures that evaluate the quality of classification decisions, including precision, recall, F_1 and accuracy. *Performance* refers to the *computational efficiency* of classification and information retrieval systems, that is, their time complexity. However, many researchers mean effectiveness, not efficiency of text classification when they use the term performance.

EFFECTIVENESS

PERFORMANCE
COMPUTATIONAL EFFICIENCY

When we process a collection with several binary classifiers as described above, we often want to compute a single aggregate measure that combines the measures for individual classifiers. There are two methods for doing this.

	class 1	
	truth: yes	truth: no
call: yes	10	10
call: no	10	970

	class 2	
	truth: yes	truth: no
call: yes	90	10
call: no	10	890

	pooled table	
	truth: yes	truth: no
call: yes	100	20
call: no	20	1860

► **Table 13.7** Macro- and microaveraging. "Truth" is the true class and "call" the decision of the classifier. In this example, macroaveraged precision is $[10/(10+10)+90/(10+90)]/2 = (0.5+0.9)/2 = 0.7$. Microaveraged precision is $100/(100+20) \approx 0.83$.

Method	F_1 micro-avg.	F_1 macro-avg.
multinomial NB	0.80	0.47
SVM	0.89	0.60

► **Table 13.8** Experimental results for F_1 on Reuters-21578 (all classes).

MACROAVERAGING
MICROAVERAGING

Macroaveraging computes a simple average over classes. *Microaveraging* pools per-document decisions across classes, and then computes an effectiveness measure on the pooled contingency table. Table 13.7 gives an example.

The differences between the two methods can be large. Macroaveraging gives equal weight to each class, whereas microaveraging gives equal weight to each per-document classification decision. Since the F_1 measure ignores true negatives and its magnitude is mostly determined by the number of true positives, large classes dominate small classes in microaveraging. In the example, microaveraged precision (0.83) is much closer to the precision of c_2 (0.9) than to the precision of c_1 (0.5) because c_2 is five times larger than c_1. Microaveraged results are therefore really a measure of effectiveness on the large classes in a test collection. To get a sense of effectiveness on small classes, compute macroaveraged results.

Table 13.8 gives microaveraged and macroaveraged effectiveness of Naive Bayes for the ModApte split of Reuters-21578. To give a sense of the relative effectiveness of Naive Bayes, we compare it to SVMs (Chapter 15), one of the most effective classifiers, but also one that is expensive to train. Naive Bayes has a microaveraged F_1 of 80% which is 9% less than the SVM (89%), a 10% relative decrease. So there is a surprisingly small effectiveness penalty for its simplicity and efficiency. However, on small classes, some of which only have on the order of ten positive examples in the training set, Naive Bayes does much worse. Its macroaveraged F_1 is 13% below the SVM, a 22% relative decrease.

When performing evaluations like the one in Table 13.8 it is important to maintain a strict separation between the training set and the test set. We can easily make correct classification decisions on the test set by using information we have gleaned from the test set, e.g., the fact that a particular word is a good predictor in the test set (even if this is not the case in the training set). A more subtle example of using knowledge about the test set is to try a large number of values of a parameter (e.g., the number of selected features) and select the value that is best for the test set.

It is important to avoid using information that was derived from the test set. As a rule, accuracy on new data – the type of data we will encounter when we use the classifier in an application – will be much lower than accuracy on a test set that the classifier has been "tuned" for.

DEVELOPMENT SET

In a clean statistical text classification experiment, you should never look at the test set. Instead, set aside a *development set* for testing while you develop your method. When such a set serves the primary purpose of finding a good value for a parameter, e.g., the number of selected features, then it is also called *held-out*. Train the classifier on the rest of the training set with different parameter values, and then select the value that gives best results on the held-out part of the training set.

HELD-OUT

Ideally, the test set should not be consulted when developing a new text classification method. At the very end, when all parameters are set and the method is fully specified, run one final experiment on the test set. Since no information about the test set was used in developing the classifier, the results of this experiment should be indicative of actual performance in practice.

13.7 References and further reading

A general introduction to statistical classification can be found in Hastie et al. (2001), including many important methods like decision trees and boosting that we do not cover. A comprehensive review of text classification methods and results is (Sebastiani 2002). An accessible introduction to text classification with coverage of decision trees, perceptrons and maximum entropy models is (Manning and Schütze 1999, ch. 16). More information on the superlinear time complexity of learning methods that are more accurate than Naive Bayes can be found in (Perkins et al. 2003, Joachims 2006).

Lewis (1998) focuses on the history of Naive Bayes classification. Bernoulli and multinomial models and their accuracy for different collections are discussed by McCallum and Nigam (1998). Friedman (1997) and Domingos and Pazzani (1997) analyze why Naive Bayes performs well although its probability estimates are poor. The latter paper also discusses NB's optimality when the independence assumptions are true of the data. Ng and Jordan (2001) show that Naive Bayes is sometimes (though rarely) superior to dis-

(1) He moved from London, Ontario, to London, England.
(2) He moved from London, England, to London, Ontario.
(3) He moved from England to London, Ontario.

► **Table 13.9** A set of documents for which the Naive Bayes independence assumptions are problematic.

criminative methods because it more quickly reaches its optimal error rate. The problem of concept drift is discussed by Forman (2006) and Hand (2006).

Early uses of mutual information and χ^2 for feature selection in text classification are Lewis and Ringuette (1994) and Schütze et al. (1995), respectively. Yang and Pedersen (1997) review feature selection methods and their impact on classification effectiveness. They find that *pointwise mutual information* is not competitive with other methods. Yang and Pedersen refer to expected mutual information (Equation (13.14)) as information gain (see Exercise 13.11, page 267). Snedecor and Cochran (1989) is a good reference for the χ^2 test in statistics, including the Yates' correction for continuity for two-by-two tables. Dunning (1993) discusses problems of the χ^2 test when counts are small. Non-greedy feature selection techniques are described by Hastie et al. (2001). Table 13.8 is based on (Li and Yang 2003).

POINTWISE MUTUAL INFORMATION

A number of approaches for hierarchical classification have been developed in order to deal with the common situation where the classes to be assigned have a natural hierarchical organization (Koller and Sahami 1997, McCallum et al. 1998, Weigend et al. 1999, Dumais and Chen 2000). In a recent large study using the Yahoo! directory, Liu et al. (2005) conclude that hierarchical classification noticeably if still modestly outperforms flat classification.

The ModApte split was defined by Apté et al. (1994). See also http://www.daviddlewis.com/resources/

UTILITY MEASURE

Lewis (1995) describes *utility measures* for the evaluation of text classification systems.

13.8 Exercises

Exercise 13.1

Which of the documents in Table 13.9 have identical and different bag of words representations for (a) the Bernoulli model (b) the multinomial model?

Exercise 13.2

The rationale for the positional independence assumption is that there is no useful information in the fact that a word occurs in position k of a document. Find exceptions. Consider formulaic documents with a fixed document structure.

	docID	words in document	in c = *China*?
training set	1	Taipei Taiwan	yes
	2	Macao Taiwan Shanghai	yes
	3	Japan Sapporo	no
	4	Sapporo Osaka Taiwan	no
test set	5	Taiwan Taiwan Sapporo	?

► **Table 13.10** Data for parameter estimation exercise.

Exercise 13.3

The class priors in Figure 13.2 are computed as the fraction of *documents* in the class as opposed to the fraction of *tokens* in the class. Why?

Exercise 13.4

Why is $|\mathbb{C}||V| < |D|L_{\text{ave}}$ in Table 13.2 expected to hold for most text collections?

Exercise 13.5

Table 13.3 gives Bernoulli and multinomial estimates for the word the. Explain the difference.

Exercise 13.6

Based on the data in Table 13.10, (i) estimate a multinomial Naive Bayes classifier, (ii) apply the classifier to the test document, (iii) estimate a Bernoulli Naive Bayes classifier, (iv) apply the classifier to the test document. You need not estimate parameters that you don't need for classifying the test document.

Exercise 13.7

Your task is to classify words as English or not English. Words are generated by a source with the following distribution:

event	word	English?	probability
1	ozb	no	4/9
2	uzu	no	4/9
3	zoo	yes	1/18
4	bun	yes	1/18

(i) Compute the parameters (priors and conditionals) of a multinomial Naive Bayes classifier that uses the letters b, n, o, u, and z as features. Assume a training set that reflects the probability distribution of the source perfectly. Make the same independence assumptions that are usually made for a multinomial classifier that uses words as features for text classification. Compute parameters using smoothing, in which computed-zero probabilities are smoothed into probability 0.01, and computed-nonzero probabilities are untouched. (This simplistic smoothing may cause $P(A) + P(\overline{A}) > 1$, which can be corrected if we correspondingly smooth all complementary probability-1 values into probability 0.99. For this exercise, solutions may omit this correction to simplify arithmetic.) (ii) How does the classifier classify the word zoo? (iii) Classify the word zoo using a multinomial classifier as in part (i), but do not make the assumption of positional independence. That is, estimate separate parameters for each

position in a word. You only need to compute the parameters you need for classifying zoo.

Exercise 13.8

Consider the following frequencies for the class *coffee* for four words in the first 100,000 documents of RCV1:

word	N_{00}	N_{10}	N_{01}	N_{11}
brazil	98,012	102	1835	51
council	96,322	133	3525	20
producers	98,524	119	1118	34
roasted	99,824	143	23	10

Select two of these four words based on (i) χ^2 (ii) mutual information (iii) frequency.

Exercise 13.9

What are the values of $I(U_w; C_c)$ and $X^2(D, w, c)$ if word and class are completely independent? What are the values if they are completely dependent?

Exercise 13.10

The feature selection method in Equation 13.14 is most appropriate for the Bernoulli model. Why? How could one modify it for the multinomial model?

Exercise 13.11

INFORMATION GAIN

Features can also be selected according to *information gain* (IG). Information gain is defined as:

$$\text{IG}(D, f) = H(p_D) - \sum_{x \in \{D_{f^+}, D_{f^-}\}} \frac{|x|}{|D|} H(p_x)$$

where H is entropy, D is the training set, and D_{f^+}, and D_{f^-} are the subset of D with feature f, and the subset of D without feature f, respectively. p_A is the class distribution in (sub)collection A, e.g., $p_A(c) = 0.25, p_A(\overline{c}) = 0.75$ if a quarter of the documents in A are in class c.

Show that mutual information and information gain are equivalent.

Exercise 13.12

Show that the two X^2 formulas (Equations (13.16) and (13.17)) are equivalent.

Exercise 13.13

In the χ^2 example on page 258 we have $|N_{11} - E_{11}| = |N_{10} - E_{10}| = |N_{01} - E_{01}| = |N_{00} - E_{00}|$. Show that this holds in general.

Exercise 13.14

χ^2 and mutual information do not distinguish between positively and negatively correlated features. Since most good text classification features are positively correlated (i.e., they occur more often in c than in $\overline{c}$), one may want to explicitly rule out the selection of "negative" indicators. How would you do this?

14 *Vector space classification*

The document representation in Naive Bayes is a vector of word counts. In this chapter we adopt a different representation for text classification, the vector space model, developed in Chapter 6. It represents each document as a vector with one real-valued component, usually a tf-idf weight, for each term. Thus, the document space, the domain of the classification function γ, is $\mathbb{R}^{|V|}$ instead of $\mathbb{N}^{|V|}$. This chapter introduces a number of classification methods that operate on real-valued vectors.

CONTIGUITY HYPOTHESIS

The basic hypothesis in using the vector space model for classification is the *contiguity hypothesis*: *documents in the same class form a contiguous region and regions of different classes do not overlap.* There are many classification tasks, in particular the type of text classification that we encountered in Chapter 13, where classes can be distinguished by word patterns. For example, documents in the class *China* tend to have high values on dimensions like Chinese, Beijing, and Mao whereas documents in the class *UK* tend to have high values for London, British and Queen. Documents of the two classes therefore form distinct contiguous regions as shown in Figure 14.1 and we can draw a line that separates them and classifies new documents. How exactly this is done is the topic of this chapter.

Whether or not a set of documents is mapped into a contiguous region depends on the particular choices we make for the document representation: type of weighting, stop list etc. To see that the document representation is crucial, consider the two classes *written by a group* vs. *written by a single person*. Frequent occurrence of the first person pronoun I is evidence for the single-person class. But that information is likely deleted from the document representation if we use a stop list. If the document representation chosen is unfavorable, the contiguity hypothesis will not hold and successful vector space classification is not possible.

Novices often use vectors of counts, but the same considerations that led us to prefer weighted representations, in particular length-normalized tf-idf representations, in Chapters 6 and 7 also apply here. For example, a word

with 5 occurrences in a document should get a higher weight than one with 1 occurrence, but a weight 5 times larger would give too much emphasis to the term. Unweighted and unnormalized counts should not be used in vector space classification.

This chapter introduces two vector space classification methods, Rocchio and kNN. Rocchio classification (Section 14.1) divides the vector space into regions centered on centroids or *prototypes*, one for each class, computed as the center of mass of all documents in the class. Rocchio classification is simple and efficient, but inaccurate if classes are not approximately spheres with similar radii.

PROTOTYPE

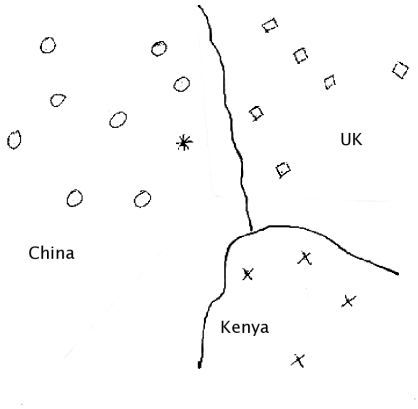
kNN or k nearest neighbor classification (Section 14.2) assigns the majority class of the k nearest neighbors to a test document. kNN requires no training, but is less efficient than other classification methods in classification. If the training set is large, then kNN can handle non-spherical and other complex classes better than Rocchio.

A large number of text classifiers can be viewed as linear classifiers – classifiers that classify based on a simple linear combination of the features (Section 14.3). Such classifiers partition the space of features into regions separated by linear *decision hyperplanes*, in a manner to be detailed below. Because of the bias-variance tradeoff (Section 14.5) more complex nonlinear models are not systematically better than linear models. Nonlinear models have more parameters to fit on a limited amount of training data and are more likely to make mistakes for small and noisy data sets.

When applying binary (or two-class) classifiers to problems with more than two classes, we distinguish *one-of* tasks – a document must be assigned to exactly one of several mutually exclusive classes – and *any-of* tasks – a document can be assigned to any number of classes (Section 14.4). Binary classifiers solve any-of problems and can be combined to solve one-of problems.

Decisions of many vector space classifiers are based on a notion of distance, e.g., when computing the nearest neighbors in kNN classification. We will use Euclidean distance in this chapter as the underlying distance measure. We observed earlier (Exercise 6.18, page 125) that there is a direct correspondence between cosine similarity and Euclidean distance for length-normalized vectors. In vector space classification, it rarely matters whether the affinity of two documents is formalized in terms of similarity or distance.

However, in addition to documents, centroids or averages of vectors also play an important role in vector space classification. Centroids are not length-normalized. For unnormalized vectors, inner product, cosine similarity and Euclidean distance all have different behavior in general (Exercise 14.1). We will be mostly concerned with small local regions when computing the similarity between a document and a centroid and the smaller the region the more similar the behavior of the three measures is.



► **Figure 14.1** Vector space classification into three classes.

14.1 Rocchio classification

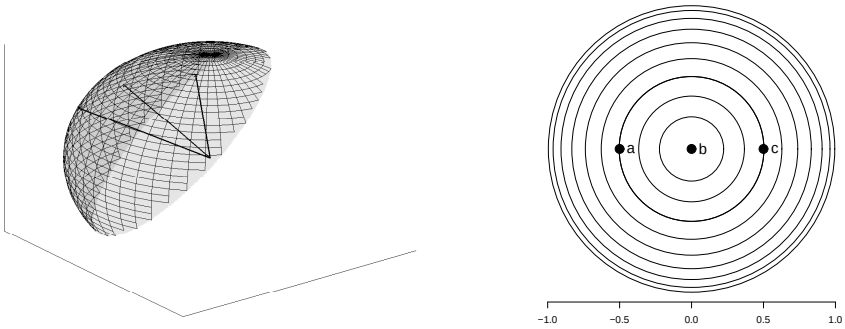
Figure 14.1 shows three classes, *China*, *UK* and *Kenya*, in a two-dimensional (2D) space. Documents are shown as circles, diamonds and X's. The boundaries in the figure, which we call *decision boundaries*, are chosen to separate the three classes, but are otherwise arbitrary. To classify a new document, depicted as a star in the figure, we determine the region it occurs in and assign it the class of that region – *China* in this case. Our task in vector space classification is to devise algorithms that compute good boundaries where "good" means high classification accuracy on data unseen during training.

DECISION BOUNDARY

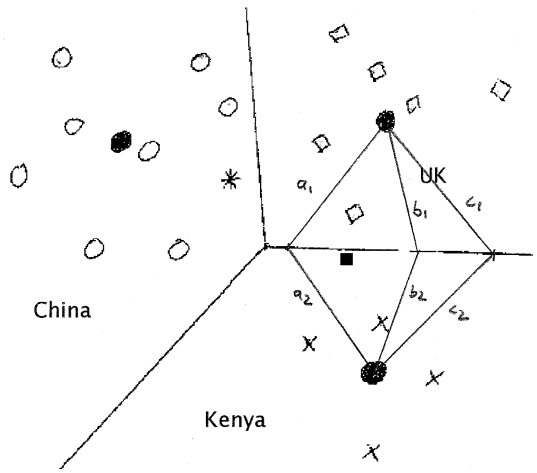
In Figure 14.1 and many other illustrations in this chapter, we show documents as points in a plane. In reality, documents in vector space are length-normalized unit vectors that point to the surface of a hypersphere. We can view the 2D planes in our figures as spherical projections of the surface of a (hyper-)sphere as shown in Figure 14.2. Distances on the surface of the sphere and on the projection plane are approximately the same as long as we restrict ourselves to small areas of the surface and choose an appropriate projection. This is not true for large areas. For example, the distance between $(-1, 0)$ and $(1, 0)$ on the unit circle is π, but it is 2 for a projection onto the x-axis. We will use 2D figures only as illustrations and mostly for local phenomena. Be aware that they can be misleading when distances are distorted.

The main work we must do in vector space classification is to define the boundaries between classes since they determine the classification decision. Perhaps the best-known way of doing this is to use *centroids*. The centroid of

CENTROID



► **Figure 14.2** Unit vectors in three dimensions and their projection onto a plane. The three unit vectors are $\vec{a} = (-0.5 \ \sqrt{0.66} \ 0.3)^T$, $\vec{b} = (0 \ \sqrt{0.9} \ 0.3)^T$ and $\vec{c} = (0.5 \ \sqrt{0.66} \ 0.3)^T$. The projection chosen here preserves the distance $\|\vec{a} - \vec{c}\| = 1$, but shortens the distances $\|\vec{a} - \vec{b}\|$ and $\|\vec{b} - \vec{c}\|$ from $\sqrt{(}0.5^2 + (\sqrt{0.66} - \sqrt{0.9})^2) \approx 0.52$ (3D space) to $1/2 = 0.5$ (2D projection). For a small area of the surface of the unit sphere, there always exists a projection that preserves distances between points with small distortions.



► **Figure 14.3** Rocchio classification. Boundaries between two classes in Rocchio classification are points of equal distance to the two centroids (e.g., $|a_1| = |a_2|, |b_1| = |b_2|, |c_1| = |c_2|$).

docID	term weights: Chinese	Japan	Tokyo	Macao	Beijing	Shanghai
$\vec{d}_1$	0	0	0	0	1.0	0
$\vec{d}_2$	0	0	0	0	0	1.0
$\vec{d}_3$	0	0	0	1.0	0	0
$\vec{d}_4$	0	0.71	0.71	0	0	0
$\vec{d}_5$	0	0.71	0.71	0	0	0
$\vec{\mu}_c$	0	0	0	0.33	0.33	0.33
$\vec{\mu}_{\overline{c}}$	0	0.71	0.71	0	0	0

► **Table 14.1** Vectors and class centroids for the data in Table 13.1.

a class c is computed as the vector average or center of mass of its members:

$$\vec{\mu}(c) = \frac{1}{|c|} \sum_{\vec{x} \in c} \vec{x} \tag{14.1}$$

Three example centroids are shown in Figure 14.3. The boundary between two classes is the set of points with equal distance from the two centroids. We classify points in accordance with the region they fall into. Equivalently, we determine the centroid $\vec{\mu}(c_j)$ that the point is closest to and then assign it to c_j. This algorithm is called *Rocchio classification* and is summarized in Figure 14.4.

ROCCHIO CLASSIFICATION

✎ **Example 14.1:** Table 14.1 shows the tf-idf vector representations of the five documents in Table 13.1 (page 244), using the formula $(1 + \log_{10} \mathrm{wf}_{t,d}) \log_{10}(4/\mathrm{df}_t)$ if $\mathrm{tf}_{t,d} > 0$ (Equation (6.11), page 114). The two class centroids are $\mu_c = 1/3 \cdot (\vec{d}_1 + \vec{d}_2 + \vec{d}_3)$ and $\mu_{\overline{c}} = 1/1 \cdot (\vec{d}_4)$. The distances of the test document from the centroids are $\|\mu_c - \vec{d}_5\| \approx 1.15$ and $\|\mu_{\overline{c}} - \vec{d}_5\| = 0.0$. Thus, Rocchio assigns d_5 to $\overline{c}$.

The assignment criterion in Figure 14.4 is Euclidean distance. An alternative is cosine similarity:

$$\text{Assign } d \text{ to class } c = \arg\max_{c_j} \cos(\vec{\mu}(c_j), \vec{d})$$

As discussed above, the two assignment criteria will sometimes make different classification decisions. We present the Euclidean distance variant of Rocchio classification here because it makes it easier to see Rocchio's close correspondence to K-means clustering (Section 16.4, page 319).

Rocchio classification is a form of Rocchio relevance feedback (Section 9.1.1, page 170). The average of the relevant documents, corresponding to the most

Training
For each class c_j
  Compute centroid $\vec{\mu}(c_j)$
Testing
Assign d to class $c = \arg\min_{c_j} \|\vec{\mu}(c_j) - \vec{d}\|$

► **Figure 14.4** Rocchio classification: Training and testing.

$\Theta(\|D\|L_{\text{ave}} + \|\mathbb{C}\|\|V\|)$	training time
$\Theta(L_{\text{ave}} + \|\mathbb{C}\|M_{\text{ave}})$	test time

► **Table 14.2** Training and test times for Rocchio classification. L_{ave} and M_{ave} are the average numbers of word tokens and types, respectively, per document. Centroid computation includes an $\Theta(|\mathbb{C}||V|)$ averaging step. Computing Euclidean distance between the class centroids and a document is $\Theta(|\mathbb{C}|M_{\text{ave}})$.

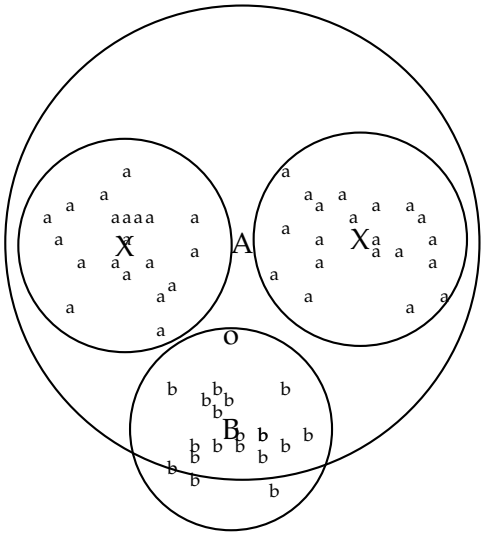
important component of the Rocchio vector in relevance feedback (Equation (9.3), page 174), is the centroid of the "class" of relevant documents. We usually omit the other two components of the Rocchio formula in Rocchio classification: the query (since there is no query in text classification) and the centroid of the negative documents since, as in Rocchio relevance feedback, positive information is much more useful than negative information. Rocchio classification can be applied to $J > 2$ classes whereas Rocchio relevance feedback is designed to distinguish only two classes, relevant and non-relevant.

In addition to respecting contiguity, the classes in Rocchio classification must also be of approximately spherical shape. In Figure 14.3, the solid square just below the boundary between *UK* and *Kenya* should intuitively be part of *UK* since *UK* is more scattered than *Kenya*. But Rocchio assigns it to *Kenya* because it ignores details of the distribution of points in a class and only uses the centroids for classification.

MULTIMODAL CLASS

The assumption of sphericity also does not hold in Figure 14.5. We cannot represent the "a" class well with a single prototype because it has two clusters. Rocchio often misclassifies this type of *multimodal class*. A text classification example for multimodality is a country like Burma, which changed its name to Myanmar in 1989. The two clusters before and after the name change need not be close to each other in space. We encountered the same problem with multimodality in relevance feedback (Section 9.1.2, page 176). In the next section, we will introduce a vector space classification method, kNN, that deals better with classes that have non-spherical, disconnected or other irregular shapes.

Table 14.2 gives the time complexity of Rocchio classification. Adding a



► **Figure 14.5** The multimodal class "a" consists of two different clusters (small upper circles centered on X's). Rocchio classification will misclassify "o" as "a" because it is closer to the centroid A of the "a" class than to the centroid B of the "b" class.

document to a centroid is $\Theta(L_{\text{ave}})$ (as opposed to $\Theta(M)$) since we need only consider non-zero entries. Overall, training time is linear in the size of the collection. Thus, Rocchio classification and Naive Bayes have the same linear training time complexity.

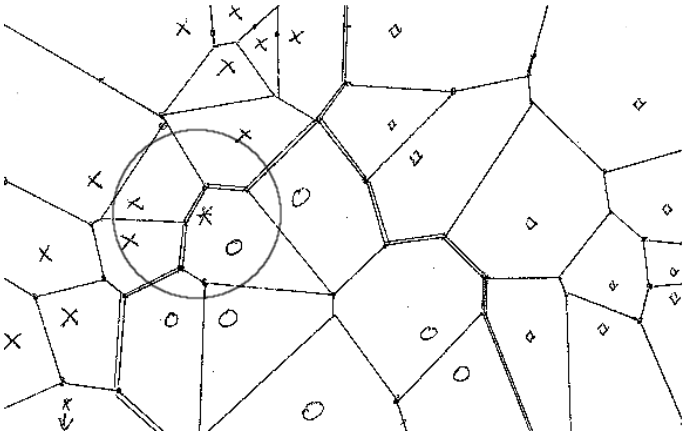
14.2 *k* nearest neighbor

k NEAREST NEIGHBOR CLASSIFICATION

Unlike Rocchio, *k nearest neighbor* or *kNN classification* determines the decision boundary locally. For 1NN we assign each document to the class of its closest neighbor. For kNN we assign each document to the majority class of its k closest neighbors. Decision boundaries are concatenated segments of the

VORONOI TESSELLATION

Voronoi tessellation as shown in Figure 14.6. The Voronoi tessellation of a set of objects decomposes space into Voronoi cells, where each object's cell consists of all points that are closer to the object than to other objects. In our case, the objects are documents. The Voronoi tessellation then partitions the plane into $|D|$ convex polygons, each containing its corresponding object (and no other) as shown in Figure 14.6. For general $k \in \mathbb{N}$, consider the region in the space for which the set of k nearest neighbors is the same. This again is a convex polygon and the space is partitioned into convex polygons, within



► **Figure 14.6** Voronoi tessellation and decision boundaries (double lines) in 1NN classification. The three classes are: X, circle and diamond.

each of which the set of k nearest neighbors is invariant (Exercise 14.8).[1]

To generalize this notion from 2-dimensional to M-dimensional spaces, we first define a hyperplane as the set of points that satisfy:

$$\vec{w}^T \vec{x} = b \tag{14.2}$$

NORMAL VECTOR

where $\vec{w}$ is the M-dimensional *normal vector*[2] of the hyperplane. This definition of hyperplanes includes lines (any line can be defined by $w_1 x_1 = b$) and 2-dimensional planes (any plane can be defined by $w_1 x_1 + w_2 x_2 = b$). A line divides a plane in two, a plane divides 3-dimensional space in two, and hyperplanes divide higher dimensional spaces in two.

1NN is not very robust. The classification decision of each document relies on the class of a single document, which may be incorrectly labeled or atypical. kNN for $k > 1$ is more robust. It assigns documents to the majority class of their k closest neighbors, with ties broken randomly. In the probabilistic version of this method, we estimate the probability of membership in the class as the proportion of the k nearest neighbors in the class.

1. The generalization of a polygon to higher dimensions is a polytope. A polygon is a convex region in 2-dimensional space bounded by lines. A polytope is a convex region in M-dimensional space bounded by $(M-1)$-dimensional hyperplanes. So in M dimensions, the decision boundaries for kNN consist of segments of $(M-1)$-dimensional hyperplanes that form the Voronoi tessellation into polytopes for the training set of documents. For our purposes, the description in terms of polygons is sufficient for understanding kNN even though it is not strictly correct for $M \neq 2$.

2. Recall from basic linear algebra that $\vec{v} \cdot \vec{w} = \vec{v}^T \vec{w}$, i.e., the inner product of $\vec{v}$ and $\vec{w}$ equals the product by matrix multiplication of the transpose of $\vec{v}$ and $\vec{w}$.

Training
Preprocess documents in training set
Select k (e.g., $k = 3$, $k = 5$ or k selected on held-out data)
Testing: Classify test document $\vec{d}$
Compute the distance of all training documents from $\vec{d}$
Identify the set S_k of the k closest training documents
For each class c
  Compute $N(S_k, c)$, the number of members of S_k in c
  Estimate $\hat{P}(c|\vec{d})$ as $N(S_k, c)/k$

► **Figure 14.7** kNN training and testing.

Figure 14.6 gives an example for $k = 3$. Probability estimates for class membership of the star are $\hat{P}(\text{circle class}|\text{star}) = 1/3$, $\hat{P}(\text{X class}|\text{star}) = 2/3$, and $\hat{P}(\text{diamond class}|\text{star}) = 0$.

The parameter k is often chosen based on experience or knowledge about the classification problem at hand. It is desirable for k to be odd to make ties less likely. $k = 3$ and $k = 5$ are common choices. An alternative way of setting the parameter is to select the k that gives best results on a held-out portion of the training set.

We can also weight the "votes" of the k nearest neighbors by their cosine similarity. In this scheme, a class's score is computed as:

$$\text{score}(c, d) = \sum_{d' \in S_k} I_c(d') \cos(\vec{d}', \vec{d})$$

where $I_c(d') = 1$ iff d' is in class c and 0 otherwise. We then assign the document to the class with the highest score. Weighting by similarities is often more accurate than simple voting. For example, if two classes have the same number of neighbors in the top k, the class with the more similar neighbors wins.

Figure 14.7 summarizes the kNN algorithm.

✎ **Example 14.2:** The distances of the test document from the four training documents in Table 14.1 are $\|\vec{d}_1 - \vec{d}_5\| = \|\vec{d}_2 - \vec{d}_5\| = \|\vec{d}_3 - \vec{d}_5\| \approx 1.41$ and $\|\vec{d}_4 - \vec{d}_5\| = 0.0$. d_5's nearest neighbor is therefore d_4 and 1NN assigns d_5 to d_4's class, $\overline{c}$.

✗

14.2.1 Time complexity and optimality of kNN

Table 14.3 gives the time complexity of kNN. kNN has properties that are quite different from most other classification algorithms. Training a kNN

kNN with preprocessing of training set	
$\Theta(\|D\|L_{\text{ave}})$	training time
$\Theta(L_{\text{ave}} + \|D\|M_{\text{ave}}) = \Theta(\|D\|M_{\text{ave}})$	test time
kNN without preprocessing of training set	
$\Theta(1)$	training time
$\Theta(L_{\text{ave}} + \|D\|L_{\text{ave}}) = \Theta(\|D\|L_{\text{ave}})$	test time

► **Table 14.3** Training and test times for kNN classification.

classifier simply consists of determining k and document preprocessing. In fact, if we preselect a value for k and do not preprocess, then kNN requires no training at all. In practice, we have to perform preprocessing steps like tokenization. It makes more sense to preprocess training documents once as part of the training phase rather than repeatedly every time we classify a new test document.

Test time is $\Theta(|D|)$ for kNN. It is linear in the size of the training set as we need to compute the distance of each training document from the test document. Test time is independent of the number of classes J. kNN therefore has a potential advantage for problems with large J.

In kNN classification, we do not perform any estimation of parameters as we do in Rocchio classification (centroids) or in Naive Bayes (priors and conditional probabilities). kNN simply memorizes all examples in the training set and then compares the test document to them. For this reason, kNN is also called *memory-based learning* or *instance-based learning*. It is usually desirable to have as much training data as possible in machine learning. But in kNN large training sets come with a severe efficiency penalty.

MEMORY-BASED LEARNING
INSTANCE-BASED LEARNING

Can kNN testing be made more efficient than $\Theta(|D|)$? There are fast kNN algorithms for small k (Exercise 14.10). There are also approximations for large k that give error bounds for specific efficiency gains (see Section 14.6). These approximations have not been extensively tested for text classification applications, so it is not clear whether they can achieve much better efficiency than $\Theta(|D|M_{\text{ave}})$ without a significant loss of accuracy.

The reader may have noticed the similarity between the problem of finding nearest neighbors of a test document and ad hoc retrieval, where we search for the documents with the highest similarity to the query (Section 6.4.2, page 119). In fact, the two problems are both k nearest neighbor problems and only differ in the relative density of (the vector of) the test document in kNN (10s or 100s of non-zero entries) versus the sparseness of (the vector of) the query in ad hoc retrieval (usually fewer than 10 non-zero entries). We introduced the inverted index for efficient ad hoc retrieval in Section 1.1 (page 6). Is the inverted index also the solution for efficient kNN?

An inverted index restricts a search to those documents that have at least

one term in common with the query. Thus in the context of kNN, the inverted index will be efficient if the test document has no term overlap with a large number of training documents. How often this is the case depends on the classification problem. If documents are long and no stop list is used, then less time will be saved. But with short documents and a large stop list, an inverted index may well cut the average test time by a factor of 10 or more.

The search time in an inverted index is a function of the length of the postings lists of the terms in the query. Postings lists grow sublinearly with the length of the collection since the vocabulary increases according to Heaps' law – if the probability of occurrence of some words increases, then the probability of occurrence of others must decrease. However, most new words are infrequent. We therefore take the complexity of inverted index search to be $\Theta(T)$ (as discussed in Section 2.3.2, page 39) and, assuming average document length does not change over time, that is equivalent to $\Theta(|D|)$.

As we will see in the next chapter, kNN's effectiveness is close to that of the most accurate learning methods in text classification (Table 15.2, page 306). A

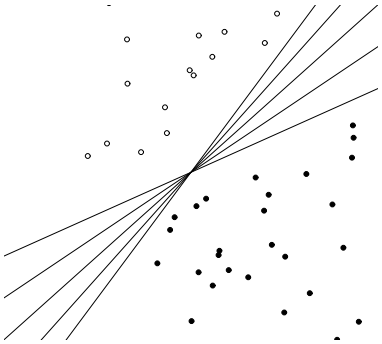
BAYES ERROR RATE

measure of the quality of a learning method is its *Bayes error rate*, the average error rate of classifiers learned by it for a particular problem, in a sense to be made precise in Section 14.5. kNN is not optimal for problems with a non-zero Bayes error rate – that is, for problems where even the best classifier has a non-zero classification error. The learning error of 1NN is asymptotically (as the training set increases) bounded by twice the Bayes error rate. That is, if the optimal classifier has an error rate of x, then 1NN has an asymptotic error rate of less than $2x$. This is due to the effect of noise – we already saw one example of noise in the form of noisy features in Section 13.5 (page 253), but noise can also take other forms as we will discuss in the next section. Noise affects two components of kNN: the test document and the closest training document. The two sources of noise are additive, so the overall error of 1NN is twice the optimal error rate. For problems with Bayes error rate 0, the error rate of 1NN will approach 0 as the size of the training set increases.

14.3 Linear vs. nonlinear classifiers

In this section, we show that the two learning methods Naive Bayes and Rocchio are instances of linear classifiers, the perhaps most important group of text classifiers, and contrast them with nonlinear classifiers. To simplify the discussion, we will only consider binary classifiers.

In two dimensions, a linear classifier is a line. Five examples are shown in Figure 14.8. These lines have the functional form $w_1x_1 + w_2x_2 = b$. The classification rule of a linear classifier is to assign a document to c if $w_1x_1 + w_2x_2 > b$ and to $\overline{c}$ if $w_1x_1 + w_2x_2 \leq b$. Here, $(x_1, x_2)^T$ is the two-dimensional



► **Figure 14.8** There is an infinite number of hyperplanes that separate two linearly separable classes.

vector representation of the document and $(w_1, w_2)^T$ is the parameter vector that defines (together with b) the decision boundary.

We can generalize this 2D linear classifier to higher dimensions by defining a hyperplane as we did in 14.2. The assignment criterion then is: assign to c if $\vec{w}^T\vec{x} > b$ and to $\overline{c}$ if $\vec{w}^T\vec{x} \leq b$. This definition of hyperplanes includes lines and planes. We call a hyperplane that we use for classification a *decision hyperplane*.

DECISION HYPERPLANE

One way of training a linear classifier is to identify a separating hyperplane between the two classes. This is only possible if the two classes are *linearly separable*, that is, at least one separating hyperplane exists. In fact, if linear separability holds, then there is an infinite number of linear separators (Exercise 14.13) as illustrated by Figure 14.8, where one can easily see that the number of possible separating hyperplanes is infinite.

LINEAR SEPARABILITY

An example of a nonlinear classifier is kNN. The nonlinearity of kNN is intuitively clear when looking at examples like Figure 14.6. The decision boundaries defined by kNN consist of linear segments, but in general have complex ragged shapes that are not lines in 2D or hyperplanes in higher dimensions.

We now show that Rocchio and Naive Bayes are linear. To see this for Rocchio, observe that a document, denoted as $\vec{x}$, is on the decision boundary if it has equal distance to the two class centroids:

$$\|\vec{\mu}(c_1) - \vec{x}\| = \|\vec{\mu}(c_2) - \vec{x}\| \tag{14.3}$$

Some basic arithmetic shows that this corresponds to a linear classifier with normal vector $\vec{w} = \vec{\mu}(c_1) - \vec{\mu}(c_2)$ and $b = 0.5 * (\|\vec{\mu}(c_1)\|^2 - \|\vec{\mu}(c_2)\|^2)$ (Exercise 14.14).

We can derive the linearity of Naive Bayes from its decision rule, which

w_i	x_i	w_i	x_i
0.70	prime	-0.71	dlrs
0.67	rate	-0.35	world
0.63	interest	-0.33	sees
0.60	rates	-0.25	year
0.46	discount	-0.24	group
0.43	bundesbank	-0.24	dlr

▶ **Table 14.4** A linear classifier. The variables x_i and parameters w_i of a linear classifier for the class *interest* (as in interest rate) in Reuters-21578. The threshold is $b = 0$. Terms like dlr and world have negative weights because they are indicators for the competing class *currency*.

chooses the category c with the largest $\hat{P}(c|d)$ (Figure 13.2, page 244) where:

$$\hat{P}(c|d) \propto \hat{P}(c) \prod_{1 \leq i \leq n_d} \hat{P}(x_i|c)$$

n_d is the number of tokens in the document that are part of the vocabulary. Denoting the complement category as $\bar{c}$, we obtain for the log odds:

$$\log \frac{\hat{P}(c|d)}{\hat{P}(\bar{c}|d)} = \log \frac{\hat{P}(c)}{\hat{P}(\bar{c})} + \sum_{1 \leq i \leq n_d} \log \frac{\hat{P}(x_i|c)}{\hat{P}(x_i|\bar{c})} \tag{14.4}$$

We choose class c if the odds are greater than 1 or, equivalently, if the log odds are greater than 0. It is easy to see that Equation (14.4) is an instance of Equation (14.2) for $w_i = \log[\hat{P}(x_i|c)/\hat{P}(x_i|\bar{c})]$, $x_i =$ number of occurrences of w_i in d, and $b = -\log[\hat{P}(c)/\hat{P}(\bar{c})]$. So in log space, Naive Bayes is a linear classifier.

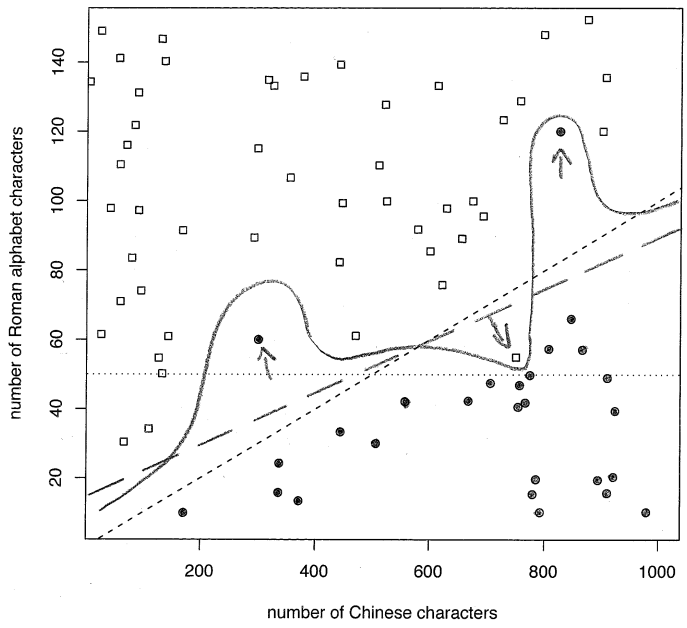
✎ **Example 14.3:** Table 14.4 defines a linear classifier for the category *interest* in Reuters-21578 (see Section 13.6, page 261). We assign document $\vec{d}_1$ "rate discount dlrs world" to *interest* since $\vec{w}^T\vec{d}_1 = 0.67 \cdot 1 + 0.46 \cdot 1 + (-0.71) \cdot 1 + (-0.35) \cdot 1 = 0.05 > 0 = b$. We assign $\vec{d}_2$ "prime dlrs" to the complement class (not in *interest*) since $\vec{w}^T\vec{d}_2 = -0.01 \leq b$. For simplicity, we assume a simple binary vector representation in this example: 1 for occurring terms, 0 for non-occurring terms.

Figure 14.9 is a graphical example of a *linear problem*, which we define to mean that the underlying distributions $P(d|c)$ and $P(d|\overline{c})$ of the two classes are separated by a line. We call this line the *class boundary*. It is the "true" boundary of the two classes and we distinguish it from the decision boundary that the learning method computes to approximate the class boundary.

CLASS BOUNDARY

NOISE DOCUMENT

As is typical in text classification, there are some *noise documents* in Fig-

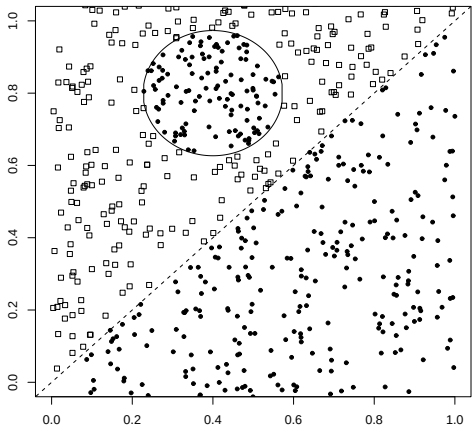


► **Figure 14.9** A linear problem with noise. In this hypothetical web page classification scenario, Chinese-only web pages are solid circles and mixed Chinese-English web pages are squares. The two classes are separated by a linear separator (dashed line, short dashes), except for three noise documents (marked with arrows).

ure 14.9 (marked with arrows) that do not fit well into the overall distribution of the classes. In Section 13.5 (page 253), we defined a noise feature as a misleading feature that, when included in the document representation, on average increases the classification error. Analogously, a noise document is a document that, when included in the training set, misleads the learning method and increases classification error. Intuitively, the underlying distribution partitions the representation space into areas with mostly homogeneous class assignments. A document that does not conform with the dominant class in its area is a noise document.

Figure 15.5 is a graphical example of a *nonlinear problem*: there is no good linear separator between the distributions $P(d|c)$ and $P(d|\overline{c})$ because of the circular "enclave" in the upper left part of the graph. Linear classifiers misclassify the enclave, whereas a nonlinear classifier like kNN will be highly accurate for this type of problem if the training set is large enough.

If a problem is nonlinear and its class boundaries cannot be approximated well with linear hyperplanes, then nonlinear classifiers are often more accu-



► **Figure 14.10** A nonlinear problem.

rate than linear classifiers. If a problem is linear, it is best to use a simpler linear classifier.

14.4 More than two classes

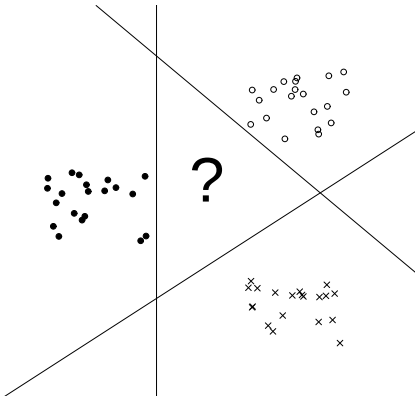
Linear classifiers are binary. What do we do if there are $J > 2$ different classes? This depends on whether the classes are mutually exclusive or not.

ANY-OF CLASSIFICATION

Classification for classes that are not mutually exclusive is called *any-of*, *multilabel*, or *multivalue classification*. In this case, a document can belong to several classes simultaneously, or to a single class, or to none of the classes. A decision on one class leaves all options open for the others. It is sometimes said that the classes are *independent* of each other, but this is misleading since the classes are rarely statistically independent. In terms of the formal definition of the classification problem in Equation (13.1) (page 240), we learn J different classifiers γ_j in any-of classification, each returning either c_j (yes) or $\overline{c}_j$ (no) for its class: $\gamma_j(\vec{d}) \in \{c_j, \overline{c}_j\}$.

Solving an any-of classification task with linear classifiers is straightforward:

1. Build a classifier for each class, where the training set consists of the set of documents in the class (positive labels) and its complement (negative labels).



► **Figure 14.11** J hyperplanes do not divide space into J disjoint regions.

2. Given the test document, apply each classifier separately. The decision of one classifier has no influence on the decisions of the other classifiers.

ONE-OF CLASSIFICATION

The second type of classification with more than two classes is *one-of classification*. Here, the classes are mutually exclusive. Each document must belong to exactly one of the classes. One-of classification is also called *multinomial*, *polytomous*[3], *multiclass*, and *single-label classification*. Formally, there is a single classification function γ in one-of classification whose range is $\mathbb{C}$, i.e., $\gamma(\vec{d}) \in \{c_1, \ldots, c_J\}$. kNN is a (nonlinear) one-of classifier.

True one-of problems are less common in text classification than any-of problems. With classes like *UK*, *China*, *poultry*, or *coffee*, a document can be relevant to many topics simultaneously – as when the prime minister of the UK visits China to talk about the coffee and poultry trade.

Nevertheless, we will often make a one-of assumption, as we did in Figure 14.1, even if classes are not really mutually exclusive. For the classification problem of identifying the language of a document, the one-of assumption is a good approximation as most text is written in only one language. In such cases, the one-of assumption simplifies the classification problem without a large decrease in classification accuracy.

J hyperplanes do not divide $\mathbb{R}^{|V|}$ into J distinct regions as illustrated in Figure 14.11. Thus, we must use a combination method when using binary linear classifiers for one-of classification. The simplest method is to rank classes and then select the top-ranked class. Geometrically, the ranking can be with respect to the distances from the J linear separators. Documents

3. A synonym of polytomous is polychotomous.

assigned class / true class	*money-fx*	*trade*	*interest*	*wheat*	*corn*	*grain*
money-fx	95	0	10	0	0	0
trade	1	1	90	0	1	0
interest	13	0	0	0	0	0
wheat	0	0	1	34	3	7
corn	1	0	2	13	26	5
grain	0	0	2	14	5	10

► **Table 14.5** A confusion matrix for Reuters-21578. For example, 14 documents from *grain* were incorrectly assigned to *wheat*. Adapted from Picca et al. (2006).

close to a class's separator are more likely to be misclassified, so the greater the distance from the separator, the more plausible it is that a positive classification decision is correct. Alternatively, we can use a direct measure of confidence to rank classes, e.g., probability of class membership. We can state this algorithm for one-of classification with linear classifiers as follows:

1. Build a classifier for each class, where the training set consists of the set of documents in the class (positive labels) and its complement (negative labels).

2. Given the test document, apply each classifier separately.

3. Assign the document to the class with

   - the maximum score,
   - the maximum confidence value,
   - or the maximum probability.

CONFUSION MATRIX

An important tool for analyzing the performance of a classifier for $J > 2$ classes is the *confusion matrix*. The confusion matrix shows for each pair of classes $< c_1, c_2 >$, how many documents from c_1 were incorrectly assigned to c_2 and vice versa. In Table 14.5, the classifier manages to distinguish the three financial classes *money-fx*, *trade*, and *interest* from the three agricultural classes *wheat*, *corn*, and *grain*, but makes many errors within these two groups. The confusion matrix can help pinpoint opportunities for improving the accuracy of the system. For example, to address the second largest error in Table 14.5, one could attempt to introduce features that distinguish *wheat* documents from *grain* documents.

14.5 The bias-variance tradeoff

Nonlinear classifiers are more powerful than linear classifiers. For some problems, there exists a nonlinear classifier with zero classification error, but no such linear classifier. Does that mean that we should always use nonlinear classifiers for optimal effectiveness in statistical text classification?

To answer this question, we introduce the bias-variance tradeoff in this section, one of the most important concepts in machine learning. Because of this tradeoff, there is no universally optimal learning method. Selecting an appropriate learning method is therefore an unavoidable part of solving a text classification problem.

We first need to state our objective in text classification more precisely. In Section 13.1 (page 239), we said that we want to minimize classification error on the test set. The implicit assumption was that training documents and test documents are generated according to the same underlying distribution. We will denote this distribution $P(< d, c >)$ where d is the document and c its label or class. Figures 13.4 and 13.5 were examples of generative models that decompose $P(< d, c >)$ into the product of $P(c)$ and $P(d|c)$. Figures 14.9 and 14.10 depict generative models for $d \in \mathbb{R}^2$ and $c \in \{\text{square, solid circle}\}$.

In this section, we do not want to use the number of correctly classified documents as evaluation measure because we need to address the inherent uncertainty of labeling. In many text classification problems, a given document representation can arise from documents belonging to different classes. This is because documents from different classes can be mapped to the same document representation. For example, the one-sentence documents d_1 = *China sues France* and d_2 = *France sues China* are mapped to the same document representation $d' = \{\text{China, France, sues}\}$ in a bag of words model. But only the latter document is relevant to the class c' = *legal actions brought by France* (which might be defined, for example, as a standing query by an international trade lawyer).

To account for this type of uncertainty, we do not simply count the number of correct classifications when evaluating a classifer, but instead look at how well the classifier estimates the conditional probability $P(c|d)$ of a document being in a class. In the above example, we might have $P(c'|d') = 0.5$.

Our goal in text classification then is to find a classifier γ such that, averaged over documents d, $\gamma(d)$ is as close as possible to the true probability $P(c|d)$. We measure this using sum-squared error:

$$\text{classification-error}(\gamma) = E_d[\gamma(d) - P(c|d)]^2 \tag{14.5}$$

where E_d is the expectation with respect to $P(d)$. The sum-squared error term gives partial credit for decisions that are close if not completely right – e.g., an estimate of $\gamma(d) = 0.9$ for $P(c|d) = 1.0$ is penalized with a smaller

$$
\begin{aligned}
(i) E(x-\alpha)^2 &= E(x^2) - 2Ex\alpha + \alpha^2 \\
&= (Ex)^2 - 2Ex\alpha + \alpha^2 \\
&+ E(x^2) - 2(Ex)^2 + (Ex)^2 \\
&= (Ex-\alpha)^2 \\
&+ E(x^2) - E2x(Ex) + E(Ex)^2 \\
&= (Ex-\alpha)^2 + E[(x-Ex)^2] \\
&= (Ex-\alpha)^2 + E[x-Ex]^2
\end{aligned}
$$

$$
\begin{aligned}
(ii) E_d E_D(\Gamma_D(d) - P(c|d))^2 &= E_D E_d(\Gamma_D(d) - P(c|d))^2 \\
&= (E_d E_D \Gamma_D(d) - P(c|d))^2 + E_d E_D[\Gamma_D(d) - E_d E_D \Gamma_D(d)]^2 \\
&= (E_D \Gamma_D(d) - P(c|d))^2 + E_D[\Gamma_D(d) - E_D \Gamma_D(d)]^2
\end{aligned}
$$

► **Figure 14.12** Arithmetic transformations for the bias-variance decomposition. We substitute $\alpha = P(c|d)$ and $x = \Gamma_D(d)$ in (i) for better readability.

squared error (0.01) than the completely incorrect estimate 0.0 (whose error is 1.0).

OPTIMAL CLASSIFIER

A classifier γ is *optimal* for a distribution $P(\langle d, c\rangle)$ if it minimizes the expected classification error. We call the classification error of the optimal classifier – the lowest possible error rate – the *Bayes error rate*.

BAYES ERROR RATE

Minimizing classification error is a desideratum for *classifiers*. For *learning methods*, our goal is to find a Γ that, averaged over training sets, learns classifers γ with minimal classification error. We can formalize this as minimizing *learning error*:

LEARNING ERROR

$$\text{learning-error}(\Gamma) = E_D[\text{classification-error}(\Gamma(D))] \tag{14.6}$$

where E_D is the expectation over labeled training sets. To keep things simple, we can assume that training sets have a fixed size – the distribution $P(\langle d, c\rangle)$ then defines a distribution $P(D)$ over training sets. Recall that D in the text classification chapters denotes labeled document sets and that we write $\gamma = \Gamma(D)$ to make γ's dependence on the training set clear.

OPTIMAL LEARNING METHOD

We can use learning error as a criterion for selecting a learning method in statistical text classification. A learning method Γ is *optimal* for a distribution $P(D)$ if it minimizes the learning error.

Writing Γ_D for $\Gamma(D)$ for better readability, we can transform Equation (14.6) as follows:

$$\text{learning-error}(\Gamma) = E_D[\text{classification-error}(\Gamma_D)]$$

$$= E_D E_d[\Gamma_D(d) - P(c|d)]^2 \tag{14.7}$$

$$= E_d(\text{bias}(\Gamma, d) + \text{variance}(\Gamma, d)) \tag{14.8}$$

$$\text{bias}(\Gamma, d) = [P(c|d) - E_D\Gamma_D(d)]^2 \tag{14.9}$$

$$\text{variance}(\Gamma, d) = E_D[\Gamma_D(d) - E_D\Gamma_D(d)]^2 \tag{14.10}$$

where the equivalence between Equation (14.7) and Equation (14.8) is shown in Figure 14.12.

BIAS *Bias* is the squared difference between $P(c|d)$, the true conditional probability of d being in c, and $\Gamma_D(d)$, the prediction of the learned classifier, averaged over training sets. Bias is large if the learning method produces classifiers that are consistently wrong. Bias is small if the classifiers are either consistently right; or if different training sets cause errors on different documents, so that for any given document $E_D\Gamma_D(d)$, the expectation over all training sets, is close to $P(c|d)$.

Linear methods like Rocchio and Naive Bayes have a high bias for nonlinear problems because linear classifiers can only model one type of class boundary, a linear hyperplane. If the generative model $P(\langle d, c\rangle)$ has a complex nonlinear class boundary, the bias term in Equation (14.8) will be high because a large number of points will be consistently misclassified. For example, the circular enclave in Figure 15.5 does not fit a linear model and will be misclassified consistently by linear classifiers.

We can think of bias as a kind of domain knowledge that we build into a classifier. If we know that the true boundary between the two classes is linear, then a learning method that produces linear classifiers is more likely to succeed than a nonlinear method. But if the true class boundary is not linear and we incorrectly bias the learning method to be linear, then classification accuracy will be low on average.

Nonlinear methods like kNN have low bias. We can see in Figure 14.6 that the decision boundaries of kNN are variable – depending on the distribution of documents in the training set, learned decision boundaries can vary greatly. As a result, no document is misclassified consistently across training sets. Each document has a chance of being classified correctly for some training sets. The average prediction $E_D\Gamma_D(d)$ is therefore closer to $P(c|d)$ and bias is smaller than for a linear learning method.

VARIANCE *Variance* is the variation of the prediction of learned classifiers: the average squared difference between $\Gamma_D(d)$ and its average $E_D\Gamma_D(d)$. Variance is large if different training sets D give rise to very different classifiers Γ_D. It is small if the training set has a minor effect on the classification decisions Γ_D makes, be they correct or incorrect. Variance measures how inconsistent the decisions are, not whether they are correct or incorrect.

Linear classifiers have low variance because most randomly drawn training sets produce similar decision hyperplanes. The decision lines produced

by linear classifiers in Figures 14.9 and 14.10 will deviate slightly from the main class boundaries, depending on the training set, but the class assignment for the vast majority of documents (with the exception of those close to the main boundary) will not be affected. The circular enclave in Figure 14.10 will be consistently misclassified.

Nonlinear methods like kNN have high variance. It is apparent from Figure 14.6 that kNN can model very complex boundaries between two classes. It is therefore sensitive to noise documents of the sort depicted in Figure 14.9. As a result the variance term in Equation (14.8) is large: Test documents are sometimes misclassified – if they happen to be close to a noise document in the training set – and sometimes correctly classified – if there are no noise documents in the training set near them. This results in high variation from training set to training set.

OVERFITTING

High-variance classifiers are prone to *overfitting* the training data. The goal in classification is to fit the training data to the extent that we capture true properties of the underlying distribution $P(\langle d, c\rangle)$. In overfitting, the classifier also learns from noise. Overfitting increases the learning error and frequently is a problem for high-variance classifiers.

We can also think of variance as the *memory capacity* of the classifier – how detailed a characterization of the training set it can remember and then apply to new data. This capacity corresponds to the number of independent parameters available to fit the training set. Each kNN neighborhood S_k makes an independent classification decision. The parameter in this case is the estimate $\hat{P}(c|S_k)$ from Figure 14.7. Thus, kNN's capacity is unlimited: it can memorize arbitrarily large training sets. In contrast, the number of parameters of Rocchio is fixed – J parameters per dimension, one for each centroid – and independent of the size of the training set. The Rocchio classifier (in form of the centroids defining it) cannot "remember" fine-grained details of the distribution of the documents in the training set.

As stated in Equation (14.6), our goal in selecting a learning method is to minimize learning error. The fundamental insight captured by Equation (14.8), which we can succinctly state as: learning-error = bias + variance, is that the learning error has two components, bias and variance, which in general cannot be minimized simultaneously. When comparing two learning methods Γ_1 and Γ_2, in most cases the comparison comes down to one method having higher bias and lower variance and the other lower bias and higher variance. The decision for one learning method vs. another is then not simply a matter of selecting the one with the minimal learning error. Instead, we have to weigh the respective merits of bias and variance in our application and choose accordingly. This tradeoff is called the *bias-variance tradeoff*.

BIAS-VARIANCE TRADEOFF

Figure 14.9 provides an illustration, which is somewhat contrived, but will be useful as an example for the tradeoff. Some Chinese text contains English words written in the Roman alphabet like CPU, ONLINE, and GPS.

Consider the task of distinguishing Chinese-only web pages from mixed Chinese-English web pages. A search engine might offer Chinese users without knowledge of English (but who understand loanwords like CPU) the option of filtering out mixed pages. We use two features for this classification task: number of Roman alphabet characters and number of Chinese characters on the web page. As stated earlier, the distribution $P(\langle d, c\rangle)$ of the generative model generates most Roman (respectively, Chinese) documents above (respectively, below) the short-dashed line, but there are a few noise documents.

In Figure 14.9, we see three classifiers:

- **One-feature classifier.** Shown as a dotted horizontal line. This classifier uses only one feature, the number of Roman alphabet characters. Assuming a learning method that minimizes the number of misclassifications in the training set, the position of the horizontal decision boundary is not greatly affected by differences in the training set (e.g., noise documents). So this classifier has low variance. But its bias is high since it will consistently misclassify squares in the lower right corner and "solid circle" documents with more than 50 Roman characters.

- **Linear classifier.** Shown as a dashed line with long dashes. This classifier has less bias since it only misclassifies noise documents and possibly a few documents close to the boundary between the two classes. Its variance is higher than that of the one-feature classifier, but still small: The dashed line with long dashes deviates only slightly from the true boundary between the two classes, and so will almost all linear decision boundaries learned from training sets. Thus, very few documents (documents close to the class boundary) will be inconsistently classified.

- **"Fit-training-set-perfectly" classifier.** Shown as a solid line. This classifier constructs a decision boundary that perfectly separates the classes in the training set. It has the lowest bias because there is no document that is consistently misclassified – the classifier sometimes even gets noise documents in the test set right. But the variance of the classifier is high. Because noise documents can move the decision boundary arbitrarily, test documents close to noise documents in the training set will be misclassified – something that the linear classifier is unlikely to do.

It is perhaps surprising that so many of the best-known text classification algorithms are linear. Some of these methods, in particular linear SVMs, regularized logistic regression and regularized linear regression, are among the most effective known methods. The bias-variance tradeoff provides insight into their success. Typical classes in text classification are complex and seem unlikely to be modelled well linearly. However, this intuition is misleading

for the high-dimensional spaces that we typically encounter in text applications. With increased dimensionality, the likelihood of linear separability increases rapidly (Exercise 14.16). Thus, linear models in high-dimensional spaces are quite powerful despite their linearity. Even more powerful nonlinear classifiers can model decision boundaries that are more complex than a hyperplane, but they are also more sensitive to noise in the training data. Nonlinear classifiers sometimes perform better if the training set is large, but by no means in all cases.

14.6 References and further reading

As discussed in Chapter 9, Rocchio relevance feedback is due to Rocchio (Rocchio 1971). It was widely used as a classification method in TREC in the 1990s (Buckley et al. 1994a;b, Voorhees and Harman 2005). Initially, Rocchio classification was a form of *routing*. Routing merely ranks documents according to relevance to a class without assigning them. Early work on *filtering*, a true classification approach that makes an assignment decision on each document, was published by Ittner et al. (1995) and Schapire et al. (1998). Joachims (1997) presents a probabilistic analysis of Rocchio classification.

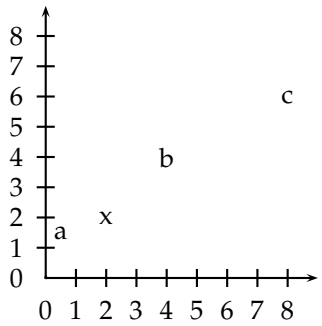
ROUTING
FILTERING

Many authors restrict the name *Roccchio classification* to binary problems and use the terms *cluster-based* Iwayama and Tokunaga (1995) and *centroid-based classification* Han and Karypis (2000), Tan and Cheng (2007) for Rocchio classification with $J > 2$.

CLUSTER-BASED CLASSIFICATION
CENTROID-BASED CLASSIFICATION

A more detailed treatment of kNN can be found in (Hastie et al. 2001), including methods for tuning the parameter k. An example of an approximate fast kNN algorithm is locality-based hashing (Andoni et al. 2007). Kleinberg (1997) presents an approximate $\Theta((M \log^2 M)(M + \log N))$ kNN algorithm (where M is the dimensionality of the space and N the number of data points), but at the cost of exponential storage requirements: $\Theta((N \log M)^{2M})$. Yang (1994) uses an inverted index to speed up kNN classification. The optimality result for 1NN (twice the Bayes error rate asymptotically) is due to Cover and Hart (1967).

See Geman et al. (1992) for a general discussion of the bias-variance tradeoff. Schütze et al. (1995) and Lewis et al. (1996) discuss linear classifiers for text and Hastie et al. (2001) linear classifiers in general. Readers interested in the algorithms mentioned, but not described in this chapter may wish to consult Bishop (2006) for neural networks, Hastie et al. (2001) for linear and logistic regression, and Minsky and Papert (1988) for the perceptron algorithm. Anagnostopoulos et al. (2006) show that an inverted index can be used for highly efficient document classification with any linear classifier, provided that the classifier is still effective when trained on a modest number of features via feature selection.



► **Figure 14.13** Example for differences between Euclidean distance, inner product similarity and cosine similarity. The vectors are $\vec{a} = (0.5 \;\; 1.5)^T$, $\vec{x} = (2 \;\; 2)^T$, $\vec{b} = (4 \;\; 4)^T$, and $\vec{c} = (8 \;\; 6)^T$.

We have only presented the simplest method for combining binary classifiers into a one-of classifier. Another important method is the use of error-correcting codes, where a vector of decisions of different binary classifiers is constructed for each document. A test document's vector is then "corrected" based on the distribution of decision vectors in the training set, a procedure that incorporates information from all binary classifiers and their correlations into the final classification decision (Dietterich and Bakiri 1995). Allwein et al. (2000) propose a general framework for combining binary classifiers.

14.7 Exercises

Exercise 14.1

In Figure 14.13, which of the three vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$ is (i) most similar to $\vec{x}$ according to inner product similarity, (ii) most similar to $\vec{x}$ according to cosine similarity, (iii) closest to $\vec{x}$ according to Euclidean distance?

Exercise 14.2

Download Reuters-21578 and train and test Rocchio and kNN classifiers for the classes *acquisitions*, *corn*, *crude*, *earn*, *grain*, *interest*, *money-fx*, *ship*, *trade*, and *wheat*. Use the ModApte split. You may want to use one of a number of software packages that implement Rocchio classification and kNN classification, for example, the Bow toolkit (McCallum 1996).

Exercise 14.3

Download 20 Newgroups (page 148) and train and test Rocchio and kNN classifiers for its 20 classes.

Exercise 14.4

Create a training set of 300 documents, 100 each from three different languages (e.g., English, French, Spanish). Create a test set by the same procedure, but also add 100

documents from a fourth language. Build (i) a one-of classifier (ii) an any-of classifier that identifies the language of a document and evaluate it on the test set. (iii) Are there any interesting differences in how the classifiers behave on this task?

Exercise 14.5

Show that Rocchio classification can assign a label to a document that is different from its training set label.

Exercise 14.6

Show that the decision boundaries in Rocchio classification are, as in kNN, given by the Voronoi tessellation.

Exercise 14.7

Computing the distance between a dense centroid and a sparse vector is $\Theta(M)$ for a naive implementation that iterates over all M dimensions. Based on the equality $\sum(x_i - \mu_i)^2 = 1.0 + \sum \mu_i^2 + \sum x_i \mu_i$ and assuming that $\sum \mu_i^2$ has been precomputed, write down an algorithm that is $\Theta(M_D)$ instead, where M_D is the average number of types per document.

Exercise 14.8 [⋆ ⋆ ⋆]

Prove that the region of the plane consisting of all points with the same k nearest neighbors is a convex polygon.

Exercise 14.9

Explain why kNN handles multimodal classes better than Rocchio.

Exercise 14.10

Design an algorithm that performs an efficient 1NN search in 1 dimension (where efficiency is with respect to the number of documents N).

Exercise 14.11 [⋆ ⋆ ⋆]

Design an algorithm that performs an efficient 1NN search in 2 dimensions (where efficiency is with respect to the number of documents N).

Exercise 14.12 [⋆ ⋆ ⋆]

Can one design an exact efficient algorithm for kNN for very large k along the ideas you used to solve the last exercise?

Exercise 14.13

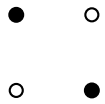
Prove that the number of linear separators of two classes is either infinite or zero.

Exercise 14.14

Show that Equation (14.3) defines a hyperplane with $\vec{w} = \vec{\mu}(c_1) - \vec{\mu}(c_2)$ and $b = 0.5 * (\|\vec{\mu}(c_1)\|^2 - \|\vec{\mu}(c_2)\|^2)$.

Exercise 14.15

We can easily construct non-separable data sets in high dimensions by embedding a non-separable set like the one shown in Figure 14.14. Assume that the number of points of the configuration is small compared to the dimensionality of the space. Explain why such an embedded configuration is likely to become separable in high dimensions after adding noise.



► **Figure 14.14** A simple non-separable set of points.

Exercise 14.16

Assuming two classes, show that the percentage of non-separable assignments of the vertices of a hypercube decreases with dimensionality M for $M > 1$. For example, for $M = 1$ the proportion of non-separable assignments is 0, for $M = 2$, it is $2/16$. One of the two non-separable cases for $M = 2$ is shown in Figure 14.14, the other is its mirror image. Solve the exercise either analytically or by simulation.

Exercise 14.17

Although we point out the similarities of Naive Bayes with linear vector space classifiers, it does not make sense to represent count vectors (the document representations in NB) in a continuous vector space. There is however a formalization of NB that is analogous to Rocchio. Show that NB assigns a document to the class (represented as a parameter vector) whose Kullback-Leibler (KL) divergence (Section 12.4, page 234) to the document (represented as a count vector, normalized to sum to 1) is smallest.

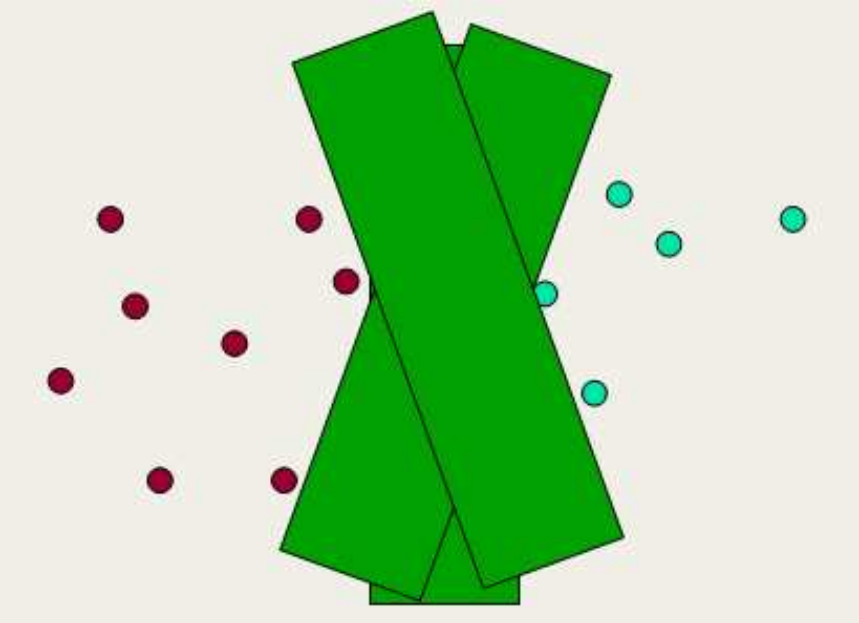
15 *Support vector machines and kernel functions*

Improving classifier effectiveness has been an area of intensive machine-learning research for the last two decades, and this work has led to a new generation of state-of-the-art classifiers, such as support vector machines, boosted decision trees, regularized logistic regression, neural networks, and random forests. Many of these methods, including support vector machines (SVMs), the main topic of this chapter, have been applied with success to information retrieval problems, particularly text classification. We will initially motivate and develop SVMs for the case of two-class data sets that are separable by a linear classifier (Section 15.1), and then extend the model to non-separable data (Section 15.2) and nonlinear models (Section 15.3). The chapter then concludes with more general discussion of experimental results for text classification (Section 15.4) and system design choices and text-specific features to be exploited in all text categorization work (Section 15.5). Support vector machines, otherwise referred to as large-margin classifiers, are not necessarily better than other methods in the above group (except perhaps in low data situations), but they perform at the state-of-the-art level and have much current theoretical and empirical appeal. No one ever got fired for using an SVM.

15.1 Support vector machines: The linearly separable case

For some training data sets, such as the one in Figure 14.8 (page 280), there are lots of possible linear separators. Intuitively, the gray/green one seems better than the black/red one because it draws the decision boundary in the middle of the void between the data. While some learning methods such as the perceptron algorithm just find any linear separator, others search for the best linear separator according to some criterion. The SVM in particular defines the criterion to be looking for a decision surface that is maximally far away from any data points. This distance from the decision surface to the closest data point determines the *margin* of the classifier.

MARGIN



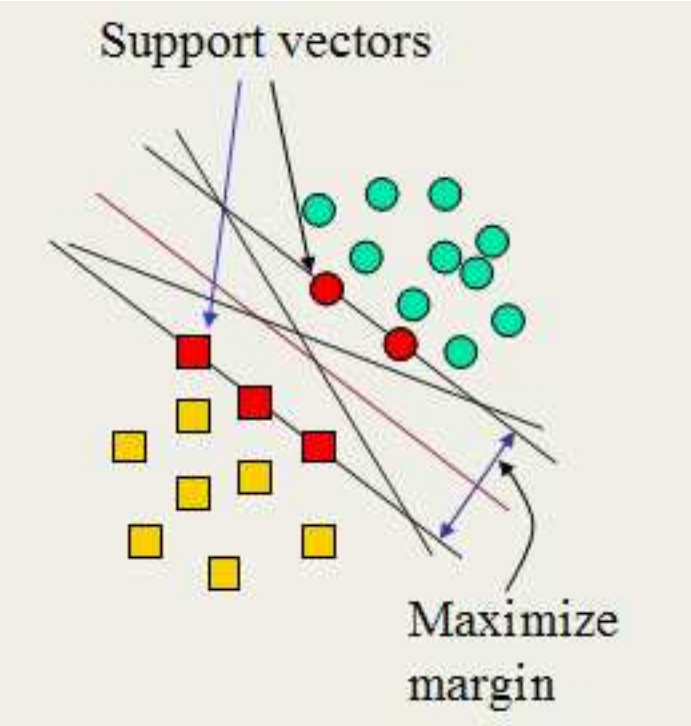
► **Figure 15.1** The intuition of large-margin classifiers. Insisting on a large margin reduces the capacity of the model: the range of angles at which the fat decision surface can be placed is smaller than for a decision hyperplane (cf. Figure 14.8 (page 280)).

This seems like a good thing to do because points near the decision surface represent very uncertain classification decisions: there is almost a 50% chance of the classifier deciding either way. A classifier with a large margin makes no very uncertain classification decisions. Another intuition motivating SVMs is shown in Figure 15.1. By construction, an SVM classifier insists on a large margin around the decision boundary. Compared to a decision hyperplane, if you have to place a fat separator between classes, you have fewer choices of where it can be put. As a result of this, the capacity of the model has been decreased, and hence we expect that its ability to correctly generalize to test data is increased (cf. the discussion of the bias-variance tradeoff in Chapter 14, page 289).

SVMs are inherently two-class classifiers. To do multiclass classification, one has to use one of the methods discussed in Section 14.4 (page 283).

An SVM is constructed to maximize the margin around the separating hyperplane. This necessarily means that the decision function for an SVM is fully specified by a (usually small) subset of the data which defines the position of the separator. These points are referred to as the *support vectors*.

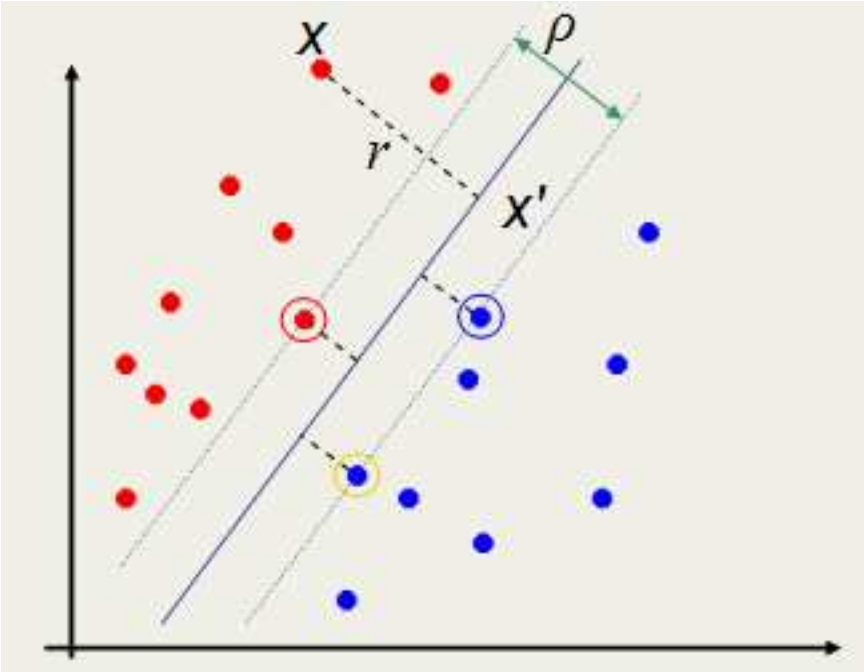
SUPPORT VECTOR



► **Figure 15.2** Support vectors are the points right up against the margin of the classifier.

Figure 15.2 shows the support vectors for a sample problem. Other data points play no part in determining the decision surface that is chosen.

Let us try to formalize this notion with algebra. A decision hyperplane (page 280) can be defined by a decision hyperplane normal vector $\vec{w}$ which is perpendicular to the hyperplane. Because of this perpendicularity, all points $\vec{x}$ on the hyperplane satisfy $\vec{w}^{\mathrm{T}}\vec{x} = 0$. To choose among all the hyperplanes that are perpendicular to the normal vector, we also specify an intercept term b. Now suppose that we have a set of training data points $\{\vec{x}_i\}$ with corresponding classes $\{y_i\}$. For SVMs, the two data classes are always named $+1$ and -1 (rather than 1 and 0), and the intercept term is always explicitly represented as b (rather than being folded into the weight vector $\vec{w}$ by adding an extra always-on feature). The math works out much more cleanly if you do things this way, as we will see almost immediately in the definition of



► **Figure 15.3** The geometric margin of a linear classifier.

functional margin. Our linear classifier is then:

$$f(\vec{x}_i) = \text{sign}(\vec{w}^{\mathrm{T}}\vec{x}_i + b) \tag{15.1}$$

FUNCTIONAL MARGIN

We are confident in the classification of a point if it is far away from the decision boundary. For a given data set and decision hyperplane, we say that the *functional margin* of the i^{th} example $\vec{x}_i$ is $y_i(\vec{w}^{\mathrm{T}}\vec{x}_i + b)$. The functional margin of a dataset is then twice the minimal functional margin of any point in the data set (the factor of 2 comes from measuring across the whole width of the margin, as in Figure 15.2). However, there is a problem with this definition: we can always make the functional margin as big as we wish by simply scaling up $\vec{w}$ and b. For example, if we replace $\vec{w}$ by $5\vec{w}$ and b by $5b$ then the functional margin $y_i(5\vec{w}^{\mathrm{T}}\vec{x}_i + 5b)$ is five times as large. This suggests that we need to place some constraint on the size of the $\vec{w}$ vector. To get a sense of how to do that, let's look at the actual geometry.

What is the Euclidean distance from a point $\vec{x}$ to the decision boundary? Look at Figure 15.3. Let us call the distance we are looking for r. We know that the shortest distance between a point and a hyperplane is perpendicu-

lar to the plane, and hence, parallel to $\vec{w}$. A unit vector in this direction is $\vec{w}/\|\vec{w}\|$. Then, the dotted line in the diagram is a translation of the vector $r\vec{w}/\|\vec{w}\|$. Let us label the point on the hyperplane closest to $\vec{x}$ as $\vec{x}'$. Then we know from the above discussion that:

$$\vec{x}' = \vec{x} - yr\frac{\vec{w}}{\|\vec{w}\|} \tag{15.2}$$

where multiplying by y again just changes the sign for the two cases where $\vec{x}$ is on either side of the decision surface. Moreover, $\vec{x}'$ lies on the decision boundary and so satisfies that $\vec{w}\vec{x}' + b = 0$. Hence:

$$\vec{w}^{\mathrm{T}}(\vec{x} - yr\frac{\vec{w}}{\|\vec{w}\|}) + b = 0$$

Solving for r gives:[1]

$$r = y\frac{\vec{w}^{\mathrm{T}}\vec{x} + b}{\|\vec{w}\|} \tag{15.3}$$

GEOMETRIC MARGIN

Again, the points closest to the separating hyperplane are support vectors. The *geometric margin* of the classifier is the maximum width of the band that can be drawn separating the support vectors of the two classes. That is, it is twice the maximal r defined above, or the maximal width of one of the fat separators shown in Figure 15.1. The geometric margin is clearly invariant to scaling of parameters: if we replace $\vec{w}$ by $5\vec{w}$ and b by $5b$, then the geometric margin is the same, because it is scaled by the length of $\vec{w}$. This means that we can impose any scaling constraint we wish on $\vec{w}$ without affecting anything. Among other choices, requiring $\|\vec{w}\| = 1$ would make the geometric margin the same as the functional margin.

Since we can scale the functional margin as we please, let us require that the functional margin of all data points is at least 1 and that this bound is tight. Then for all items in the data:

$$y_i(\vec{w}^{\mathrm{T}}\vec{x}_i + b) \geq 1$$

and for the support vectors the inequality is an equality. Since each example's distance from the hyperplane is $r_i = y_i(\vec{w}^{\mathrm{T}}\vec{x}_i + b)/\|\vec{w}\|$, the geometric margin is $\rho = 2/\|\vec{w}\|$. Our desire is still to maximize this geometric margin. That is, we want to find $\vec{w}$ and b such that:

- $\rho = 2/\|\vec{w}\|$ is maximized
- For all $\{(\vec{x}_i, y_i)\}$, $y_i(\vec{w}^{\mathrm{T}}\vec{x}_i + b) \geq 1$

1. Recall that $\|\vec{w}\| = \sqrt{\vec{w}^{\mathrm{T}}\vec{w}}$.

Now noting that maximizing $2/\|\vec{w}\|$ is the same as minimizing $\|\vec{w}\|/2$, we have the standard final formulation as a minimization problem:

(15.4) Find $\vec{w}$ and b such that:

- $\frac{1}{2}\vec{w}^{\mathrm{T}}\vec{w}$ is minimized
- and for all $\{(\vec{x}_i, y_i)\}$, $y_i(\vec{w}^{\mathrm{T}}\vec{x}_i + b) \geq 1$

QUADRATIC PROGRAMMING

This is now optimizing a quadratic function subject to linear constraints. *Quadratic optimization* problems are a standard, well-known class of mathematical optimization problem, and many algorithms exist for solving them. We could in principle build our SVM using standard quadratic programming (QP) libraries, though in practice there are more specialized and much faster libraries available especially for building SVMs. There has been much research in this area and many fast but intricate algorithms exist for this problem. However, we will not present the details here. It is enough to understand how the problem is set up as a QP problem. Thereafter, there are only about 20 people in the world who don't use one of the standard SVM software packages to build models.

Nevertheless, to understand the mechanism for doing nonlinear classification with SVMs, we need to present a fraction more of how SVMs are solved although we will omit the details. The solution involves constructing a dual problem where a Lagrange multiplier α_i is associated with every constraint in the primary problem:

(15.5) Find $\alpha_1, \ldots \alpha_N$ such that $\sum \alpha_i - \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j \vec{x}_i^{\mathrm{T}} \vec{x}_j$ is maximized, and

- $\sum_i \alpha_i y_i = 0$
- $\alpha_i \geq 0$ for all $1 \leq i \leq N$

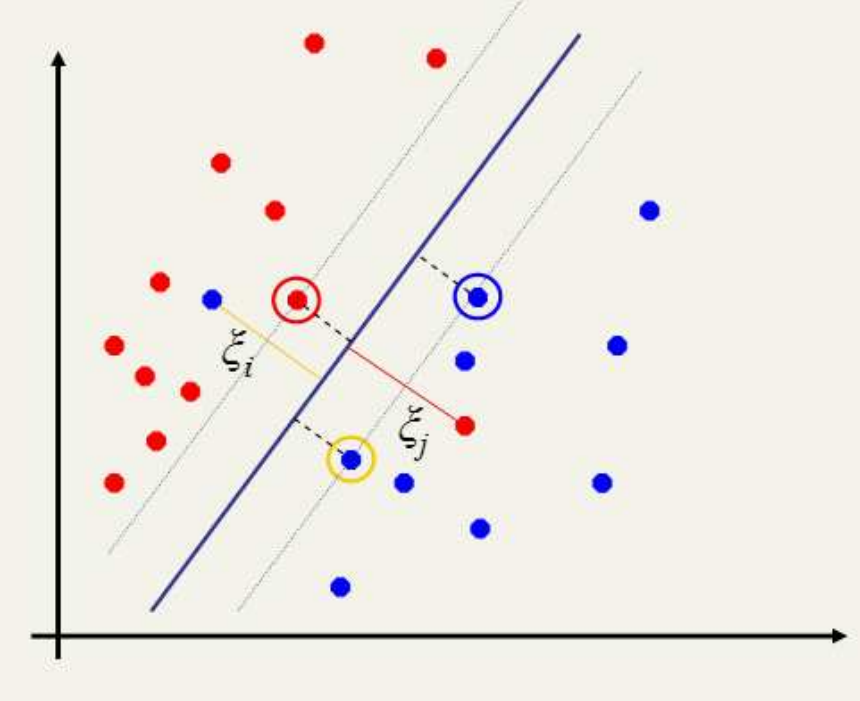
The solution is then of the form:

(15.6) $\vec{w} = \sum \alpha_i y_i \vec{x}_i$
$b = y_k - \vec{w}^{\mathrm{T}}\vec{x}_k$ for any $\vec{x}_k$ such that $\alpha_k \neq 0$

In the solution, most of the α_i are zero. Each non-zero α_i indicates that the corresponding $\vec{x}_i$ is a support vector. The classification function is then:

$$f(\vec{x}) = \text{sign}(\sum \alpha_i y_i \vec{x}_i^{\mathrm{T}} \vec{x} + b)$$

Notice that both the term to be maximized in the dual problem and the classifying function involve an *inner product* between pairs of points ($\vec{x}$ and $\vec{x}_i$ or $\vec{x}_i$ and $\vec{x}_j$), and that is the only way the data is used – we will return to the significance of this later.



► **Figure 15.4** Large margin classification with slack variables.

15.2 Soft margin classification

For the very high dimensional problems common in text classification, sometimes the data is linearly separable. But in the general case it is not, and even if it is, we might prefer a solution that better separates the bulk of the data while ignoring a couple of weird outlier points.

SLACK VARIABLES

If the training set is not linearly separable, the standard approach is to introduce *slack variables* ξ_i which allow misclassification of difficult or noisy examples. In this model, the fat decision margin is allowed to make a few mistakes, and we pay a cost for each misclassified example which depends on how far away from the decision surface it is. See Figure 15.4.

The formulation of the optimization problem with slack variables is then:

(15.7) Find $\vec{w}$, b, and $\xi_i \geq 0$ such that:

- $\frac{1}{2}\vec{w}^{\mathrm{T}}\vec{w} + C\sum_i \xi_i$ is minimized
- and for all $\{(\vec{x}_i, y_i)\}$, $y_i(\vec{w}^{\mathrm{T}}\vec{x}_i + b) \geq 1 - \xi_i$

The optimization problem is then trading off how fat it can make the margin versus how many points have to be moved around to allow this margin. The margin can be less than 1 for a point $\vec{x}_i$ by setting $\xi_i > 0$, but then one pays a penalty of $C\xi_i$ in the minimization for having done that. The parameter C is a *regularization* term, which provides a way to control overfitting: as C becomes large, it is unattractive to not respect the data at the cost of reducing the geometric margin, while when it is small, it is easy to account for some data points with the use of slack variables and to have the fat margin placed so it models the bulk of the data.

REGULARIZATION

The dual problem for soft margin classification becomes:

(15.8) Find $\alpha_1, \ldots \alpha_N$ such that $\sum \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j \vec{x}_i^{\mathrm{T}} \vec{x}_j$ is maximized, and

- $\sum_i \alpha_i y_i = 0$
- $0 \leq \alpha_i \leq C$ for all $1 \leq i \leq N$

Note that neither the slack variables ξ_i nor Lagrange multipliers for them appear in the dual problem. All we are left with is the constant C bounding the possible size of the Lagrange multipliers for the support vector data points. Again, the $\vec{x}_i$ with non-zero α_i will be the support vectors, and typically they will be a small proportion of the data. The solution of the dual problem is of the form:

(15.9) $\vec{w} = \sum \alpha y_i \vec{x}_i$
$b = y_k(1 - \xi_k) - \vec{w}^{\mathrm{T}} \vec{x}_k$ for $k = \arg\max_k \alpha_k$

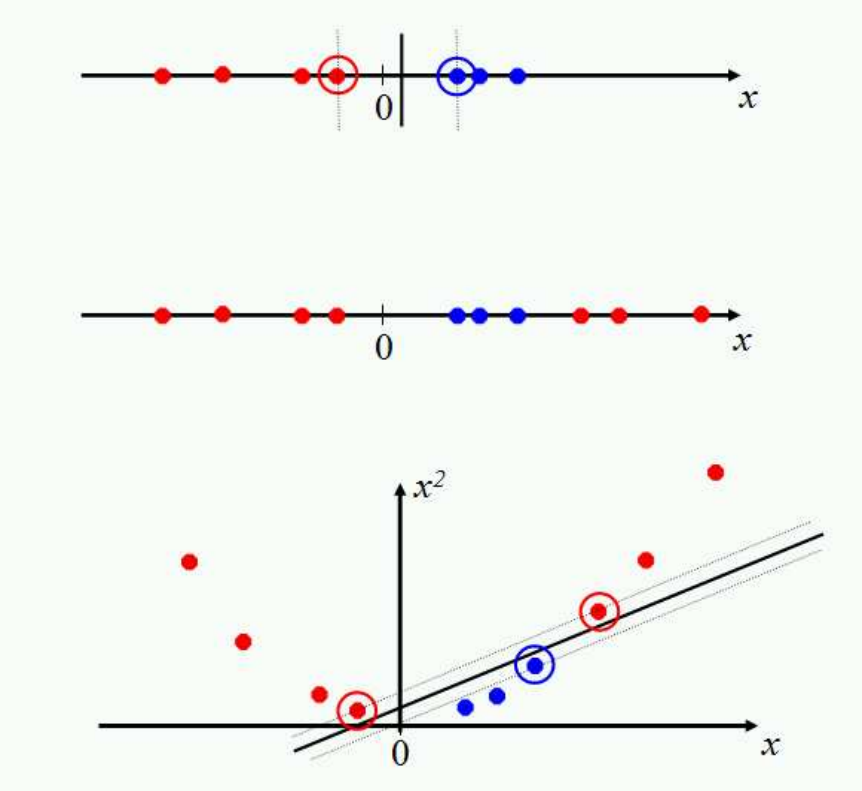
Again $\vec{w}$ is not needed explicitly for classification, which can be done simply in terms of the dot product of data points:

$$f(\vec{x}) = \sum_i \alpha_i y_i \vec{x}_i^{\mathrm{T}} \vec{x} + b$$

Given a new point $\vec{x}$ to classify, the classification function is computing the projection of the point onto the hyperplane normal. This will determine which class to assign to the point. If the point is within the margin of the classifier (or another confidence threshold t that we might have determined to avoid classification mistakes) then the classifier can return "don't know" rather than one of the two classes.

15.3 Nonlinear SVMs

With what we have presented so far, data sets that are linearly separable (perhaps with a few exceptions or some noise) are well-handled. But what are we going to do if the data set is just too hard – in the sense that it just doesn't allow classification by a linear classifier. Let us look at a one-dimensional case



► **Figure 15.5** Projecting nonlinearly separable data into a higher dimensional space can make it linearly separable.

for motivation. The top data set in Figure 15.5 is straightforwardly classified by a linear classifier but the middle data set is not. We instead need to be able to pick out an interval. One way to solve this problem is to map the data on to a higher dimensional space and then to use a linear classifier in the higher dimensional space. For example, the bottom part of the figure shows that a linear separator can easily classify the data if we use a quadratic function to map the data into two dimensions (a polar coordinates projection would be another possibility). The general idea is to map the original feature space to some higher-dimensional feature space where the training set is separable. Though, of course, we would want to do so in ways that preserve relevant notions of data point relatedness, so that the resultant classifier should still generalize well. Kernels can make a non-separable problem separable, and they can map data into a better representational space.

KERNEL TRICK

SVMs, and also a number of other linear classifiers, provide an easy and efficient way of doing this mapping to a higher dimensional space, which is referred to as "the *kernel trick*". It's not really a trick: it just exploits the math that we have seen. The SVM linear classifier relies on an inner product between data point vectors. Let $K(\vec{x}_i, \vec{x}_j) = \vec{x}_i^{\mathrm{T}} \vec{x}_j$. Then the classifier is

$$f(\vec{x}) = \sum_i \alpha_i y_i K(\vec{x}_i, \vec{x}) + b \tag{15.10}$$

KERNEL FUNCTION

Now consider if we decided to map every data point into a higher dimensional space via some transformation $\Phi: \vec{x} \mapsto \phi(\vec{x})$. Then the inner product becomes $\phi(\vec{x}_i)^{\mathrm{T}} \phi(\vec{x}_j)$. If it turned out that this inner product (which is just a real number) could be computed simply and efficiently in terms of the original data points, then we wouldn't have to actually map from $\vec{x} \mapsto \phi(\vec{x})$. Rather, we could simply compute the quantity $K(\vec{x}_i, \vec{x}_j) = \phi(\vec{x}_i)^{\mathrm{T}} \phi(\vec{x}_j)$, and then use the function's value in Equation (15.10). A *kernel function* K is such a function that corresponds to an inner product in some expanded feature space.

For example, for 2-dimensional vectors $\vec{x} = (x_1, x_2)$, let $K(\vec{x}_i, \vec{x}_j) = (1 + \vec{x}_i^{\mathrm{T}} \vec{x}_j)^2$. We wish to show that this is a kernel, i.e., that $K(\vec{x}_i, \vec{x}_j) = \phi(\vec{x}_i)^{\mathrm{T}} \phi(\vec{x}_j)$ for some ϕ. Consider $\phi(\vec{x}) = (1, x_1^2, \sqrt{2}x_1 x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2)$. Then:

$$\begin{aligned} K(\vec{x}_i, \vec{x}_j) = (1 + \vec{x}_i^{\mathrm{T}} \vec{x}_j)^2 &= 1 + x_{i1}^2 x_{j1}^2 + 2x_{i1}x_{j1}x_{i2}x_{j2} + x_{i2}^2 x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} \\ &= [1 \; x_{i1}^2 \; \sqrt{2}x_{i1}x_{i2} \; x_{i2}^2 \sqrt{2}x_{i1} \; \sqrt{2}x_{i2}]^{\mathrm{T}} [1 \; x_{j1}^2 \; \sqrt{2}x_{j1}x_{j2} \; x_{j2}^2 \sqrt{2}x_{j1} \; \sqrt{2}x_{j2}] \\ &= \phi(\vec{x}_i)^{\mathrm{T}} \phi(\vec{x}_j) \end{aligned}$$

KERNEL
MERCER KERNELS

What kinds of functions are valid *kernel functions* (sometimes more precisely referred to as *Mercer kernels*, because they satisfy Mercer's condition)? The function K must be continuous, symmetric, and have a positive definite gram matrix. Such a K means that there exists a mapping to a reproducing kernel Hilbert space (a Hilbert space is a vector space closed under dot products) such that the dot product there equals the value of K. If you know a fair amount of functional analysis, those last two sentences might have made sense; if you don't but would like to, you should consult the books on SVMs in the references; and if you're in neither of those two groups, you can content yourself with knowing that 90% of work with kernels uses one of two straightforward families of functions of two vectors, which do define valid kernels.

These two common families of kernels are polynomial kernels and radial basis functions. Polynomial kernels are of the form $K(\vec{x}, \vec{z}) = (1 + \vec{x}^{\mathrm{T}} \vec{z})^d$. The case of $d = 1$ is a linear kernel, which is what we had before we started talking about kernels (the constant 1 just changing the threshold). The case

of $d = 2$ gives a quadratic kernel, and is very commonly used. We illustrated the quadratic kernel above. The most common form of radial basis function is a Gaussian distribution, calculated as:

$$K(\vec{x}, \vec{z}) = e^{-\|\vec{x}-\vec{z}\|^2/(2\sigma^2)}$$

A radial basis function is equivalent to mapping the data into an infinite dimensional Hilbert space, and so we can't illustrate the radial basis function in the same way as we did for a quadratic kernel. Beyond these two families, there has been interesting work developing other kernels, some of which is promising for text applications. In particular, there has been investigation of string kernels.

The world of SVMs comes with its own language, which is rather different from the language otherwise used in machine learning. The terminology does have deep roots in mathematics, even though most people who use SVMs don't really understand those roots and just use the terminology because others do and it sounds cool. It's important not to be too awed by that terminology. Really, we are talking about some quite simple things. A polynomial kernel allows you to model feature conjunctions (up to the order of the polynomial). Simultaneously you also get the powers of the basic features – for most text applications, that probably isn't useful, but just comes along with the math and hopefully doesn't do harm. A radial basis function (RBF) allows one to have features that pick out circles (hyperspheres) – although the decision boundaries become much more complex as multiple such features interact. A string kernel lets you have features that are character subsequences of words. All of these are straightforward notions which have also been used in many other places under different names.

15.4 Experimental data

Experiments have shown SVMs to be a very effective text classifier. Dumais et al. (1998) compared a Rocchio variant, Naive Bayes, a more general Bayes Net classifier, Decision Trees, and SVM classifiers on the 10 largest classes in the Reuters-21578 Test Collection, which was introduced in Chapter 13 (page 261). Some of their results are shown in Table 15.1, with SVMs clearly performing best. This was one of several pieces of work that established the strong reputation of SVMs for text classification. Another comparison from around the same time was work by Joachims (1998). Some of his results are shown in Table 15.2. Joachims uses a large number of word features and reports notable gains from using higher order polynomial or RBF kernels. However, Dumais et al. (1998) used MI feature selection (Section 13.5.1, page 254) to build classifiers with a much more limited number of features (300) and got as good or better results than Joachims with just linear SVMs.

	Rocchio	NB	BayesNets	Trees	SVM (poly degree = 1)
earn	92.9%	95.9%	95.8%	97.8%	98.0%
acq	64.7%	87.8%	88.3%	89.7%	93.6%
money-fx	46.7%	56.6%	58.8%	66.2%	74.5%
grain	67.5%	78.8%	81.4%	85.0%	94.6%
crude	70.1%	79.5%	79.6%	85.0%	88.9%
trade	65.1%	63.9%	69.0%	72.5%	75.9%
interest	63.4%	64.9%	71.3%	67.1%	77.7%
ship	49.2%	85.4%	84.4%	74.2%	85.6%
wheat	68.9%	69.7%	82.7%	92.5%	91.8%
corn	48.2%	65.3%	76.4%	91.8%	90.3%
micro-Avg Top 10	64.6%	81.5%	85.0%	88.4%	92.0%
micro-Avg All Cat	61.7%	75.2%	80.0%	N/A	87.0%

► **Table 15.1** SVM classifier break-even F_1 from Dumais et al. (1998). Results are shown for the 10 largest categories and over all categories on the Reuters-21578 data set. Micro- and macro-averaging were defined in Table 13.7 (page 263).

					SVM (poly degree)					SVM (rbf width)			
	NB	Rocchio	Trees	kNN	1	2	3	4	5	0.6	0.8	1.0	1.2
earn	95.9	96.1	96.1	97.3	98.2	98.4	98.5	98.4	98.3	98.5	98.5	98.4	98.3
acq	91.5	92.1	85.3	92.0	92.6	94.6	95.2	95.2	95.3	95.0	95.3	95.3	95.4
money-fx	62.9	67.6	69.4	78.2	66.9	72.5	75.4	74.9	76.2	74.0	75.4	76.3	75.9
grain	72.5	79.5	89.1	82.2	91.3	93.1	92.4	91.3	89.9	93.1	91.9	91.9	90.6
crude	81.0	81.5	75.5	85.7	86.0	87.3	88.6	88.9	87.8	88.9	89.0	88.9	88.2
trade	50.0	77.4	59.2	77.4	69.2	75.5	76.6	77.3	77.1	76.9	78.0	77.8	76.8
interest	58.0	72.5	49.1	74.0	69.8	63.3	67.9	73.1	76.2	74.4	75.0	76.2	76.1
ship	78.7	83.1	80.9	79.2	82.0	85.4	86.0	86.5	86.0	85.4	86.5	87.6	87.1
wheat	60.6	79.4	85.5	76.6	83.1	84.5	85.2	85.9	83.8	85.2	85.9	85.9	85.9
corn	47.3	62.2	87.7	77.9	86.0	86.5	85.3	85.7	83.9	85.1	85.7	85.7	84.5
microavg.	72.0	79.9	79.4	82.3	84.2	85.1	85.9	86.2	85.9	86.4	86.5	86.3	86.2

► **Table 15.2** SVM classifier break-even F_1 from Joachims (1998). Results are shown for the 10 largest categories on the Reuters-21578 data set.

This mirrors the results discussed in Chapter 14 (page 279) on other linear approaches like Naive Bayes. At a minimum, it seems that working with simple word features can get one a long way. It is also noticeable the degree to which the two papers' results for other learning methods differ. In text classification, there's always more to know than simply which machine learning algorithm was used.

These and other results have shown that simple classifiers such as Naive Bayes classifiers are uncompetitive with classifiers like SVMs when trained

and tested on independent and identically distributed (i.i.d.) data, that is, uniform data with all the good properties of statistical sampling. However, these differences may often be invisible or even reverse themselves when working in the real world where, usually, the training sample is drawn from a subset of the data to which the classifier will be applied, the nature of the data drifts over time rather than being stationary, and there may well be errors in the data (among other problems). For general discussion of this issue see Hand (2006). Many practitioners have had the experience of being unable to build a fancy classifier for a certain problem that consistently performs as well as Naive Bayes.

15.5 Issues in the classification of text documents

Most of our discussion of classification has focused on introducing various machine learning methods rather than discussing particular features of text documents relevant to classification. This bias is appropriate for a textbook, but is misplaced for an application developer. It is frequently the case that greater performance gains can be achieved from exploiting domain-specific text features than from changing from one machine learning classifier to another. In this section we wish to step back a little and consider the applications of text classification, the space of possible solutions, and the utility of application-specific heuristics.

There are lots of applications of text classification in the commercial world; email spam filtering is perhaps now the most ubiquitous.

15.6 References and further reading

There are now a number of books dedicated to SVMs, large margin learning, and kernels of which currently the two best are probably Schölkopf and Smola (2001) and Shawe-Taylor and Cristianini (2004). Well-known, good article length introductions are Burges (1998) and Chen et al. (2005), the latter of which introduces the more recent ν-SVM, which provides an alternative parameterization for dealing with inseparable problems, whereby rather than specifying a penalty C, one specifies a parameter ν which bounds the number of examples which can appear on the wrong side of the decision surface. For the foundations by their originator, see Vapnik (1998). Other recent, more general books on statistical learning also give thorough coverage to SVMs, for example, Hastie et al. (2001).

The kernel trick was first presented in (Aizerman et al. 1964). For more about string kernels and other kernels for structured data, see (Lodhi et al. 2002, Gaertner et al. 2002). The Advances in Neural Information Processing (NIPS) conferences have become the premier venue for theoretical machine

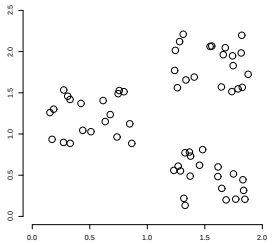
learning work, such as on SVMs. Other venues such as SIGIR are much stronger on experimental methodology and using text-specific features to improve classifier effectiveness.

A recent comparison of most current machine learning classifiers (though on problems rather different from typical text problems) can be found in Caruana and Niculescu-Mizil (2006). Older examinations of a more limited set of classifiers on text classification problems can be found in (Yang 1999, Yang and Liu 1999, Dumais et al. 1998). Joachims (2002a) presents his work on SVMs applied to text problems in detail. Zhang and Oles (2001) have insightful comparisons of Naive Bayes, regularized logistic regression and SVM classifiers.

16 *Flat clustering*

CLUSTER

Clustering algorithms group a set of documents into subsets or *clusters*. The algorithms' goal is to create clusters that are coherent internally, but clearly different from each other. In other words, documents within a cluster should be as similar as possible; and documents in one cluster should be as dissimilar as possible from documents in other clusters.



► **Figure 16.1** An example of a data set with a clear cluster structure.

UNSUPERVISED LEARNING

Clustering is the most common form of *unsupervised learning*. No supervision means that there is no human expert who has assigned documents to classes. In clustering, it is the distribution and makeup of the data that will determine cluster membership. A simple example is Figure 16.1. It is visually clear that there are three distinct clusters of points. This chapter and Chapter 17 introduce algorithms that find such clusters in an unsupervised fashion.

The difference between clustering and classification may not seem great at first. After all, in both cases we have a partition of a set of documents into groups. But as we will see the two problems are fundamentally different. In supervised classification (Chapter 13, page 240), our goal is to replicate a categorical distinction that a human supervisor imposes on the data. In

unsupervised learning, of which clustering is the most important example, we have no such teacher that would guide us.

The key input to a clustering algorithm is the similarity measure. In Figure 16.1, it is the different degrees of closeness of points to each other that define three different clusters. In document clustering, the similarity measure is usually vector space similarity (Chapter 6) or a similarity measure based on Euclidean distance. Different similarity measures give rise to different clusterings. Thus, the similarity measure is an important means by which we can influence the outcome of clustering.

FLAT CLUSTERING

Flat clustering creates a flat set of clusters without any explicit structure that would relate clusters to each other. *Hierachical algorithms* create a hierarchy of clusters and will be covered in Chapter 17. Chapter 17 also addresses the difficult problem of labeling clusters automatically.

HARD CLUSTERING
HARD ASSIGNMENT
SOFT CLUSTERING
SOFT ASSIGNMENT

A second important distinction is between hard and soft clustering algorithms. *Hard clustering* computes a *hard assignment* – each document is a member of exactly one cluster. The assignment of *soft clustering algorithms* is *soft* – a document's assignment is a distribution over all clusters. In a soft assignment, a document has fractional membership in several clusters. Latent semantic indexing, a form of dimensionality reduction, is a soft clustering algorithm (Chapter 18, page 371).

This chapter motivates the use of clustering in information retrieval by introducing a number of applications (Section 16.1), defines the problem we are trying to solve in clustering (Section 16.2) and discusses measures for evaluating cluster quality (Section 16.3). It then describes two flat clustering algorithms, K-means (Section 16.4), a hard clustering algorithm, and the Expectation-Maximization (or EM) algorithm (Section 16.5), a soft clustering algorithm. K-means is perhaps the most widely used flat clustering algorithm due to its simplicity and efficiency. The EM algorithm is a generalization of K-means and can be applied to a large variety of document representations and distributions.

16.1 Clustering in information retrieval

CLUSTER HYPOTHESIS

The *cluster hypothesis* states the fundamental assumption we make when using clustering in information retrieval.

> **Cluster hypothesis.** Documents in the same cluster behave similarly with respect to relevance to information needs.

The hypothesis states that if there is a document from a cluster that is relevant to a search request, then it is likely that other documents from the same cluster are also relevant. This is because clustering puts together documents that share many words. The cluster hypothesis essentially is the contigu-

Application	What is clustered?	Benefit	Example
Search result clustering	search result	more effective information presentation to user	Figure 16.2
Scatter-Gather	(subsets of) collection	alternative user interface: "search without typing"	Figure 16.3
Collection clustering	collection	effective information presentation for exploratory browsing	McKeown et al. (2002), http://news.google.com
Language modeling	collection	increased precision and/or recall	Liu and Croft (2004)
Cluster-based retrieval	collection	higher efficiency: faster search	Salton (1971a)

► **Table 16.1** Some applications of clustering in information retrieval.

ity hypothesis in Chapter 14 (page 269). In both cases, we posit that similar documents behave similarly with respect to relevance.

Table 16.1 shows some of the main applications of clustering in information retrieval. They differ in the set of documents that they cluster – search result, collection or subsets of the collection – and the aspect of an information retrieval system they try to improve – user experience, user interface, effectiveness or efficiency of the search system. But they are all based on the basic assumption stated by the cluster hypothesis.

The first application mentioned in Table 16.1 is *search result clustering* where search result refers to the set of documents that were returned for the query. The default presentation of search results in information retrieval is a simple list. Users scan the list from top to bottom until they have found the information they are looking for. Instead, search result clustering clusters the search result, so that similar documents appear together. It is often easier to scan a few coherent groups than many individual documents. This is particularly useful if a search term has different word senses. The example in Figure 16.2 is jaguar. Three frequent senses on the web refer to the car, the animal and an Apple operating system. The *Clustered Results* panel returned by the Vivísimo search engine (http://vivisimo.com) can be a more effective user interface for understanding what is in the search result than a simple list of documents.

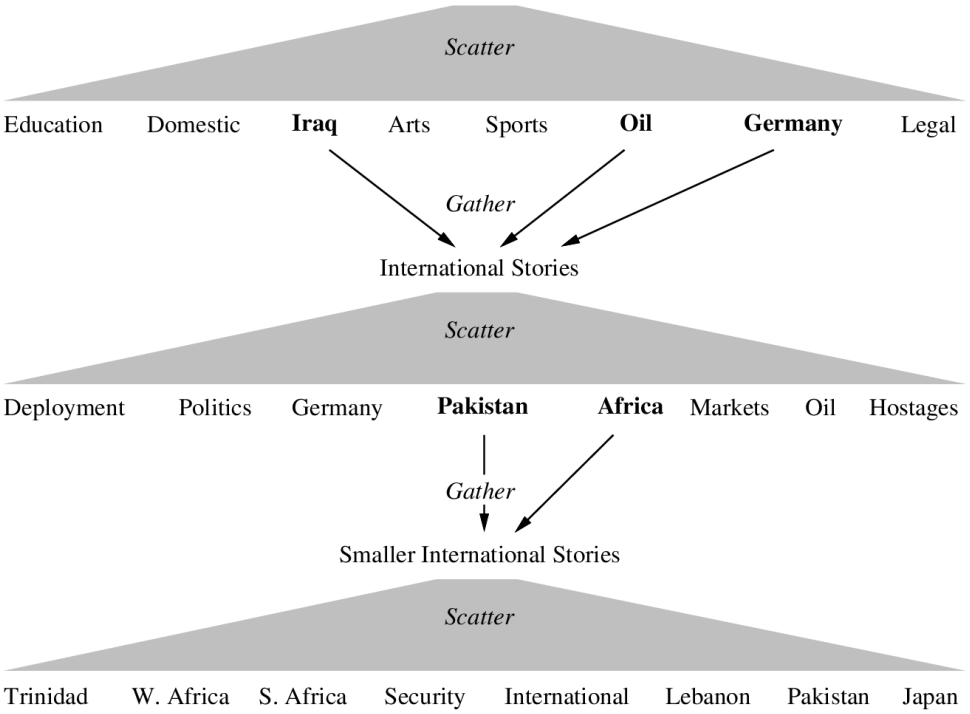
SCATTER-GATHER

A better user interface is also the goal of *Scatter-Gather*, the second application in Table 16.1. Scatter-Gather clusters the whole collection to get groups of documents that the user can select or *gather*. The selected groups are merged and the resulting set is again clustered. This process is repeated until a cluster of interest is found. An example is shown in Figure 16.3.

► **Figure 16.2** Clustering of search results to improve user recall. None of the top hits cover the animal sense of jaguar, but users can easily access it by clicking on the *cat* cluster in the *Clustered Results* panel on the left (third arrow from the top).

Automatically generated clusters like those in Figure 16.3 are not as neatly organized as a manually constructed hierarchical tree like the Open Directory at http://dmoz.org. Also, finding descriptive labels for clusters automatically is a difficult problem (Section 17.7, page 353). But cluster-based navigation is an interesting alternative to keyword searching, the standard information retrieval paradigm. This is especially true in scenarios where users prefer browsing over searching because they are unsure about which search terms to use.

As an alternative to the user-mediated iterative clustering in Scatter-Gather, we can also compute a static hierarchical clustering of a collection that is not influenced by user interactions ("Collection clustering" in Table 16.1). Google News and its precursor, the Columbia NewsBlaster system, are examples of this approach. In the case of news, we need to frequently recompute the clustering to make sure that users can access the latest breaking stories. Clustering is well suited for access to a collection of news stories since news reading is not really search, but rather a process of selecting a subset of stories about recent events.



► **Figure 16.3** An example of a user session in Scatter-Gather. A collection of New York Times news stories is clustered ("scattered") into eight clusters (top row). The user manually *gathers* three of these into a smaller collection *International Stories* and performs another scattering operation. This process repeats until a small cluster with relevant documents is found (e.g., *Trinidad*).

The fourth application of clustering exploits the cluster hypothesis directly for improving search results, based on a clustering of the entire collection. We use a standard inverted index to identify an initial set of documents that match the query, but we then add other documents from the same clusters even if they have low similarity to the query. For example, if the query is car and several car documents are taken from a cluster of automobile documents, then we can add documents from this cluster that use terms other than car (automobile, vehicle etc). This can increase recall since a group of documents with high mutual similarity is often relevant as a whole.

More recently this idea has been used for language modeling. Equation (12.5), page 230, showed that to avoid sparse data problems in the language modeling approach to IR, the model of document d can be interpolated with a

collection model. But the collection contains many documents with words untypical of d. By replacing the collection model with a model derived from d's cluster, we get more accurate estimates of the occurrence probabilities of words in d.

Clustering can also speed up search. As we saw in Section 6.4.2, page 119, search in the vector space model amounts to finding the nearest neighbors to the query. The inverted index supports fast nearest-neighbor search for the standard IR setting. However, sometimes we may not be able to use an inverted index efficiently, e.g., in latent semantic indexing (Chapter 18). In such cases, we could compute the similarity of the query to every document, but this is slow. The cluster hypothesis offers an alternative: Find the clusters that are closest to the query and only consider documents from these clusters. Within this much smaller set, we can compute similarities exhaustively and rank documents in the usual way. Since there are many fewer clusters than documents, finding the closest cluster is fast; and since the documents matching a query are all similar to each other, they tend to be in the same clusters. While this algorithm is inexact, the expected decrease in search quality is small. This is essentially the application of clustering that was covered in Section 7.1.6 (page 133).

16.2 Problem statement

We can define the goal in hard flat clustering as follows. Given (i) a set of documents $D = \{d_1, \ldots, d_N\}$, (ii) a desired number of clusters K, and (iii) an *objective function* that evaluates the quality of a clustering, we want to compute an assignment $\gamma : D \rightarrow \{1, \ldots, K\}$ that minimizes (or, in other cases, maximizes) the objective function. In most cases, we also demand that γ is surjective, i.e., that none of the K clusters is empty.

OBJECTIVE FUNCTION

The objective function is often defined in terms of similarity or distance between documents. Below, we will see that the objective in K-means clustering is to minimize the average distance between documents and their centroids or, equivalently, to maximize the average similarity between documents and their centroids. The discussion of similarity measures and distance metrics in Chapter 14 (page 270) also applies to this chapter. As in Chapter 14, we use both similarity and distance to talk about relatedness between documents.

For documents, the type of similarity we want is usually topic similarity or common high values on the same dimensions in the vector space model. For example, documents about China have high values on dimensions like Chinese, Beijing, and Mao whereas documents about the UK tend to have high values for London, Britain and Queen. We approximate topic similarity with cosine similarity or Euclidean distance in vector space (Chapter 6). If the intended similarity is something else, for example, language, then a differ-

ent representation may be appropriate. When computing topic similarity, stop words can be safely ignored, but they are important cues for separating clusters of English (in which the occurs frequently and la infrequently) and French documents (in which the occurs infrequently and la frequently).

16.2.1 Cardinality – the number of clusters

CARDINALITY

A difficult issue in clustering is determining the *cardinality* of a clustering, the number K of clusters. Often K is nothing more than a good guess based on experience or domain knowledge. But for K-means, we will also introduce a heuristic method for choosing K and an attempt to incorporate the selection of K into the objective function. Sometimes the application puts constraints on the range of K. For example, the Scatter-Gather interface in Figure 16.3 could not display more than about $K = 10$ clusters per layer because of the size and resolution of computer monitors in the early 1990s.

Since our goal is to optimize an objective function, clustering is essentially a search problem. The brute force solution would be to enumerate all possible clusterings and pick the best. However, for N documents and K clusters, there are $\leq K^N$ different partitions, so this approach is not feasible.[1] For this reason, most flat clustering algorithms refine an initial partitioning iteratively. If the search starts at an unfavorable initial point, we may miss the global optimum. Finding a good starting point is therefore another important problem we have to solve in flat clustering.

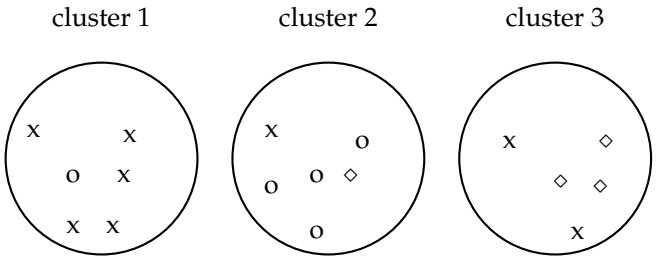
16.3 Evaluation of clustering

Typical objective functions in clustering formalize the goal of attaining high intra-cluster similarity (documents within a cluster are similar) and low inter-cluster similarity (documents from different clusters are dissimilar). This is an *internal criterion* for the quality of a clustering. But good scores on an internal criterion do not necessarily translate into good effectiveness in an application. An alternative to internal criteria is direct evaluation in the application of interest. For search result clustering, we may want to measure the time it takes users to find an answer with different clustering algorithms. This is the most direct evaluation, but it is expensive, especially if large user studies are necessary.

INTERNAL CRITERION OF QUALITY

As a surrogate for user judgments, we can use a set of classes in an evaluation benchmark or gold standard (see Section 8.5, page 155, and Section 13.6, page 261). The gold standard is ideally produced by human judges with a

1. A tigher bound is $\leq K^N/N!$. The exact number of different partitions of N documents into K clusters is the Stirling number of the second kind. See http://mathworld.wolfram.com/StirlingNumberoftheSecondKind.html or Comtet (1974).



► **Figure 16.4** Purity as an external evaluation criterion for cluster quality. Majority class and number of members of the majority class for the three clusters are: X, 5 (cluster 1); circle, 4 (cluster 2); and diamond, 3 (cluster 3). Purity is $(1/17) * (5 + 4 + 3) \approx 0.71$.

EXTERNAL CRITERION OF QUALITY

good level of inter-judge agreement (see Chapter 8, page 146). We can then compute an *external criterion* that evaluates how well the clustering matches the gold standard classes. For example, we may want to say that the optimal clustering of the search result for jaguar in Figure 16.2 consists of three classes corresponding to the three senses *car*, *animal*, and *operating system*.

This section introduces four external criteria of clustering quality. *Purity* is a simple and transparent evaluation measure. *Normalized mutual information* is information-theoretically motivated and can therefore be more easily interpreted than other measures. The *Rand index* penalizes both false positive and false negative decisions during clustering. The *F measure* in addition supports differential weighting of these two types of errors.

PURITY

To compute *purity*, each cluster is assigned to the class which is most frequent in the cluster, and then the accuracy of this assignment is measured by counting the number of correctly assigned documents and dividing by N. Formally:

$$\text{purity}(\Omega, \mathbb{C}) = \frac{1}{N} \sum_k \max_j |\omega_k \cap c_j| \tag{16.1}$$

where $\Omega = \{\omega_1, \omega_2, \ldots, \omega_K\}$ is the set of clusters and $\mathbb{C} = \{c_1, c_2, \ldots, c_J\}$ is the set of classes. We present an example of how to compute purity in Figure 16.4[2]. Bad clusterings have purity values close to 0, a perfect clustering has a purity of 1.0. Purity is compared with the other three measures discussed in this chapter in Table 16.2.

High purity is easy to achieve when the number of clusters is large – in particular, purity is 1.0 if each document gets its own cluster. Thus, we can-

2. Recall our note of caution from Figure 14.2 (page 272) when looking at this and other 2D figures in this and the following chapter: these illustrations can be misleading because 2D projections of length-normalized vectors distort similarities and distances between points.

	purity	NMI	RI	F_5
minimum	0.0	0.0	0.0	0.0
maximum	1.0	1.0	1.0	1.0
value for Figure 16.4	0.71	0.36	0.68	0.46

► **Table 16.2** The four external evaluation measures applied to the clustering in Figure 16.4.

not use purity to trade off the quality of the clustering against the number of clusters.

NORMALIZED MUTUAL INFORMATION

A measure that allows us to make this tradeoff is *normalized mutual information* or *NMI*:

$$\text{NMI}(\Omega, \mathbb{C}) = \frac{I(\Omega;\mathbb{C})}{[H(\Omega) + H(\mathbb{C})]/2} \tag{16.2}$$

I is mutual information (cf. Chapter 13, page 254):

$$I(\Omega;\mathbb{C}) = \sum_k \sum_j P(\omega_k \cap c_j) \log \frac{P(\omega_k \cap c_j)}{P(\omega_k)P(c_j)} \tag{16.3}$$

$$= \sum_k \sum_j \frac{|\omega_k \cap c_j|}{N} \log \frac{N|\omega_k \cap c_j|}{|\omega_k||c_j|} \tag{16.4}$$

where $P(\omega_k)$, $P(c_j)$, and $P(\omega_k \cap c_j)$ are the probabilities of a document being in ω_k, c_j, and in the intersection of ω_k and c_j, respectively. Equation (16.4) is equivalent to Equation (16.3) for maximum likelihood estimates of the probabilities (i.e., the estimate of each probability is the corresponding relative frequency).

H is entropy as defined in Chapter 5 (page 93):

$$H(\Omega) = -\sum_k P(\omega_k) \log P(\omega_k) \tag{16.5}$$

$$= -\sum_k \frac{|\omega_k|}{N} \log \frac{|\omega_k|}{N} \tag{16.6}$$

where, again, the second equation is based on maximum likelihood estimates of the probabilities.

$I(\Omega;\mathbb{C})$ in Equation (16.3) measures the amount of information by which our knowledge about the classes increases when we are told what the clusters are. The minimum of $I(\Omega;\mathbb{C})$ is 0 if the clustering is random with respect to the classes. In that case, knowing that a document is in a particular cluster does not give us any new information about what class it might be in. Maximum mutual information is reached for a clustering Ω_{exact} that perfectly

recreates the classes – but also if clusters in Ω_{exact} are further subdivided into smaller clusters (Exercise 16.4). In particular, a clustering with $K = N$ one-document clusters has maximum MI. So MI has the same problem as purity: it does not penalize large cardinalities and thus does not formalize our bias that, other things being equal, fewer clusters are better.

The normalization by the denominator $[H(\Omega) + H(\mathbb{C})]/2$ in Equation (16.2) fixes this problem since entropy tends to increase with the number of clusters. For example, $H(\Omega)$ reaches its maximum $\log_2 N$ for $K = N$, which ensures that NMI is low for $K = N$. Because NMI is normalized, we can use it to compare clusterings with different numbers of clusters. The particular form of the denominator is chosen because $[H(\Omega) + H(\mathbb{C})]/2$ is a tight upper bound on $I(\Omega; \mathbb{C})$ (Exercise 16.5). Thus, NMI is always a number between 0 and 1.

An alternative to this information-theoretic interpretation of clustering is to view it as a series of decisions, one for each of the $N(N-1)/2$ pairs of documents in the collection. We want to assign two documents to the same cluster if and only if they are similar. A true positive (TP) decision assigns two similar documents to the same cluster, a true negative (TN) decision assigns two dissimilar documents to different clusters. There are two types of errors we can commit. A false positive (FP) decision assigns two dissimilar documents to the same cluster. A false negative (FN) decision assigns two similar documents to different clusters. The *Rand index* RI measures the percentage of decisions that are correct. That is, it is simply accuracy (Section 8.3, page 149).

RAND INDEX
RI

$$\text{RI} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{FN} + \text{TN}}$$

As an example, we compute RI for Figure 16.4. We first compute TP + FP. The three clusters contain 6, 6, and 5 points, respectively, so the total number of "positives" or pairs of documents that are in the same cluster is:

$$\text{TP} + \text{FP} = \binom{6}{2} + \binom{6}{2} + \binom{5}{2} = 40$$

Of these, the X pairs in cluster 1, the circle pairs in cluster 2, the diamond pairs in cluster 3, and the X pair in cluster 3 are true positives:

$$\text{TP} = \binom{5}{2} + \binom{4}{2} + \binom{3}{2} + \binom{2}{2} = 20$$

Thus, FP $= 40 - 20 = 20$.

FN and TN are computed similarly, resulting in the following contingency table:

	Same cluster	Different clusters
Same class	TP = 20	FN = 24
Different classes	FP = 20	TN = 72

RI is then $(20+72)/(20+20+24+72) \approx 0.68$.

The Rand index gives equal weight to false positives and false negatives. Separating similar documents is sometimes worse than putting pairs of dissimilar documents in the same cluster. We can use the *F measure* (Section 8.3, page 148) to penalize false negatives more strongly than false positives by selecting a value $\beta > 1$, thus giving more weight to recall.

F MEASURE

$$P = \frac{\text{TP}}{\text{TP}+\text{FP}} \qquad R = \frac{\text{TP}}{\text{TP}+\text{FN}} \qquad F_\beta = \frac{(\beta^2+1)PR}{\beta^2 P + R}$$

Based on the numbers in the contingency table, $P = 20/40 = 0.5$ and $R = 20/44 \approx 0.455$. This gives us $F_1 \approx 0.48$ for $\beta = 1$ and $F_5 \approx 0.456$ for $\beta = 5$. In information retrieval, evaluating clustering with F has the advantage that the measure is already familiar to the research community.

16.4 *K*-means

K-means is the most important flat clustering algorithm. Its objective is to minimize the average squared distance of documents from their cluster centers where a cluster center is defined as the mean or *centroid* $\vec{\mu}$ of the documents in a cluster ω:

CENTROID

$$\vec{\mu}(\omega) = \frac{1}{|\omega|} \sum_{\vec{x} \in \omega} \vec{x}$$

This definition assumes that documents are represented as vectors in a real-valued space in the familiar way. We used centroids for Rocchio classification in Chapter 14 (page 271). They play a similar role here. The ideal cluster in *K*-means is a sphere with the centroid as its center of gravity. Ideally, the clusters should not overlap. Our desiderata for classes in Rocchio classification were the same. The difference is that we have no labeled training set in clustering for which we know which documents should be in the same cluster.

A measure of how well the centroids represent the members of their clusters is the *residual sum of squares* or *RSS*, the squared distance of each vector from its centroid summed over all vectors:

RESIDUAL SUM OF SQUARES

$$\text{RSS}_k = \sum_{\vec{x} \in \omega_k} \|\vec{x} - \vec{\mu}(\omega_k)\|^2$$

$$\text{RSS} = \sum_{k=1}^{K} \text{RSS}_k \tag{16.7}$$

Given:
  D: a set of N vectors
  K: desired number of clusters

Select K random seeds $\{\vec{s}_1, \vec{s}_2, \ldots, \vec{s}_K\}$ from D
Let $\vec{\mu}(\omega_k) := \vec{s}_k, 1 \leq k \leq K$
Repeat until stopping criterion is met:
  Reassignment step
    Assign each $\vec{x}_n$ to cluster ω_k s.t. $\|\vec{x}_n - \vec{\mu}(\omega_k)\|$ is minimal
  Recomputation step: For each ω_k:
    $\vec{\mu}(\omega_k) = \frac{1}{|\omega_k|} \sum_{\vec{x} \in \omega_k} \vec{x}$

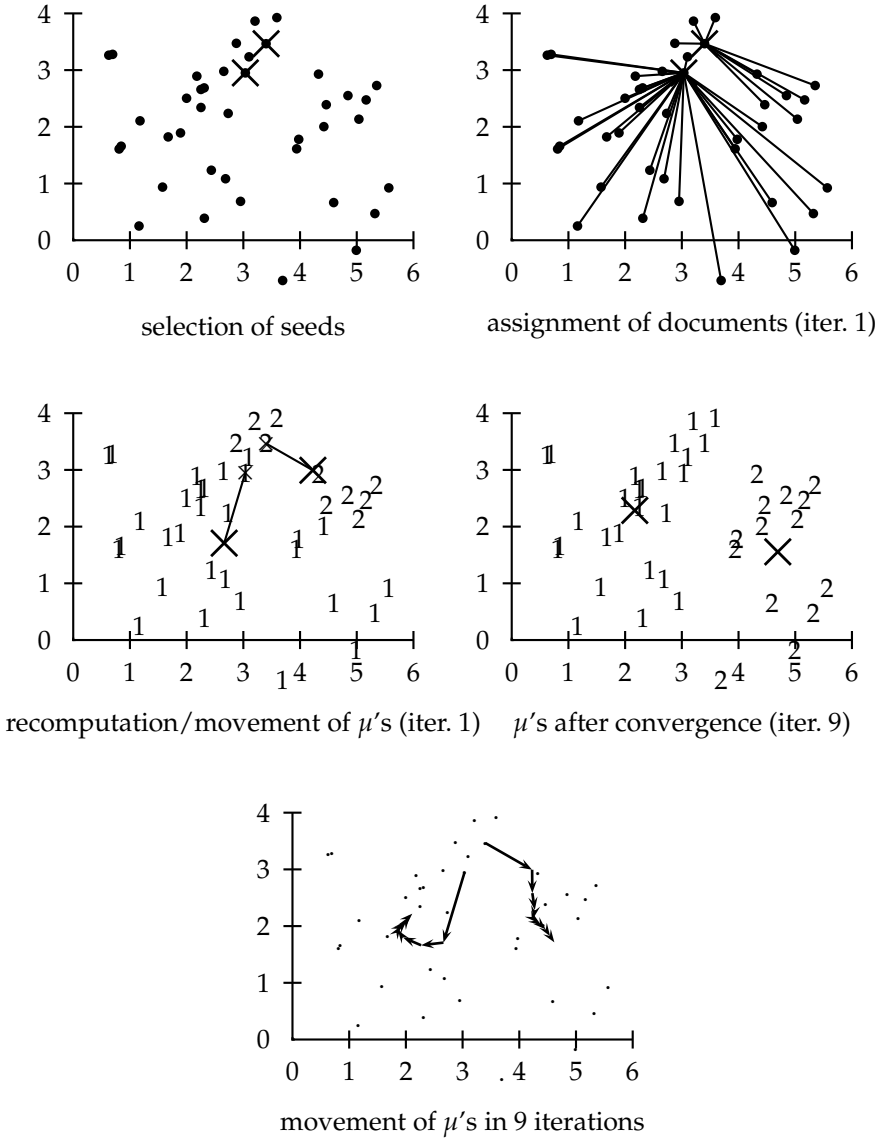
► **Figure 16.5** The K-means algorithm. Alternative methods of seed selection are discussed on page 322.

RSS is the objective function in K-means and our goal is to minimize it. Since N is fixed, minimizing RSS is equivalent to minimizing the average squared distance, a measure of how well centroids represent their documents.

SEED One way to get K-means started is to select as initial cluster centers K randomly selected documents, the *seeds*. It then moves the cluster centers around in space in order to minimize RSS. As shown in Figure 16.5, this is done iteratively by repeating two steps until a stopping criterion is met: reassigning documents to the cluster with the closest centroid; and recomputing each centroid based on the current members of its cluster. Figure 16.6 shows snapshots from nine iterations of the K-means algorithm for a set of points. The "centroid" column of Table 17.2 (page 354) shows examples of centroids.

We can apply one of the following termination conditions.

- A fixed number of iterations I has been completed. This condition limits the runtime of the clustering algorithm, but in some cases the quality of the clustering will be poor because of an insufficient number of iterations.
- Assignment of documents to clusters (the partitioning function γ) does not change between iterations. Except for cases with a bad local minimum, this produces a good clustering, but runtime may be unacceptably long.
- Centroids $\vec{\mu}_k$ do not change between iterations. This is equivalent to γ not changing (Exercise 16.8).
- Terminate when RSS falls below a threshold. This criterion makes sure that the clustering is of a desired quality after termination. In practice, we need to combine it with a bound on the number of iterations to guarantee termination.



► **Figure 16.6** A *K*-means example in $\mathbb{R}^2$. The position of the two centroids (μ's shown as x's) converges after nine iterations.

- Terminate when the decrease in RSS falls below a threshold θ. For small θ, this indicates that we are close to convergence. Again, we need to combine it with a bound on the number of iterations to prevent very long runtimes.

We now show that *K*-means converges by proving that RSS monotonically decreases in each iteration where we will use *decrease* in the meaning *decrease or does not change* in this section. First, RSS decreases in the reassignment step since each vector is assigned to the closest centroid, so the distance it contributes to RSS decreases. Secondly, it decreases in the recomputation step because the new centroid is the vector $\vec{v}$ for which RSS_k reaches its minimum.

$$\text{RSS}_k(\vec{v}) = \sum_{\vec{x}\in\omega_k} \|\vec{v}-\vec{x}\|^2 = \sum_{\vec{x}\in\omega_k} \sum_{m=1}^{M} (v_m - x_m)^2 \tag{16.8}$$

$$\frac{\partial \text{RSS}_k(\vec{v})}{\partial v_m} = \sum_{\vec{x}\in\omega_k} 2(v_m - x_m) \tag{16.9}$$

where x_m, v_m and $\mu_m(\omega_k)$ are the m^{th} components of their respective vectors. Setting the partial derivative to zero, we get:

$$v_m = \frac{1}{|\omega_k|} \sum_{\vec{x}\in\omega_k} x_m \tag{16.10}$$

which is the componentwise definition of the centroid. Thus, we minimize RSS_k when the old centroid is replaced with the new centroid. RSS, the sum of the RSS_k, must then also decrease during recomputation.

Since there is only a finite set of possible clusterings, a monotonically decreasing algorithm will eventually arrive at a (local) minimum. Take care, however, to break ties consistently, e.g., by assigning a document to the cluster with the lowest index if there are several equidistant centroids. Otherwise, the algorithm can cycle forever in a loop of clusterings that have the same cost.

This proves the convergence of *K*-means, but there is unfortunately no guarantee that a *global minimum* in the objective function will be reached.

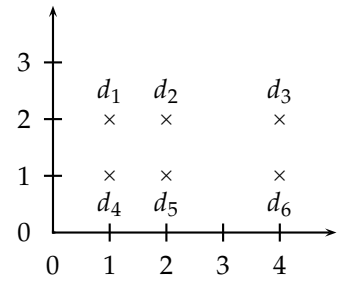
OUTLIER

This is a particular problem if a document set contains many *outliers*, documents that are far from any other documents and therefore do not fit well into any cluster. Frequently, if an outlier is chosen as an initial seed, then no other vector is assigned to it during subsequent iterations. We end up

SINGLETON CLUSTER

with a *singleton cluster* (a cluster with only one document) even though there is probably a clustering with lower RSS. Figure 16.7 shows an example of a suboptimal clustering resulting from a bad choice of initial seeds.

Effective heuristics for seed selection include excluding outliers from the seed set; trying out multiple starting points and choosing the clustering with



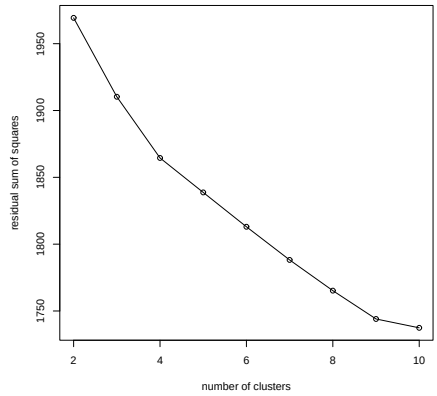
► **Figure 16.7** The outcome of clustering in K-means depends on the initial seeds. For seeds d_2 and d_5, K-means converges to $\{\{d_1, d_2, d_3\}, \{d_4, d_5, d_6\}\}$, a suboptimal clustering. For seeds d_2 and d_3, it converges to $\{\{d_1, d_2, d_4, d_5\}, \{d_3, d_6\}\}$, the global optimum for $K = 2$.

lowest cost; and obtaining seeds from another method such as hierarchical clustering. Since deterministic hierarchical clustering methods are more predictable than K-means, a hierarchical clustering of a small random sample of size iK (e.g., for $i = 5$ or $i = 10$) often provides good seeds (see the description of the Buckshot algorithm, Chapter 17, page 356).

Other initialization methods compute seeds that are not selected from the vectors to be clustered. A robust method that works well for a large variety of document distributions is to select i (e.g., $i = 10$) random vectors for each cluster and use their centroid as the seed for this cluster. This method is recommended unless prior knowledge can guide the selection of good inital seeds.

What is the time complexity of K-means? Most of the time is spent on computing vector distances. One such operation costs $\Theta(M)$. The reassignment step computes KN distances, so its overall complexity is $\Theta(KNM)$. In the recomputation step, each vector gets added to a centroid once, so the complexity of this step is $\Theta(NM)$. For a fixed number of iterations I, the overall complexity is therefore $\Theta(IKNM)$. Thus, K-means is linear in all relevant factors: iterations, number of clusters, number of vectors and dimensionality of the space. This means that K-means is more efficient than the hierachical algorithms in Chapter 17. We had to fix the number of iterations I, but this rarely does harm in practice. In most cases, K-means converges quickly.

There is one subtlety in the preceding argument. Even a linear algorithm can be quite slow if one of the arguments of $\Theta(\ldots)$ is large, and M usually is large. High dimensionality is not a problem for computing the distance of two documents. Their vectors are sparse, so that only a small fraction of the theoretically possible M componentwise differences need to be computed. Centroids, however, are dense since they pool all terms that occur in any of



► **Figure 16.8** Estimated minimal residual sum of squares ($\widehat{\text{RSS}}$) as a function of the number of clusters in K-means. In this clustering of 1203 Reuters-RCV1 documents, there are two points where the $\widehat{\text{RSS}}$ curve flattens: at 4 clusters and at 9 clusters. The documents were selected from the categories *China*, *Germany*, *Russia* and *Sports*, so the $K = 4$ clustering is closest to the Reuters categorization.

the documents of their clusters. As a result, distance computations are time consuming in a naive implementation of K-means. But there are simple and effective heuristics for making centroid-document similarities as fast to compute as document-document similarities. Truncating centroids to the most significant k terms (e.g., $k = 1000$) hardly decreases cluster quality while achieving a significant speedup of the reassignment step (see references in Section 16.6).

K-MEDOIDS

The same efficiency problem is addressed by *k-medoids*, a variant of K-means that computes medoids instead of centroids as cluster centers. We

MEDOID

define the *medoid* of a cluster as the document vector that is closest to the centroid. Since medoids are sparse document vectors, distance computations are fast.

16.4.1 Cluster cardinality in K-means

We stated in Section 16.2 that the number of clusters K is an input to most flat clustering algorithms. What do we do if we cannot come up with a plausible guess for K?

A naive approach would be to select the optimal number of K according to the objective function, i.e., the number K that minimizes RSS. Defining $\text{RSS}_{\text{min}}(K)$ as the minimal RSS of all clusterings with K clusters, we observe

that $\text{RSS}_{\text{min}}(K)$ is a monotonically decreasing function in K (Exercise 16.11), which reaches its minimum 0 for $K = N$ where N is the number of documents. We would end up with each document being in its own cluster. Clearly, this is not an optimal clustering.

A heuristic method that gets around this problem is to estimate $\text{RSS}_{\text{min}}(K)$ by computing RSS for i (e.g., $i = 10$) different clusterings with K clusters and taking the minimum. We denote this estimate by $\widehat{\text{RSS}}_{\text{min}}(K)$. We can then inspect the values $\widehat{\text{RSS}}_{\text{min}}(K)$ as K increases and find the "knee" in the curve – the point where successive decreases in $\widehat{\text{RSS}}_{\text{min}}$ become noticeably smaller. There are two such points in Figure 16.8, one at $K = 4$, where the gradient flattens slightly, and a clearer flattening at $K = 9$. This is typical: there is seldom a single best number of clusters. We still need to employ an external constraint to choose from a number of possible values of K (4 and 9 in this case).

A second type of criterion for cluster cardinality imposes a penalty for each new cluster – where conceptually we start with a single cluster containing all documents and then search for the optimal number of clusters K by successively increasing K. To determine the cluster cardinality in this way, we

DISTORTION

create a generalized objective function that combines two elements: *distortion*, a measure of how much documents deviate from the prototype of their

COMPLEXITY

clusters (e.g., RSS for K-means); and a measure of the *complexity* of the clustering, which is usually a function of the number of clusters. For K-means, we get this selection criterion for K:

$$K = \arg\min_K [\text{RSS}_{\text{min}}(K) + \lambda K] \tag{16.11}$$

where λ is a weighting factor. A large value of λ favors solutions with few clusters. For $\lambda = 0$, there is no penalty for more clusters and $K = N$ is the best solution.

The obvious difficulty with Equation (16.11) is that we need to determine λ. Unless this is easier than determining K directly, then we are back to square one. In some cases, we can choose values of λ that have worked well for similar data sets in the past. For example, if we periodically cluster news stories from a newswire, there is likely to be a fixed value of λ that gives us the right K in each successive clustering. In this application, we would not be able to determine K based on past experience since K changes.

AKAIKE INFORMATION CRITERION

A theoretical justification for Equation (16.11) is the *Akaike Information Criterion* or AIC, an information-theoretic measure which trades off model fit against model complexity. The general form of AIC is:

$$\textbf{AIC:} \qquad K = \arg\min_K [-2L(K) + 2q(K)] \tag{16.12}$$

where $-L(K)$, the negative maximum log likelihood of the data for K clus-

ters, is a measure of distortion and $q(K)$ is the number of parameters of a model with K clusters. For K-means it can be stated as follows:

$$\textbf{AIC:} \qquad K = \arg\min_K [\mathrm{RSS}_{\min}(K) + 2 \cdot M \cdot K] \tag{16.13}$$

Equation (16.13) is a special case of Equation (16.11) for $\lambda = 2M$.

To derive Equation (16.13) from Equation (16.12) observe that $q(K) = KM$ in K-means since each element of the K centroids is a parameter that can be varied independently; and that $L(K) = -(1/2)\mathrm{RSS}_{\min}(K)$ (modulo a constant) if we view the model underlying K-means as a Gaussian mixture with hard assignment, uniform cluster priors and identical spherical covariance matrices (see Exercise 16.17).

The derivation of AIC is based on a number of assumptions, e.g., that the data are independently and identically distributed. These assumptions are only approximately true for data sets in information retrieval. As a consequence, the AIC can rarely be applied as is in text clustering. In Figure 16.8, the dimensionality of the vector space is $M \approx 50{,}000$. Thus, $q(K) > 50{,}000$ dominates the smaller RSS-based term ($\widehat{\mathrm{RSS}}_{\min}(1) < 5000$, not shown in the figure) and the minimum of the expression is reached for $K = 1$. But as we know, $K = 4$ (corresponding to the four classes *China*, *Germany*, *Russia* and *Sports*) is a better choice than $K = 1$. In practice, Equation (16.11) is often more useful than Equation (16.13) – with the caveat that we need to come up with an estimate for λ.

16.5 Model-based clustering

In this section, we describe a generalization of K-means, the EM algorithm. It can be applied to a larger variety of document representations and distributions than K-means.

In K-means, we attempt to find centroids that are good representatives. We can view the set of K centroids as a model that generates the data. Generating a document in this model consists of first picking a centroid at random and then adding some noise. If the noise is normally distributed, this procedure will result in clusters of spherical shape. *Model-based clustering* assumes that the data were generated by a model and then tries to recover the original model from the data. The model then defines clusters and an assignment of documents to clusters.

MODEL-BASED CLUSTERING

A commonly used criterion for selecting the model is maximum likelihood. In K-means, the quantity $\exp(-\mathrm{RSS})$ is proportional to the likelihood that a particular model (i.e., a set of centroids) generated the data. For K-means, maximum likelihood and minimal RSS are equivalent criteria.

More generally, we write Θ for the parameters that describe the model. In K-means, $\Theta = \{\vec{\mu}_1, \ldots, \vec{\mu}_K\}$. The maximum likelihood criterion is then to

select the model Θ that maximizes the log likelihood of generating the data D:

$$\Theta = \arg\max_{\Theta} L(D|\Theta) = \arg\max_{\Theta} \log \prod_{n=1}^{N} P(d_n|\Theta) = \arg\max_{\Theta} \sum_{n=1}^{N} \log P(d_n|\Theta)$$

$L(D|\Theta)$ is the objective function that measures the goodness of the clustering. Given two clusterings with the same number of clusters, we prefer the one with higher $L(D|\Theta)$.

This is the same approach we took in Chapter 12 (page 225) for language modeling and in Section 13.1 (page 248) for text classification. In text classification, we chose the class that maximizes the likelihood of generating a particular document. Here, we choose the clustering Θ that maximizes the likelihood of generating a given set of documents. Once we have Θ, we can compute an assignment probability $P(d|\omega_k; \Theta)$ for each document-cluster pair.

Because cluster membership is a probability distribution in model-based clustering, assignment to clusters is soft (as defined earlier in this chapter on page 310). A document about Chinese cars may get soft assignments of 0.5 to each of the two clusters *China* and *automobiles*, reflecting the fact that both topics are pertinent. A hard clustering like K-means cannot model this simultaneous relevance to two topics.

Model-based clustering provides a framework for incorporating our knowledge about a domain. K-means and the hierarchical algorithms in Chapter 17 make fairly rigid assumptions about the data. For example, clusters in K-means are assumed to be spheres. Model-based clustering offers more flexibility. The clustering model can be adapted to what we know about the underlying distribution of the data, be it binomial (as in the example below), Gaussian with non-spherical variance (another model that is important in document clustering) or a member of a different family.

EXPECTATION-MAXIMIZATION ALGORITHM
EM ALGORITHM

A commonly used algorithm for model-based clustering is the *Expectation-Maximization algorithm* or *EM algorithm*. EM clustering is an iterative algorithm that maximizes $L(D|\Theta)$. EM can be applied to many different types of probabilistic modeling. We will work with a mixture of multivariate Bernoulli distributions here, the distribution we know from Section 11.3 (page 210) and Section 13.3 (page 246):

$$P(d|\omega_k, \Theta) = \left(\prod_{w_m \in d} q_{mk} \right) \left(\prod_{w_m \notin d} (1 - q_{mk}) \right)$$

where $\Theta = \{\Theta_1, \ldots, \Theta_K\}$, $\Theta_k = (\alpha_k, q_{1k}, \ldots, q_{Mk})$, and $q_{mk} = P(U_m = 1|\omega_k)$

are the parameters of the model.[3] $P(U_m = 1|\omega_k)$ is the probability that a document from cluster k contains word w_m. α_k is the prior probability of cluster ω_k: the probability that a document d is in ω_k if we have no information about d.

The mixture model then is:

$$P(d|\Theta) = \sum_{k=1}^{K} \alpha_k \left(\prod_{w_m \in d} q_{mk} \right) \left(\prod_{w_m \notin d} (1 - q_{mk}) \right) \tag{16.14}$$

In this model, we generate a document by first picking a cluster k with probability α_k and then generating the words of the document according to the parameters q_{mk}. Recall that the document representation of the multivariate Bernoulli is a vector of M Boolean values (and not a real-valued vector).

How do we use EM to infer the parameters of the clustering from the data? That is, how do we choose parameters Θ that maximize $L(D|\Theta)$? EM is quite similar to K-means in that it alternates between an *expectation step*, corresponding to reassignment, and a *maximization step*, corresponding to recomputation of the parameters of the models. The parameters of K-means are the centroids, the parameters of the instance of EM in this section are the α_k and q_{mk}.

EXPECTATION STEP
MAXIMIZATION STEP

The maximization step recomputes the conditional parameters q_{mk} and the priors α_k as follows:

$$\textbf{Maximization Step:} \quad q_{mk} = \frac{\sum_{n=1}^{N} r_{nk} I(w_m \in d_n)}{\sum_{n=1}^{N} r_{nk}} \qquad \alpha_k = \frac{\sum_{n=1}^{N} r_{nk}}{N} \tag{16.15}$$

$I(w_m \in d_n) = 1$ if $w_m \in d_n$ and 0 otherwise. r_{nk} is the soft assignment of document d_n to cluster k as computed in the preceding iteration. (We'll address the issue of initialization in a moment.) These are the maximum likelihood estimates for the parameters of the multivariate Bernoulli from Table 13.3 (page 252) except that documents are assigned fractionally to clusters here. These maximum likelihood estimates maximize the likelihood of the data given the model.

The expectation step computes the soft assignment of documents to clusters given the current parameters q_{mk} and α_k:

$$\textbf{ExpectationStep}: \quad r_{nk} = \frac{\alpha_k (\prod_{w_m \in d_n} q_{mk})(\prod_{w_m \notin d_n} (1 - q_{mk}))}{\sum_{k=1}^{K} \alpha_k (\prod_{w_m \in d_n} q_{mk})(\prod_{w_m \notin d_n} (1 - q_{mk}))} \tag{16.16}$$

3. U is the random variable we defined in Section 13.3 (page 249) for the Bernoulli Naive Bayes model.

This expectation step applies Equation (16.14) to computing the likelihood that ω_k generated document d_n. It is the classification procedure for the multivariate Bernoulli in Table 13.3. Thus, the expectation step is nothing else but (Bernoulli) Naive Bayes classification.

We clustered a set of 11 documents into two clusters using EM in Table 16.3. After convergence in iteration 25, the first 5 documents are assigned to cluster 1 ($r_{i,1} = 1.00$) and the last 6 to cluster 2 ($r_{i,1} = 0.00$). Somewhat atypically, the final assignment is a hard assignment here. EM usually converges to a soft assignment. In iteration 25, the prior for cluster 1 is $5/11 \approx 0.45$ because 5 of the 11 documents are in cluster 1. Some words are quickly associated with one cluster because the initial assignment can "spread" to them unambiguously. For example, membership in cluster 2 spreads from document 7 to document 8 in the first iteration because they share sugar. ($r_{8,1} = 0$ in iteration 1.) For parameters of words occurring in ambiguous contexts, convergence takes longer. Seed documents 6 and 7 both contain sweet. As a result, it takes 25 iterations for the word to be unambiguously associated with one cluster (cluster 2: $q_{\text{sweet},1} = 0$ in iteration 25).

Finding good seeds is even more critical for EM than for K-means. EM is prone to get stuck in local optima if the seeds are not chosen well. This is a general problem which also occurs in other applications of EM.[4] Therefore, as with K-means, the initial assignment of documents to clusters is often computed by a different algorithm. For example, a hard K-means clustering may provide the initial assignment, which EM can then "soften up."

16.6 References and further reading

A more general introduction to clustering, covering both K-means and EM, but without reference to text-specific issues, can be found in (Duda et al. 2000). Rasmussen (1992) gives an introduction to clustering from an information retrieval perspective. An alternative definition of hard clustering is that a document can be a full member of more than one cluster. *Partitional clustering* always means that each document belongs to exactly one cluster (but in a partitional hierarchical clustering (Chapter 17) all members of a cluster are of course also members of its parent). On the definition of hard clustering that permits multiple membership, the difference between soft clustering and hard clustering is that membership values in hard clustering are either 0 or 1 whereas they can take on any non-negative value in soft clustering.

PARTITIONAL CLUSTERING

The cluster hypothesis is due to Jardine and van Rijsbergen (1971) who

4. For example, this problem is common when EM is applied to natural language processing problems using hidden Markov models, probabilistic grammars, or machine translation models (Manning and Schütze 1999).

docID	document text	docID	document text
1	hot chocolate cocoa beans	7	sweet sugar
2	cocoa ghana africa	8	sugar cane brazil
3	beans harvest ghana	9	sweet sugar beet
4	cocoa butter	10	sweet cake icing
5	butter truffles	11	cake black forest
6	sweet chocolate		

Parameter	Iteration of clustering							
	0	1	2	3	4	5	15	25
α_1		0.50	0.45	0.52	0.56	0.55	0.53	0.45
$r_{1,1}$		1.00	1.00	1.00	1.00	1.00	1.00	1.00
$r_{2,1}$		0.50	0.73	0.97	1.00	1.00	1.00	1.00
$r_{3,1}$		0.50	0.80	0.99	1.00	1.00	1.00	1.00
$r_{4,1}$		0.50	0.71	0.87	0.98	1.00	1.00	1.00
$r_{5,1}$		0.50	0.53	0.61	0.78	0.96	1.00	1.00
$r_{6,1}$	1.00	1.00	1.00	1.00	1.00	1.00	0.74	0.00
$r_{7,1}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$r_{8,1}$		0.00	0.00	0.00	0.00	0.00	0.00	0.00
$r_{9,1}$		0.00	0.00	0.00	0.00	0.00	0.00	0.00
$r_{10,1}$		0.50	0.42	0.19	0.02	0.00	0.00	0.00
$r_{11,1}$		0.50	0.56	0.53	0.28	0.02	0.00	0.00
$q_{\text{africa},1}$		0.000	0.036	0.046	0.057	0.061	0.064	0.071
$q_{\text{africa},2}$		0.000	0.031	0.019	0.002	0.000	0.000	0.000
$q_{\text{brazil},1}$		0.000	0.000	0.000	0.000	0.000	0.000	0.000
$q_{\text{brazil},2}$		0.000	0.062	0.071	0.077	0.074	0.070	0.062
$q_{\text{cocoa},1}$		0.000	0.143	0.152	0.167	0.181	0.191	0.214
$q_{\text{cocoa},2}$		0.000	0.063	0.040	0.012	0.001	0.000	0.000
$q_{\text{sugar},1}$		0.000	0.000	0.000	0.000	0.000	0.000	0.000
$q_{\text{sugar},2}$		0.500	0.187	0.214	0.231	0.221	0.210	0.187
$q_{\text{sweet},1}$		0.500	0.107	0.089	0.070	0.062	0.054	0.000
$q_{\text{sweet},2}$		0.500	0.156	0.185	0.216	0.219	0.220	0.250

► **Table 16.3** The EM clustering algorithm. The table shows a set of documents (above) and parameter values for selected iterations during EM clustering (below). Parameters shown are prior α_1, soft assignment scores $r_{n,1}$ (both omitted for cluster 2), and lexical parameters $q_{m,k}$ for a few words. The authors initially assigned document 6 to cluster 1 and document 7 to cluster 2 (iteration 0). EM converges after 25 iterations. For smoothing, the r_{nk} in Equation 16.15 were replaced with $r_{nk} + \epsilon$ where $\epsilon = 0.0001$.

state it as follows: *Associations between documents convey information about the relevance of documents to requests.* Croft (1978) shows that cluster-based retrieval can be more accurate as well as more efficient than regular search. However, Voorhees (1985a) presents evidence that accuracy does not improve consistently across collections.

There is good evidence that clustering of search results improves user experience and search result quality (Hearst and Pedersen 1996, Zamir and Etzioni 1999, Tombros et al. 2002, Käki 2005), although not as much as search result structuring based on carefully edited category hierarchies (Hearst 2006). The Scatter-Gather interface for browsing collections was presented by Cutting et al. (1992). A theoretical framework for analyzing the properties of Scatter/Gather and other information seeking user interfaces is presented by Pirolli (2007). The cluster-based language modeling approach was pioneered by Liu and Croft (2004). Schütze and Silverstein (1997) evaluate LSI (Chapter 18) and truncated representations of centroids for efficient K-means clustering.

The Columbia NewsBlaster system (McKeown et al. 2002), a forerunner to the now much more famous and refined Google News (http://news.google.com), used hierarchical clustering (Chapter 17) to give two levels of news topic granularity. See Hatzivassiloglou et al. (2000) for details, and (Chen and Lin 2000, Radev et al. 2001) for related systems. Other applications of clustering in information retrieval are duplicate detection (Yang and Callan (2006), (Section 19.6.1, page 387)), novelty detection (see references in (Section 17.9, page 356)) and metadata discovery on the semantic web (Alonso et al. 2006).

The discussion of external evaluation measures is partially based on Strehl (2002). Dom (2002) proposes a measure Q_0 that is better motivated theoretically than NMI. Q_0 is the number of bits needed to transmit class memberships assuming cluster memberships are known. The Rand index is due to Rand (1971). Hubert and Arabie (1985) propose an *adjusted* Rand index that ranges between -1 and 1 and is 0 if there is only chance agreement between clusters and classes (similar to κ in Chapter 8, page 156). Basu et al. (2004) argue that the three evaluation measures NMI, Rand index and F measure give very similar results. Stein et al. (2003) propose *expected edge density* as an internal measure and give evidence that it is a good predictor of the quality of a clustering. Kleinberg (2002) and Meilă (2005) present axiomatic frameworks for comparing clusterings.

ADJUSTED RAND INDEX

Authors that are often credited with the invention of the K-means algorithm include Lloyd (1982) (first distributed in 1957), Ball (1965), MacQueen (1967), and Hartigan and Wong (1979). Arthur and Vassilvitskii (2006) investigate the worst-case complexity of K-means. Dhillon and Modha (2001) compare K-means clusters to SVD-based clusters (Chapter 18). The k-medoid algorithm was presented by Kaufman and Rousseeuw (1990). The EM algorithm was originally introduced by Dempster et al. (1977). An in-depth

treatment of EM is (McLachlan and Krishnan 1996).

AIC is due to Akaike (1974) (see also Burnham and Anderson (2002)). An alternative to AIC is BIC, which can be motivated as a Bayesian model selection procedure (Schwarz 1978). Fraley and Raftery (1998) show how to choose an optimal number of clusters based on BIC. An application of BIC to *K*-means is (Pelleg and Moore 2000). Hamerly and Elkan (2003) propose an alternative to BIC that performs better in their experiments. Another influential Bayesian approach for determining the number of clusters (simultaneously with cluster assignment) is decribed by Cheeseman and Stutz (1996). Two methods for determining cardinality without external criteria are presented by Tibshirani et al. (2001).

We only have space here for classical completely unsupervised clustering. An important current topic of research is how to use prior knowledge to guide clustering (e.g., Ji and Xu (2006)) and how to incorporate interactive feedback during clustering (e.g., Huang and Mitchell (2006)). Fayyad et al. (1998) propose an initialization for EM clustering. For algorithms that can cluster very large data sets in one scan through the data see (Bradley et al. 1998).

The applications in Table 16.1 all cluster documents. Other information retrieval applications cluster words (e.g., Crouch 1988) or contexts of words (e.g., Schütze and Pedersen 1995).

16.7 Exercises

Exercise 16.1

Define two documents as similar if they have n content words in common (for, say, $n = 5$). What are some examples of documents for which the cluster hypothesis does not hold?

Exercise 16.2

Why are documents that do not use the same word for the concept *car* likely to end up in the same cluster in *K*-means clustering?

Exercise 16.3

Make up a simple one-dimensional example (i.e. points on a line) with two clusters where the inexactness of cluster-based retrieval shows up. In your example, retrieving clusters close to the query should do worse than direct nearest neighbor search.

Exercise 16.4

Let Ω be a clustering that exactly reproduces a class structure $\mathbb{C}$ and Ω' a clustering that further subdivides some clusters in Ω. Show that $I(\Omega;\mathbb{C}) = I(\Omega';\mathbb{C})$.

Exercise 16.5

Show that $I(\Omega;\mathbb{C}) \leq [H(\Omega) + H(\mathbb{C})]/2$.

Exercise 16.6

Replace every point d in Figure 16.4 with two points in the same class as d. Compute purity, NMI, RI, and F_5 for this clustering. Do the measures increase or decrease after doubling the number of points? Does this correspond to your intuition as to the relative difficulty of clustering a set twice as large?

Exercise 16.7

Which of the four evaluation measures introduced above are symmetric in the sense that the measure's value does not change if the roles of clusters and classes are switched?

Exercise 16.8

Two of the possible termination conditions for K-means were (1) assignment does not change, (2) centroids do not change (page 320). Do these two conditions imply each other?

Exercise 16.9

Compute RSS for the two clusterings in Figure 16.7.

Exercise 16.10

Download Reuters-21578. (i) Compute a K-means clustering of the entire collection (training and test sets) into 10 clusters. There are a number of software packages that implement K-means, e.g., WEKA (Witten and Frank 2005) and R (R Development Core Team 2005). (ii) Compute purity, normalized mutual information, F_1 and RI for the classes *acquisitions*, *corn*, *crude*, *earn*, *grain*, *interest*, *money-fx*, *ship*, *trade*, and *wheat*. You can exclude documents that are in two or more of these classes from the evaluation. (iii) Compile a confusion matrix (Table 14.5, page 285) for the 10 classes and 10 clusters (again excluding documents with more than one assignment). Identify classes that give rise to false positives and false negatives.

Exercise 16.11

Show that $\text{RSS}_{\text{min}}(K)$ as defined above is monotonically decreasing in K.

Exercise 16.12

There is a soft version of K-means that computes the assignment strength of a document to a cluster as a monotonically decreasing function of the distance Δ from its centroid, e.g., as $e^{-\Delta}$. Modify reassignment and recomputation steps of hard K-means for this soft version.

Exercise 16.13

In the last iteration in Table 16.3, document 6 is in cluster 2 even though it was the initial seed for cluster 1. Why does the document change membership?

Exercise 16.14

The values of the parameters q_{mk} in iteration 25 in Table 16.3 are rounded. What are the exact values that EM will converge to?

Exercise 16.15

Perform a K-means clustering for the documents in Table 16.3. After how many iterations does K-means converge? Compare the result to the EM clustering in Table 16.3 and discuss the differences.

Exercise 16.16

Modify the expectation and maximization steps of EM for a Gaussian mixture. As with Naive Bayes, the maximization step computes the maximum likelihood parameter estimates α_k, $\vec{\mu}_k$, and Σ_k for each of the clusters. The expectation step computes for each vector a soft assignment to clusters (Gaussians) based on their current parameters. Write down the corresponding equations.

Exercise 16.17

Show that K-means can be viewed as the limiting case of EM for Gaussian mixtures if variance is very small and all covariances are 0.

Exercise 16.18

We saw above that the time complexity of K-means is $\Theta(IKNM)$. What is the time complexity of EM?

Exercise 16.19

WITHIN-POINT SCATTER

The *within-point scatter* of a cluster ω is defined as $\frac{1}{2}\sum_{\vec{x}_i \in \omega}\sum_{\vec{x}_j \in \omega} \|\vec{x}_i - \vec{x}_j\|^2$. Show that minimizing RSS and minimizing within-point scatter are equivalent.

Exercise 16.20

Derive an AIC criterion for the multivariate Bernoulli mixture model from Equation (16.12).

17 *Hierarchical clustering*

HIERARCHICAL CLUSTERING

HIERARCHY

Flat clustering is efficient and conceptually simple, but as we saw in Chapter 16 it has a number of drawbacks. It returns a flat unstructured set of clusters; and the flat clustering algorithms K-means and EM require a prespecified number of clusters as input and are nondeterministic. *Hierarchical clustering* (or *hierarchic clustering*) outputs a hierarchy, a structure that is more informative than the unstructured set of clusters in flat clustering. In this chapter, we only consider *hierarchies* that are binary trees as in Figure 17.1 – but hierarchical clustering can be easily extended to other types of trees. Hierarchical clustering does not require us to prespecify the number of clusters. And most hierarchical algorithms are deterministic. These advantages of hierarchical clustering come at the cost of lower efficiency. The most common hierarchical clustering algorithms have a complexity that is at least quadratic in the number of documents compared to the linear complexity of K-means and EM (cf. Section 16.4, page 323).

This chapter first introduces *agglomerative* hierarchical clustering (Section 17.1) and presents four different agglomerative algorithms, in Sections 17.2–17.4, which differ in the similarity measures they employ: single-link, complete-link, group-average, and centroid similarity. We then discuss the optimality conditions of hierarchical clustering in Section 17.5. Section 17.6 introduces top-down (or *divisive*) hierarchical clustering. Section 17.7 looks at automatic labeling of clusters, which is important whenever humans interact with the output of clustering. Finally, we discuss implementation issues in Section 17.8. Section 17.9 provides pointers to further reading, including references to soft hierarchical clustering, which we do not cover in this book. (In a soft hierarchical clustering, sibling nodes can share documents; see Chapter 16, page 310)

There are few differences between the applications of flat and hierarchical clustering in information retrieval. In particular, hierarchical clustering is appropriate for any of the applications shown in Table 16.1 (page 311; see also Section 16.6, page 329). In fact, the example we gave for collection clustering is hierarchical. In general, we select flat clustering when efficiency

is important and hierarchical clustering when one of the potential problems of flat clustering (not enough structure, predetermined number of clusters, non-determinism) is a concern. In addition, many researchers believe that hierarchical clustering produces better clusters than flat clustering. But there is no consensus on this issue (see references in Section 17.9).

17.1 Hierarchical agglomerative clustering

Hierarchical algorithms are either top-down or bottom-up. Bottom-up algorithms treat each document as a singleton cluster at the outset and then successively merge (or *agglomerate*) pairs of clusters until all clusters have been merged into a single cluster that contains all documents. Bottom-up clustering is therefore called *hierarchical agglomerative clustering* or *HAC*. Top-down clustering requires a method for splitting a cluster and proceeds by splitting clusters recursively until individual documents are reached (see Section 17.6). HAC is more frequently used than top-down clustering and is the main subject of this chapter.

HIERARCHICAL AGGLOMERATIVE CLUSTERING
HAC

Before looking at specific similarity measures used in hierarchical clustering in Sections 17.2–17.4, we first introduce the general idea of hierarchical clustering and discuss a few key properties.

A HAC (hierarchical agglomerative) clustering is typically visualized as a *dendrogram* as shown in Figure 17.1. A merge of two clusters is represented as a horizontal line that connects two clusters (where documents are viewed as singleton clusters). The y-axis represents *combination similarity*, the similarity of the two clusters connected by the horizontal line at a particular y. We define the combination similarity of a single-document cluster as the document's self-similarity (which is 1.0 for cosine similarity). By moving up from the bottom layer to the top node, we can reconstruct the history of mergers that resulted in the depicted clustering.

DENDROGRAM

COMBINATION SIMILARITY

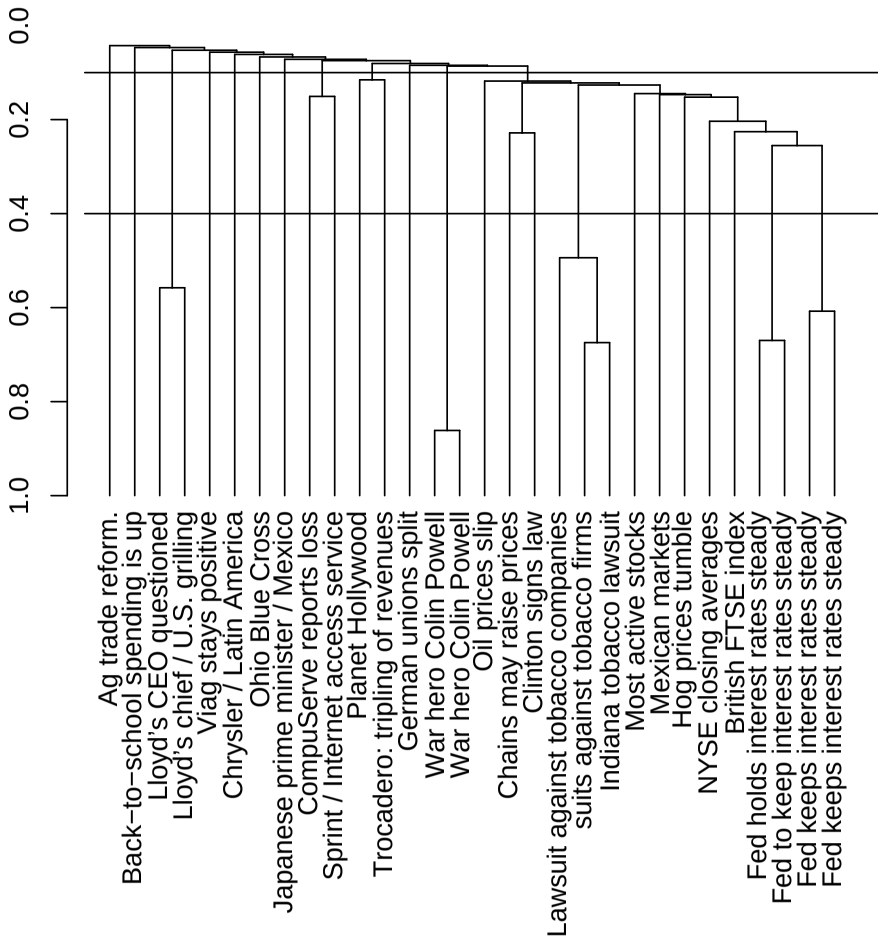
A fundamental assumption in HAC is that the merge operation is *monotonic*. If $s_1, s_2, \ldots, s_{K-1}$ are the successive combination similarities, then $s_1 \geq s_2 \geq \ldots \geq s_{K-1}$ holds for a monotonic hierarchical clustering algorithm. A non-monotonic hierarchical clustering contains at least one *inversion* $s_i < s_{i+1}$ and contradicts the fundamental assumption that we chose the best merger available at each step. We will see an example of an inversion later in this chapter in Figure 17.12.

MONOTONICITY

INVERSION

Hierarchical clustering does not require a prespecified number of clusters. But in some applications we want a partition of disjoint clusters just as in flat clustering. In those cases, the hierarchy needs to be cut at some point. A number of criteria can be used to determine the cutting point:

- Cut at a prespecified level of similarity. For example, we cut the dendrogram at 0.4 if we want clusters with a minimum combination similarity



► **Figure 17.1** A dendrogram of a single-link clustering of 30 documents from Reuters-RCV1. The y-axis represents combination similarity, the similarity of the two component clusters that gave rise to the corresponding merge. For example, the combination similarity of *Lloyd's CEO questioned* and *Lloyd's chief / U.S. grilling* is ≈ 0.56. Two possible cuts of the dendrogram are shown: at 0.4 into 24 clusters and at 0.1 into 12 clusters.

Given: N one-document clusters
Compute similarity matrix
for $k = 1$ to N:
  for $\ell = 1$ to N:
    $C[k][\ell] = \text{sim}(d_k, d_\ell)$
Initialization
A=[] *(for collecting merge sequence)*
for $k = 1$ to N:
  $I[k] = 1$ *(keeps track of active clusters)*
Compute clustering
for $k = 1$ to $N - 1$:
  $(\ell, m) = \arg\max_{(\ell,m),\ell\neq m,I[\ell]=I[m]=1} C[\ell][m]$
  A.append($\langle \ell, m \rangle$) *(Execute and store merger)*
  for $j = 1$ to N:
    $C[\ell][j] = C[j][\ell] = \text{sim}(j, \ell, m)$
  $I[m] = 0$ *(deactivate cluster)*

► **Figure 17.2** A simple, but inefficient HAC algorithm.

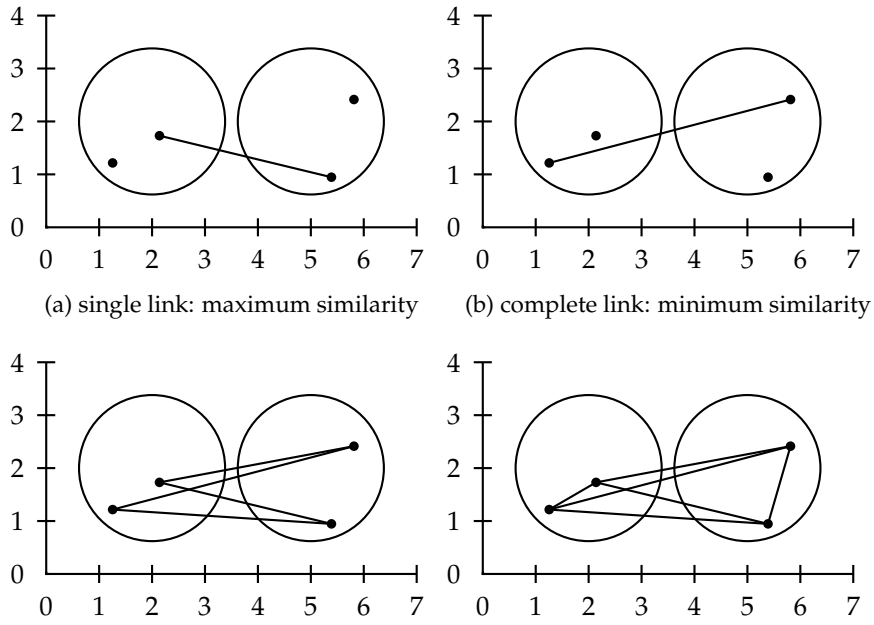
of 0.4. In Figure 17.1, cutting the diagram at $y = 0.4$ yields 24 clusters (grouping only documents with high similarity together) and cutting it at $y = 0.1$ yields 12 clusters (one large financial news cluster and 11 smaller clusters).

- Cut the dendrogram where the gap between two successive combination similarities is largest. Such large gaps arguably indicate "natural" clusterings. Adding one more cluster decreases the quality of the clustering significantly, so cutting before this steep decrease occurs is desirable. This strategy is analogous to looking for the knee in the K-means graph in Figure 16.8 (page 324).
- Apply Equation (16.11) (page 325):

$$K = \arg\min_K [\text{RSS}_{\min}(K) + \lambda K] \tag{17.1}$$

  where K refers to the cut of the hierarchy that results in K clusters, RSS is the residual sum of squares and λ is a penalty for each additional cluster. Instead of RSS, another measure of distortion can be used.
- As in flat clustering, we can also prespecify the number of clusters K and select the cutting point that produces K clusters.

A simple, naive HAC algorithm is shown in Figure 17.2. It consists of $N - 1$ steps of merging the currently most similar clusters. In each iteration, the two



(a) single link: maximum similarity (b) complete link: minimum similarity

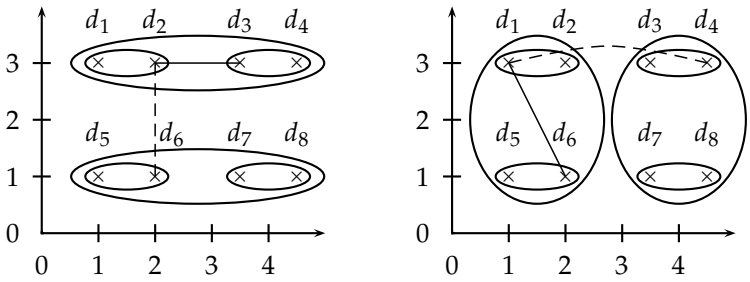
(c) centroid: average inter-similarity (d) group-average: average of all similarities

► **Figure 17.3** The different notions of cluster similarity used by the four HAC algorithms. An intersimilarity is a similarity between two documents from different clusters.

most similar clusters are merged and the rows and columns of the merged cluster ℓ in C are updated.[1] The clustering is stored as a list of mergers in A. I indicates which clusters are still available to be merged. The function $\text{sim}(j, \ell, m)$ computes the similarity of cluster j with the merger of clusters ℓ and m. For some HAC algorithms $\text{sim}(j, \ell, m)$ is simply a function of $C[j][\ell]$ and $C[j][m]$, for example, the maximum of these two values for single-link.

We will now refine this algorithm for the different similarity measures of single-link and complete-link clustering (Section 17.2) and group-average and centroid clustering (Sections 17.3 and 17.4). The merge criteria of these four variants of HAC are shown in Figure 17.3.

1. We assume that we use a deterministic method for breaking ties, e.g., always choose the merger that is the first cluster with respect to a total ordering of the subsets of D.



► **Figure 17.4** A single-link (left) and complete-link (right) clustering of eight documents. The ellipses correspond to successive clustering stages. Left: The single-link similarity of the two upper two-point clusters is the similarity (proximity) of d_2 and d_3 (solid line), which is greater than the single-link similarity of the two left pairs (dashed line). Right: The complete-link similarity of the two upper two-point clusters is the similarity of d_1 and d_4 (dashed line), which is smaller than the complete-link similarity of the two left pairs (solid line).

17.2 Single-link and complete-link clustering

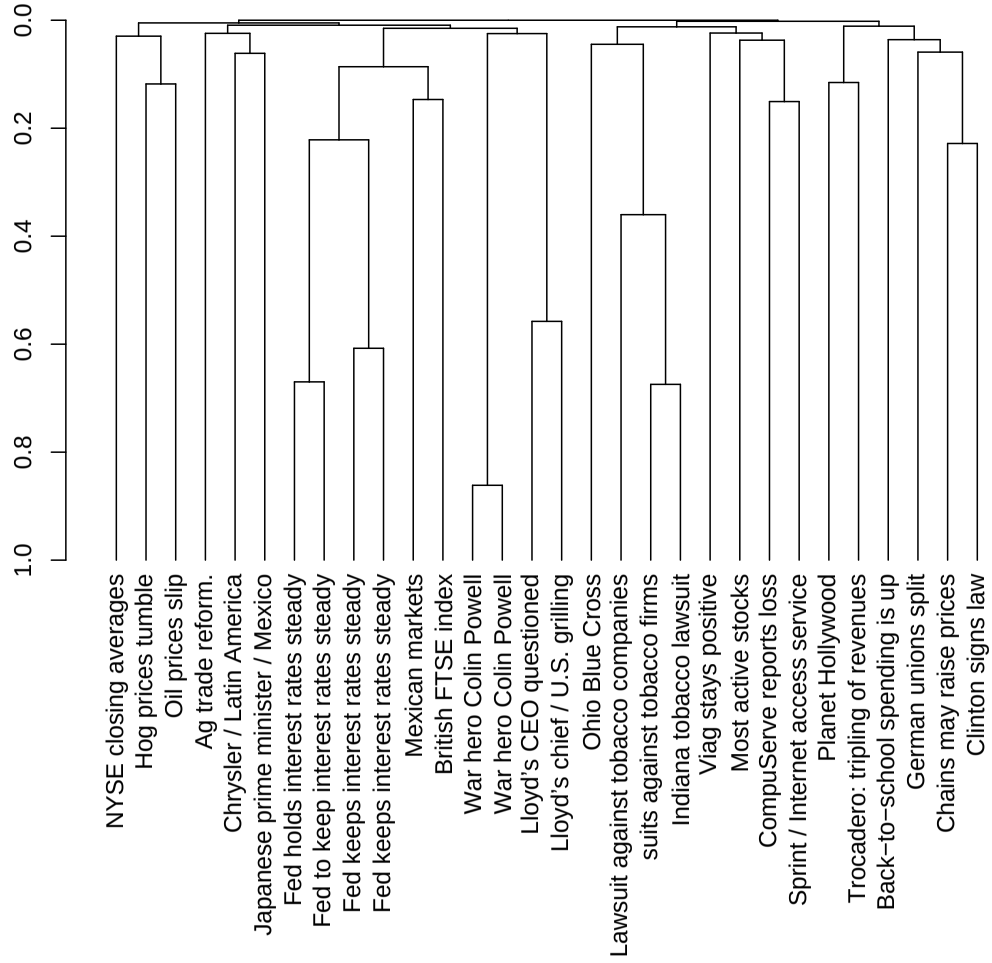
SINGLE-LINK CLUSTERING

In *single-link clustering* or *single-linkage clustering*, the similarity of two clusters is the similarity of their *most similar* members (see Figure 17.3, (a)). This single-link merge criterion is *local*. We pay attention solely to the area where the two clusters come closest to each other. Other, more distant parts of the cluster and the clusters' overall structure are not taken into account.

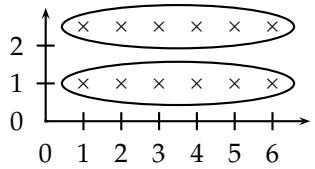
COMPLETE-LINK CLUSTERING

In *complete-link clustering* or *complete-linkage clustering*, the similarity of two clusters is the similarity of their *most dissimilar* members (see Figure 17.3, (b)). This is equivalent to choosing the cluster pair whose merger has the smallest diameter. This complete-link merge criterion is non-local: the entire structure of the clustering is taken into account. We prefer compact clusters with small diameters over long, straggly clusters. Complete-link clustering is sensitive to outliers. A single document far from the center can increase diameters of candidate merge clusters dramatically and completely change the final clustering.

Figure 17.4 depicts a single-link and a complete-link clustering of eight documents. The first four steps, each producing a cluster consisting of a pair of two documents, are identical. Then single-link clustering joins the upper two pairs (and after that the lower two pairs) because on the maximum-similarity definition of cluster similarity, those two clusters are closest. Complete-link clustering joins the left two pairs (and then the right two pairs) because



► **Figure 17.5** A dendrogram of a complete-link clustering of the 30 documents in Figure 17.1.



► **Figure 17.6** Chaining in single-link clustering. The local criterion in single-link clustering can cause undesirable elongated clusters.

those are the closest pairs according to the minimum-similarity definition of cluster similarity.[2]

Figure 17.1 is an example of a single-link clustering of a set of documents while Figure 17.5 is a complete-link clustering of the same set. When cutting the last merger in Figure 17.5, we obtain two clusters of similar size (documents 1–16, i.e. from *NYSE closing averages* to *Lloyd's chief / U.S. grilling*, and documents 17–30, from *Ohio Blue Cross* to *Clinton signs law*). There is no cut of the dendrogram in Figure 17.1 that would give us an equally balanced clustering.

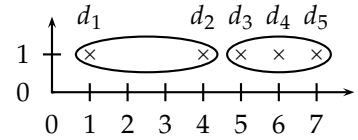
Both single-link and complete-link clustering have graph-theoretic interpretations. Define s_k to be the combination similarity of the two clusters merged in step k and $G(s_k)$ the graph that links all data points with a similarity of at least s_k. Then the clusters after step k in single-link clustering are the *connected components* of $G(s_k)$ and the clusters after step k in complete-link clustering are the maximal *cliques* of $G(s_k)$.[3]

CONNECTED COMPONENT
CLIQUE

These graph-theoretic interpretations motivate the terms single-link and complete-link clustering. Single-link clusters at step k are maximal sets of points that are linked via at least one link (a single link) of similarity $s \geq s_k$; complete-link clusters at step k are maximal sets of points that are completely linked with each other via links of similarity $s \geq s_k$.

Single-link and complete-link clustering reduce the assessment of cluster quality to a single similarity between a pair of documents: the two most similar documents in single-link clustering and the two most dissimilar documents in complete-link clustering. A measurement based on one pair cannot fully reflect the distribution of documents in a cluster. It is therefore not surprising that both algorithms often produce undesirable clusters. Single-link clustering can produce straggling clusters as shown in Figure 17.6. Since the merge criterion is strictly local, a chain of points can be extended for long

2. If you are bothered by the possibility of ties, assume that d_1 has coordinates $(1+\epsilon, 3-\epsilon)$ and that all other points have integer coordinates.
3. A connected component is a maximal set of points such that there is a path connecting each pair. A clique is a set of points that are completely linked with each other.



► **Figure 17.7** Outliers in complete-link clustering. The five documents have the coordinates $1 + 2\epsilon, 4, 5 + 2\epsilon, 6$ and $7 - \epsilon$. Complete-link clustering creates the two clusters shown as ellipses. The most intuitive two-cluster clustering is $\{\{d_1\}, \{d_2, d_3, d_4, d_5\}\}$, but in complete-link clustering, the outlier d_1 splits $\{d_2, d_3, d_4, d_5\}$ as shown.

CHAINING

distances without regard to the overall shape of the emerging cluster. This effect is called *chaining*.

The chaining effect is also apparent in Figure 17.1. The last 12 mergers of the single-link clustering (those above the 0.1 line) add on single documents or pairs of documents, corresponding to a chain. The complete-link clustering in Figure 17.5 avoids this problem. Documents are split into two groups of roughly equal size when we cut the dendrogram at the last merger. In general, this is a more useful organization of the data than a clustering with chains.

But complete-link clustering has a different problem. It pays too much attention to outliers, points that do not fit well into the global structure of the cluster. In the example in Figure 17.7 the four documents d_2, d_3, d_4, d_5 are split because of the outlier d_1 at the left edge (Exercise 17.2). Complete-link clustering does not find the most intuitive cluster structure in this example.

17.2.1 Time complexity

The complexity of the naive HAC algorithm in Figure 17.2 is $\Theta(N^3)$ because we exhaustively search the $N \times N$ matrix C for the largest similarity in each of $N - 1$ iterations.

For the four HAC algorithms discussed in this chapter a more efficient algorithm is the priority-queue algorithm shown in Figure 17.8. Its time complexity is $\Theta(N^2 \log N)$. The rows $C[k]$ of the $N \times N$ matrix C are sorted in decreasing order of similarity in the priority queues P. $P[k]$.max() then returns the element of $C[k]$ that currently has the highest similarity with k. After creating the merged cluster of k_1 and k_2, k_1 is used as its representative. The function sim computes the similarity function for potential merger pairs: largest similarity for single-link, smallest similarity for complete-link, average similarity for GAAC (Section 17.3), and centroid similarity for centroid clustering (Section 17.4). We give an example of how a row of C is processed (Figure 17.8, bottom panel). The first k-loop is $\Theta(N^2)$, the sec-

Given: N length-normalized vectors $\vec{v}_i$
Compute matrix C
for $k = 1$ to N:
  for $\ell = 1$ to N:
    $C[k][\ell].\text{sim} = \vec{v}_k \cdot \vec{v}_\ell$
    $C[k][\ell].\text{index} = \ell$
for $k = 1$ to N:
  $P[k]$:= priority queue for $C[k]$ sorted on sim
  Delete $C[k][k]$ from $P[k]$ *(don't want self-similarities)*
Initialization
$A = [\,]$
for $k = 1$ to N:
  $I[k] = 1$
Compute clustering
for $k = 1$ to $N - 1$:
  $k_1 = \arg\max_{k, I[k]=1} P[k].\text{max}().\text{sim}$
  $k_2 = P[k_1].\text{max}().\text{index}$
  $A.\text{append}(\langle k_1, k_2 \rangle)$
  $I[k_2] = 0$
  $P[k_1] = \emptyset$
  for all ℓ with $I[\ell] = 1, \ell \neq k_1$:
    $C[k_1][\ell].\text{sim} = C[\ell][k_1].\text{sim} = \text{sim}(\ell, k_1, k_2)$
    Delete $C[\ell][k_1]$ and $C[\ell][k_2]$ from $P[\ell]$
    Insert $C[\ell][k_1]$ in $P[\ell]$, $C[k_1][\ell]$ in $P[k_1]$

clustering algorithm	$\text{sim}(\ell, k_1, k_2)$
single-link	$\max(\text{sim}(\ell, k_1), \text{sim}(\ell, k_2))$
complete-link	$\min(\text{sim}(\ell, k_1), \text{sim}(\ell, k_2))$
centroid	$(\frac{1}{N_m}\vec{v}_m) \cdot (\frac{1}{N_\ell}\vec{v}_\ell)$
group-average	$\frac{1}{(N_m+N_\ell)(N_m+N_\ell-1)}[(\vec{v}_m + \vec{v}_\ell)^2 - (N_m + N_\ell)]$

compute $C[5]$	1	2	3	4
	0.2	0.8	0.6	0.4
create $P[5]$ (by sorting)	2	3	4	1
	0.8	0.6	0.4	0.2
merge 2 and 3, update	2	4	1	
similarity of 2, delete 3	0.3	0.4	0.2	
reinsert 2	4	2	1	
	0.4	0.3	0.2	

► **Figure 17.8** The priority-queue algorithm for HAC. Top: The algorithm. Center: Four different similarity measures. Bottom: An example of a sequence of processing steps for a priority queue. This is a made up example showing $P[5]$ for a 5×5 matrix C.

```
SINGLELINKCLUSTERING(d⃗_1, ..., d⃗_N)
 1  for n ← 1 to N
 2  do for i ← 1 to N
 3     do C[n][i].idx ← i
 4        C[n][i].sim ← d⃗_n · d⃗_i
 5     I[n] ← n
 6     NBM[n] ← arg max_{X∈{C[n][i] | n≠i}} X.sim
 7  A ← []
 8  for n ← 1 to N − 1
 9  do i_1 ← arg max_{i|I[i]=i} NBM[i].sim
10     i_2 ← I[NBM[i_1].idx]
11     A.APPEND(⟨i_1, i_2⟩)
12     for i ← 1 to N
13     do if I[i] = i ∧ i ≠ i_1 ∧ i ≠ i_2
14           then C[i_1][i].sim ← C[i][i_1].sim ← max{C[i_1][i].sim, C[i_2][i].sim}
15        if I[i] = i_2
16           then I[i] ← i_1
17     NBM[i_1] ← arg max_{X∈{C[i_1][i] | I[i]=i∧i≠i_1}} X.sim
18  return A
```

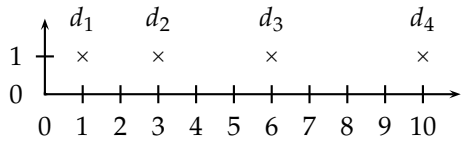
▶ **Figure 17.9** Single-link clustering algorithm using an NBM array. When merging two clusters i_1 and i_2, one of the two (i_1) is selected as the representative of the merged cluster. If $I[i] = i$, then i is the representative of its current cluster. If $I[i] \neq i$, then i has been merged into the cluster represented by $I[i]$ and will therefore be ignored when updating $NBM[i_1]$.

ond and third are $\Theta(N^2 \log N)$ for an implementation of priority queues that supports deletion and insertion in $\Theta(\log N)$. Overall complexity of the algorithm is therefore $\Theta(N^2 \log N)$. In the definition of the merge functions, $\vec{v}_m$ and $\vec{v}_\ell$ are the vector sums of $\omega_{k_1} \cup \omega_{k_2}$ and ω_ℓ, respectively, and N_m and N_ℓ are the number of documents in $\omega_{k_1} \cup \omega_{k_2}$ and ω_ℓ, respectively.

For single-link, we can introduce a next-best-merge array (NBM) as a further optimization as shown in Figure 17.9. NBM keeps track of what the best merge is for each cluster. Each of the two top level for-loops in Figure 17.9 are $\Theta(N^2)$, thus the overall complexity of single-link clustering is $\Theta(N^2)$.

BEST-MERGE PERSISTENCE

Can we also speed up the other three HAC algorithms with an NBM array? Single-link clustering is *best-merge persistent*. Suppose that the best merge cluster for ω_k is ω_j. Then after merging ω_j with a third cluster $\omega_i \neq \omega_k$, the merger of ω_i and ω_j will be ω_k's best merge cluster (Exercise 17.3). As a consequence, the best-merge candidate for the merged cluster is one of the



► **Figure 17.10** Complete-link clustering is not best-merge persistent. At first, d_2 is the best-merge cluster for d_3. But after merging d_1 and d_2, d_4 becomes d_3's best-merge candidate. In a best-merge persistent algorithm like single-link, the d_3's best-merge cluster would be $\{d_1, d_2\}$.

two best-merge candidates of its components in single-link clustering. This means that C can be updated in $\Theta(N)$ in each iteration – by taking a simple max of two values on line 14 in Figure 17.9, for each of the remaining $\leq N$ clusters.

Figure 17.10 demonstrates that best-merge persistence does not hold for complete-link clustering, which means that we cannot use an NBM array to speed up clustering. After merging d_3's best merge candidate d_2 with cluster d_1, an unrelated cluster d_4 becomes the best merge candidate for d_3. This is because the complete-link merge criterion is non-local and can be affected by points at a great distance from the area where two merge candidates meet.

In practice, the efficiency penalty of the $\Theta(N^2 \log N)$ algorithm is small compared to the $\Theta(N^2)$ single-link algorithm since computing the similarity between two documents (e.g., as a dot product) is an order of magnitude slower than a comparison of two values in sorting. All the HAC algorithms we present are $\Theta(N^2)$ with respect to similarity computations. So the difference in complexity is rarely a concern in practice when choosing one of the algorithms.

17.3 Group-average agglomerative clustering

GROUP-AVERAGE AGGLOMERATIVE CLUSTERING
GAAC

For clustering in a vector space, there is a clustering method that evaluates cluster quality based on *all* similarities between documents, thus avoiding the pitfalls of the single-link and complete-link criteria: *group-average agglomerative clustering* or *GAAC* (see Figure 17.3, (d)). It is also called *group-average clustering* and *average-link clustering*. GAAC computes the average similarity sim-ga of all pairs of documents, including pairs from the same cluster. Self-similarities are not included in the average:

$$\text{sim-ga}(\omega_i, \omega_j) = \frac{1}{(N_i + N_j)(N_i + N_j - 1)} \sum_{d_k \in \omega_i \cup \omega_j} \sum_{d_\ell \in \omega_i \cup \omega_j, d_\ell \neq d_k} \vec{d}_k \cdot \vec{d}_\ell \tag{17.2}$$

where $\vec{d}$ is the length-normalized vector of document d, $\cdot$ denotes the scalar or dot product, and N_i and N_j are the number of documents in ω_i and ω_j, respectively.

We can compute the measure sim-ga efficiently because the sum of individual vector similarities is equal to the similarities of their sums:

$$\sum_{d_k \in \omega_i} \sum_{d_\ell \in \omega_j} (\vec{d}_k \cdot \vec{d}_\ell) = (\sum_{d_k \in \omega_i} \vec{d}_k) \cdot (\sum_{d_\ell \in \omega_j} \vec{d}_\ell) \tag{17.3}$$

With (17.3), we have:

$$\text{sim-ga}(\omega_i, \omega_j) = \frac{1}{(N_i + N_j)(N_i + N_j - 1)} [(\sum_{d_k \in \omega_i \cup \omega_j} \vec{d}_k)^2 - (N_i + N_j)] \tag{17.4}$$

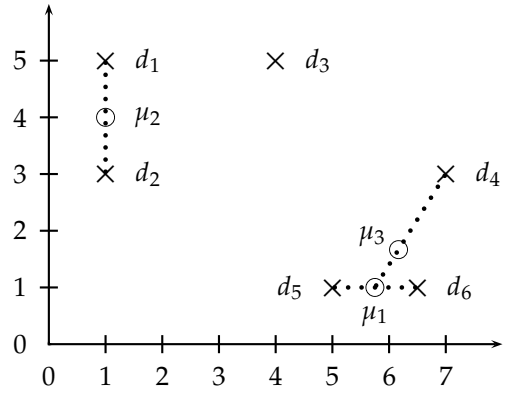
The term $(N_i + N_j)$ is the sum of $N_i + N_j$ self-similarities of value 1.0. With this trick we can compute cluster similarity in constant time (assuming we have available the two vector sums $\sum_{d_k \in \omega_i} \vec{d}_k$ and $\sum_{d_k \in \omega_j} \vec{d}_k$) instead of in $\Theta(N_i N_j)$. Note that for two single-document clusters, 17.4 is equivalent to the dot product.

Equation (17.3) relies on the distributivity of the scalar product with respect to vector addition. Since this is crucial for the efficient computation of a GAAC clustering, the method cannot be easily applied to representations of documents that are not real-valued vectors. Also, Equation (17.3) only holds for the dot product (the term $(\ldots)^2$ is a dot product). While many algorithms introduced in this book have near-equivalent descriptions in terms of dot product, cosine similarity and Euclidean distance (see discussion in Chapter 14, page 270), Equation (17.3) can only be expressed using the dot product. This is a fundamental difference between single-link/complete-link clustering and GAAC. The first two only require a square matrix of similarities as input and do not care how these similarities were computed. To summarize, GAAC requires (i) documents represented as vectors, (ii) length normalization of vectors, so that self-similarities are 1.0, and (iii) the dot product for computing the similarity between vectors and sums of vectors.

The merge algorithm for GAAC is the same as Figure 17.8 for complete-link except that we use as the similarity function Equation 17.4. So the overall time complexity of GAAC is the same as for complete-link clustering: $\Theta(N^2 \log N)$. Like complete-link clustering, GAAC is not best-merge persistent (Exercise 17.3). This means that there is no $\Theta(N^2)$ algorithm for GAAC that would be analogous to the $\Theta(N^2)$ algorithm for single-link.

We can also define group-average similarity as including self-similarities:

$$\text{sim-ga}'(\omega_i, \omega_j) = \frac{1}{(N_i + N_j)^2} (\sum_{d_k \in \omega_i \cup \omega_j} \vec{d}_k)^2 = \frac{1}{N_i + N_j} \sum_{d_k \in \omega_i \cup \omega_j} \vec{d}_k \cdot \vec{\mu}(\omega_i \cup \omega_j) \tag{17.5}$$



► **Figure 17.11** Three iterations of centroid clustering. Each iteration merges the two clusters whose centroids are closest.

where the centroid $\mu(\omega)$ is defined as in Equation (14.1) (page 273). This definition is equivalent to the intuitive definition of cluster quality as average similarity of documents $\vec{d}_k$ to the cluster's centroid $\vec{\mu}$.

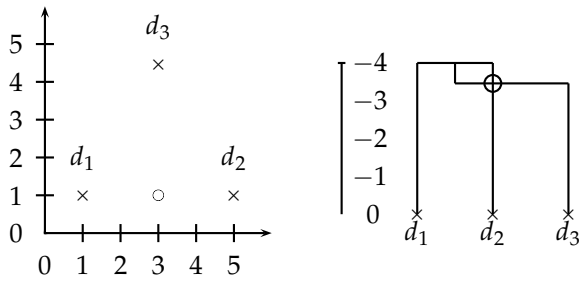
Self-similarities are always equal to 1.0, the maximum possible value for length-normalized vectors. The proportion of self-similarities in Equation (17.5) is $i/i^2 = 1/i$ for a cluster of size i. This gives an unfair advantage to small clusters since they will have proportionally more self-similarities. For two documents d_1, d_2 with a similarity s, we have sim-ga$'(d_1, d_2) = (1+s)/2$. In contrast, sim-ga$(d_1, d_2) = s \leq (1+s)/2$. The sim-ga similarity s is the same as in single-link, complete-link and centroid clustering. We prefer the definition in Equation (17.4), which excludes self-similarities from the average, because we do not want to penalize large clusters for their smaller proportion of self-similarities and because we want a consistent similarity value s for document pairss for all four HAC algorithms.

17.4 Centroid clustering

In centroid clustering, the similarity of two clusters is defined as the similarity of their centroids:

$$\text{sim-cent}(\omega_i, \omega_j) = (\frac{1}{N_i} \sum_{d_k \in \omega_i} \vec{d}_k) \cdot (\frac{1}{N_j} \sum_{d_\ell \in \omega_j} \vec{d}_\ell) = \frac{1}{N_i N_j} \sum_{d_k \in \omega_i} \sum_{d_\ell \in \omega_j} \vec{d}_k \cdot \vec{d}_\ell \tag{17.6}$$

The first part of the equation is centroid similarity. The second part shows that centroid similarity is equivalent to average similarity of all pairs of documents from *different* clusters. Thus, the difference between GAAC and cen-



► **Figure 17.12** Centroid clustering is not monotonic. The documents d_1 at $(1+\epsilon, 1)$, d_2 at $(5, 1)$, and d_3 at $(3, 1+2\sqrt{3})$ are almost equidistant, with d_1 and d_2 closer to each other than to d_3. The non-mononotonic inversion in the hierarchical clustering of the three points appears as an intersecting merge line in the dendrogram (intersection is circled).

troid clustering is that GAAC considers all pairs of documents in computing average pairwise similarity (Figure 17.3, (d)) whereas centroid clustering excludes pairs from the same cluster (Figure 17.3, (c)).

Figure 17.11 shows the first three steps of a centroid clustering. The first two iterations form the clusters $\{d_5, d_6\}$ with centroid μ_1 and $\{d_1, d_2\}$ with centroid μ_2 because the pairs (d_5, d_6) and (d_1, d_2) have the highest centroid similarities. In the third iteration, the highest centroid similarity is between μ_1 and d_4 producing the cluster $\{d_4, d_5, d_6\}$ with centroid μ_3.

Like GAAC, centroid clustering is not best-merge persistent and therefore $\Theta(N^2 \log N)$ (Exercise 17.3).

INVERSION

In contrast to the other three HAC algorithms, centroid clustering is not monotonic. So-called *inversions* can occur: Similarity can increase during clustering as in the example in Figure 17.12, where we define similarity as negative distance. In the first merger, the similarity of d_1 and d_2 is $-(4-\epsilon)$. In the second merger, the similarity of the centroid of d_1 and d_2 (the circle) and d_3 is $\approx -\cos(\pi/6) \times 4 = -\sqrt{3}/2 \times -4 \approx -3.46 > -4$. This is an example of an inversion: similarity *increases* in this sequence of two clustering steps. In a monotonic HAC algorithm, similarity is monotonically *decreasing* from iteration to iteration.

Increasing similarity in a series of HAC clustering steps contradicts the fundamental assumption that small clusters are more coherent than large clusters. An inversion in a dendrogram shows up as a horizontal merge line that is *lower* than the previous merge line. All merge lines in Figures 17.1 and 17.5 are higher than their predecessors because single-link and complete-link clustering are monotonic clustering algorithms.

Despite its non-monotonicity, centroid clustering is often used because its similarity measure – the similarity of two centroids – is conceptually simpler

than the average of all pairwise similarities in GAAC. Figure 17.11 is all one needs to understand centroid clustering. There is no equally simple graph that would explain how GAAC works.

17.5 Optimality of HAC

To state the optimality conditions of hierarchical clustering precisely, we first define the combination similarity comb-sim of a clustering $\Omega = \{\omega_1, \ldots, \omega_K\}$ as the smallest combination similarity of any of its K clusters:

$$\text{comb-sim}(\{\omega_1, \ldots, \omega_K\}) = \min_k \text{comb-sim}(\omega_k)$$

Recall that the combination similarity of a cluster ω that was created as the merger of ω_1 and ω_2 is the similarity of ω_1 and ω_2 (page 336).

OPTIMAL CLUSTERING

We then define $\Omega = \{\omega_1, \ldots, \omega_K\}$ to be *optimal* if all clusterings Ω' with k clusters, $k \leq K$, have lower combination similarities:

$$|\Omega'| \leq |\Omega| \Rightarrow \text{comb-sim}(\Omega') \leq \text{comb-sim}(\Omega)$$

Figure 17.12 shows that centroid clustering is not optimal. The clustering $\{\{d_1, d_2\}, \{d_3\}\}$ (for $K = 2$) has combination similarity $-(4 - \epsilon)$ and $\{\{d_1, d_2, d_3\}\}$ (for $K = 1$) has combination similarity -3.46. So the clustering $\{\{d_1, d_2\}, \{d_3\}\}$ produced in the first merger is not optimal since there is a clustering with fewer clusters ($\{\{d_1, d_2, d_3\}\}$) that has higher combination similarity. Centroid clustering is not optimal because inversions can occur.

The above definition of optimality would be of limited use if it was only applicable to a clustering together with its merging history. But we can easily show (Exercise 17.4) that combination similarity for the three non-inversion algorithms can be read off from the cluster without knowing its history. These direct definitions of combination similarity are as follows.

COMBINATION SIMILARITY

single-link The combination similarity of a cluster ω is the smallest similarity of any bipartition of the cluster, where the similarity of a bipartition is the largest similarity between any two documents from the two parts:

$$\text{comb-sim}(\omega) = \min_{\{\omega' | \omega' \subset \omega\}} \max_{d_i \in \omega'} \max_{d_j \in \omega - \omega'} \text{sim}(d_i, d_j)$$

where each $< \omega', \omega - \omega' >$ is a possible bipartition of ω.

complete-link The combination similarity of a cluster ω is the smallest similarity of any two points in ω: $\min_{d_i \in \omega} \min_{d_j \in \omega} \text{sim}(d_i, d_j)$

GAAC The combination similarity of a cluster ω is the average of all pairwise similarities in ω (where self-similarities are not included in the average): Equation (17.4)

If we use these definitions of combination similarity, then optimality is a property of a set of clusters and not of a process that produced a set of clusters.

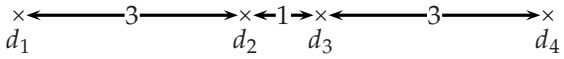
We can now prove the optimality of single-link clustering by induction over the number of clusters K. We will give a proof for the case where no two pairs of documents have the same similarity, but it can easily be extended to the case with ties. The inductive basis of the proof is that a clustering with $K = N$ clusters has combination similarity 1.0, which is the largest value possible. The induction hypothesis is that a clustering Ω_K with K clusters is optimal: comb-sim$(\Omega_K) >$ comb-sim(Ω'_K) for all Ω'_K. Assume for contradiction that the clustering Ω_{K-1} we obtain by merging the two most similar clusters in Ω_K is not optimal and that instead a different sequence of mergers Ω'_K, Ω'_{K-1} leads to the optimal clustering with $K-1$ clusters. We can write the assumption that Ω'_{K-1} is optimal and that Ω_{K-1} is not as comb-sim$(\Omega'_{K-1}) >$ comb-sim(Ω_{K-1}).

Case 1: The two documents linked by $s =$ comb-sim(Ω'_{K-1}) are in the same cluster in Ω_K. They can only be in the same cluster if a merge with similarity smaller than s has occurred in the merge sequence producing Ω_K. This implies $s >$ comb-sim(Ω_K). Thus, comb-sim$(\Omega'_{K-1}) = s >$ comb-sim$(\Omega_K) >$ comb-sim$(\Omega'_K) >$ comb-sim(Ω'_{K-1}). Contradiction.

Case 2: The two documents linked by $s =$ comb-sim(Ω'_{K-1}) are not in the same cluster in Ω_K. But $s =$ comb-sim$(\Omega'_{K-1}) >$ comb-sim(Ω_{K-1}), so the single-link merging rule should have merged these two clusters when processing Ω_K. Contradiction.

Thus, Ω_{K-1} is optimal.

In contrast to single-link clustering, complete-link clustering and GAAC are not optimal as this example shows:



Both algorithms merge the two points with distance 1 (d_2 and d_3) first and thus cannot find the two-cluster clustering $\{\{d_1, d_2\}, \{d_3, d_4\}\}$. But $\{\{d_1, d_2\}, \{d_3, d_4\}\}$ is optimal on the optimality criteria of complete-link clustering and GAAC.

However, the merge criteria of complete-link clustering and GAAC approximate the desideratum of approximate sphericity better than the merge criterion of single-link clustering. In most applications, we want spherical clusters. Thus, even though single-link clustering may seem preferable at first because of its optimality, it is optimal with respect to the wrong criterion in most document clustering applications.

Table 17.1 summarizes the properties of the four HAC algorithms intro-

method	combination similarity	time compl.	optimal?	comment
single-link	max inter-sim of any two docs	$\Theta(N^2)$	yes	chaining effect
complete-link	min inter-sim of any two docs	$\Theta(N^2 \log N)$	no	sensitive to outliers
group-average	average of all sims	$\Theta(N^2 \log N)$	no	best choice for most applications
centroid	average inter-sim	$\Theta(N^2 \log N)$	no	inversions can occur

► **Table 17.1** Comparison of HAC algorithms. Inter-sim refers to the similarity of two documents, one from each of the two clusters (i.e., excluding pairs from the same cluster).

duced in this chapter. We recommend GAAC for document clustering because it is generally the method that produces the clustering with the best properties for applications. It does not suffer from chaining, sensitivity to outliers and inversions.

There are two exceptions to this recommendation. First, for non-vector representations, GAAC is not applicable and clustering should typically be performed with the complete-link method.

Secondly, in some applicatinos the purpose of clustering is not to create a complete hierarchy or exhaustive partition of the entire document set. For instance, *first story detection* or *novelty detection*novelty detection is the task of detecting the first occurrence of an event in a stream of news stories. One approach to this task is to find a tight cluster within the documents that were sent across the wire in a short period of time and are dissimilar from all previous documents. For example, the documents sent over the wire in the minutes after the World Trade Center attack on September 11, 2001 form such a cluster. Variations of single-link clustering can do well on this task since it is the structure of small parts of the vector space – and not gloal structure – that is important in this case.

FIRST STORY DETECTION

Similarly, we will describe an approach to duplicate detection on the web in Section 19.6.1 (page 389) where single-link clustering is used in the guise of the union-find algorithm. Again, the decision whether a group of documents are duplicates of each other is not influenced by documents that are located far away and single-link clustering is a good choice for duplicate detection.

17.6 Divisive clustering

So far we've only looked at agglomerative clustering, but a cluster hierarchy can also be generated top-down. This variant of hierarchical clustering is called *top-down clustering* or *divisive clustering*. We start at the top with all

TOP-DOWN CLUSTERING
DIVISIVE CLUSTERING

documents in one cluster. The cluster is split using a flat clustering algorithm. This procedure is applied recursively until individual documents are reached (see Section 17.6).

Top-down clustering is conceptually more complex than bottom-up clustering since we need a second, flat clustering algorithm as a "subroutine". It has the advantage of being more efficient if we do not generate a complete hierarchy all the way down to individual document leaves. For a fixed number of top levels, using an efficient flat algorithm like K-means, top-down algorithms are linear in the number of documents and clusters. So they run much faster than HAC algorithms, which are at least quadratic.

There is evidence that divisive algorithms produce more accurate hierarchies than bottom-up algorithms in some circumstances (see reference to bisecting K-means in Section 17.9). Bottom-up methods make clustering decisions based on local patterns without initially taking into account the global distribution. These early decisions cannot be undone. Top-down clustering benefits from complete information about the global distribution when making top-level partitioning decisions.

17.7 Cluster labeling

In many applications of flat clustering and hierarchical clustering, particularly in analysis tasks and in user interfaces (see applications in Table 16.1, page 311), human users interact with clusters. In such settings, we must label clusters, so that users can see what a cluster is about.

DIFFERENTIAL CLUSTER LABELING

Differential cluster labeling selects cluster labels by comparing the distribution of words in one cluster with that of other clusters. The feature selection methods we introduced in Section 13.5 (page 253) can all be used for differential cluster labeling.[4] In particular, mutual information (MI) (Section 13.5.1, page 254) or, equivalently, information gain and the χ^2-test (Section 13.5.2, page 257) will identify cluster labels that characterize one cluster in contrast to other clusters. A combination of a differential test with a penalty for rare words often gives the best labeling results because rare words are not necessarily representative of the cluster as a whole.

We apply three labeling methods to a K-means clustering in Table 17.2. In this example, there was almost no difference between MI and χ^2. We therefore omit the latter.

CLUSTER-INTERNAL LABELING

Cluster-internal labeling computes a label that solely depends on the cluster itself, not on other clusters. Labeling a cluster with the title of the document closest to the centroid is one cluster-internal method. Titles are easier to read than a list of words. A full title can also contain important context that didn't

4. Selecting the most frequent words is non-differential feature selection technique we discussed in Section 13.5. It can also be used for labeling clusters.

	# docs	labeling method		
		centroid	mutual information	title
4	622	oil plant mexico production crude **power 000 refinery gas** bpd	plant oil production **barrels** crude bpd mexico **dolly capacity petroleum**	MEXICO: Hurricane Dolly heads for Mexico coast
9	1017	police security **russian** people military peace killed told **grozny court**	police killed military security peace told **troops forces rebels** people	RUSSIA: Russia's Lebed meets rebel chief in Chechnya
10	1259	00 000 tonnes traders futures wheat prices **cents september** tonne	**delivery** traders futures tonne tonnes **desk** wheat prices 000 00	USA: Export Business - Grain/oilseeds complex

► **Table 17.2** Automatically computed cluster labels. This is for three of ten clusters (4, 9, and 10) in a *K*-means clustering of the first 10,000 documents in Reuters-RCV1. The last three columns show cluster summaries computed by three labeling methods: most highly weighted words in centroid (centroid), mutual information, and the title of the document closest to the centroid of the cluster (title). Words selected by only one of the first two methods are in bold.

make it into the top 10 terms selected by MI. On the web, anchor text can play a role similar to a title since the anchor text pointing to a page can serve as a concise summary of its contents.

In Table 17.2, the title for cluster 9 suggests that many of its documents are about the Chechnya conflict, a fact the MI words do not reveal; but a single document is unlikely to be representative of all documents in a cluster. An example is cluster 4, whose selected title is misleading. The main topic of the cluster is oil. Articles about hurricane Dolly only ended up in this cluster because of its effect on oil prices.

We can also use a list of words with high weights in the centroid of the cluster as a label. Such highly weighted words (or, even better, phrases, especially noun phrases) are often more representative of the cluster than a few titles can be, even if they are not filtered for distinctiveness as in the differential methods. But a list of phrases takes more time to digest for users than a well crafted title.

Cluster-internal methods are efficient, but they fail to distinguish words that are frequent in the collection as a whole from those that are frequent only in the cluster. Words like year or Tuesday may be among the most frequent in a cluster, but they are not helpful in understanding the contents of a cluster with a specific topic like oil.

In Table 17.2, the centroid method selects a few more uninformative words

(000, court, cents, september) than MI (forces, desk), but most of the words selected by either method are good descriptors. We get a good sense of the documents in a cluster from scanning the selected words.

For hierarchical clustering, additional complications arise in cluster labeling. Not only do we need to distinguish an internal node in the tree from its siblings, but also from its parent and its children. Documents in child nodes are by definition also members of their parent node, so we cannot use a naive differential method to find labels that distinguish the parent from its children. However, more complex criteria, based on a combination of overall collection frequency and prevalence in a given cluster, can determine whether a term is a more informative label for a child node or a parent node (see Section 17.9).

17.8 Implementation notes

Most problems that require the computation of a large number of dot products benefit from an inverted index. This is also the case for HAC clustering. Computational savings due to the inverted index are large if there are many zero similarities – either because many documents do not share any words or because an agressive stop list is used.

In low dimensions, more aggressive optimizations are possible that make the computation of most pairwise similarities unnecessary (Exercise 17.9). Because of the curse of dimensionality, more efficient algorithms are not known in higher dimensions. We encountered the same problem in kNN classification (see Section 14.6, page 291).

When computing a GAAC of a large document set in high dimensions, we have to take care to avoid dense centroids. For dense centroids, clustering can take time $\Theta(MN^2 \log N)$ where M is the size of the vocabulary whereas complete-link clustering is $\Theta(M_{\text{ave}} N^2 \log N)$ where M_{ave} is the average vocabulary of a document. So for large vocabularies complete-link can be more efficient than an unoptimized implementation of GAAC. We discussed this problem in the context of K-means clustering in Chapter 16 (page 324) and suggested two solutions: truncating centroids (keeping only highly weighted terms) and representing clusters by means of sparse medoids instead of dense centroids. This optimization can also be applied to GAAC and centroid clustering.

Even with these optimizations, HAC algorithms are all $\Theta(N^2)$ or $\Theta(N^2 \log N)$ and therefore infeasible for large document sets of 1,000,000 or more documents. For such large sets, HAC can only be used in combination with a flat clustering algorithm like K-means. Recall that K-means requires a set of seeds as initialization (Figure 16.5, page 320). If these seeds are badly chosen, then the resulting clustering will be of poor quality. We can employ an

HAC algorithm to compute seeds of high quality. If the HAC algorithm is applied to a document subset of size $\sqrt{N}$, then the overall run time of *K*-means cum HAC seed generation is $\Theta(N)$. This is because the application of a quadratic algorithm to a sample of size $\sqrt{N}$ has an overall complexity of $\Theta(N)$. An appropriate adjustment can be made for an $\Theta(N^2 \log N)$ algorithm to guarantee linearity. This algorithm is referred to as the *Buckshot algorithm*. It combines the determinism and higher reliability of HAC with the efficiency of *K*-means.

BUCKSHOT ALGORITHM

17.9 References and further reading

An excellent general review of clustering is (Jain et al. 1999). Early references for specific HAC algorithms are (King 1967) (single-link), (Sneath and Sokal 1973) (complete-link, GAAC) and (Lance and Williams 1967) (discussing a large variety of hierarchical clustering algorithms). The single-link algorithm in Figure 17.9 is similar to *Kruskal's algorithm* for constructing a minimum spanning tree. A graph-theoretical proof of the correctness of Kruskal's algorithm (which is analogous to the proof in Section 17.5) is provided in (Cormen et al. 1990, Theorem 23.1). See Exercise 17.1 for the connection between minimum spanning trees and single-link clusterings.

KRUSKAL'S ALGORITHM

It is often claimed that hierarchical clustering algorithms produce better clusterings than flat algorithms (Jain and Dubes 1988, p. 140), (Cutting et al. 1992, Larsen and Aone 1999) although more recently there have been experimental results suggesting the opposite (Zhao and Karypis 2002). Even without a consensus on average behavior, there is no doubt that results of EM and *K*-means are highly variable since they will often converge to a local optimum of poor quality. The hierarchical algorithms we have presented here are deterministic and thus more predictable.

The complexity of complete-link, group-average and centroid clustering is sometimes given as $\Theta(N^2)$ (Day and Edelsbrunner 1984, Voorhees 1985b, Murtagh 1983) because a document similarity computation is an order of magnitude more expensive than a simple comparison, the main operation executed in the merging steps after the $N \times N$ similarity matrix has been computed.

The centroid algorithm described here is due to Voorhees (1985b). Voorhees recommends complete-link and centroid clustering over single-link for a retrieval application. The Buckshot algorithm was originally published by Cutting et al. (1993). Allan et al. (1998) apply the single-link clustering to first story detection.

An important HAC technique not discussed here is *Ward's method* (Ward 1963, El-Hamdouchi and Willett 1986), also called *minimum variance clustering*. In each step, it selects the merger with the smallest RSS (Chapter 16,

WARD'S METHOD
MINIMUM VARIANCE CLUSTERING

page 319). The merge criterion in Ward's method (a function of all individual distances from the centroid) is closely related to the merge criterion in GAAC (a function of all individual similarities to the centroid).

Despite its importance for making the results of clustering useful, comparatively little work has been done on labeling clusters. Popescul and Ungar (2000) obtain good results with a combination of χ^2 and collection frequency of a term. Glover et al. (2002b) use information gain for labeling clusters of web pages. Stein and zu Eissen's approach is ontology-based (2004). The more complex problem of labeling nodes in a hierarchy (which requires distinguishing more general labels for parents from more specific labels for children) is tackled by Glover et al. (2002a) and Treeratpituk and Callan (2006). Some clustering algorithms attempt to find a set of labels first and then build (often overlapping) clusters around the labels, thereby avoiding the problem of labeling altogether (Zamir and Etzioni 1999, Käki 2005, Osiński and Weiss 2005). We know of no comprehensive study that compares the quality of such "label-based" clustering to the clustering algorithms discussed here and in Chapter 16. In principle, work on multi-document summarization (McKeown and Radev 1995) is also applicable to cluster labeling, but multi-document summaries are usually longer than the short text fragments needed when labeling clusters. Cluster labeling is ultimately a UI problem. We recommend reading (Baeza-Yates and Ribeiro-Neto 1999, ch. 10) for an introduction to user interfaces in IR.

An example of an efficient divisive algorithm is bisecting *K*-means (Steinbach et al. 2000). The *principal direction divisive partitioning* (PDDP) algorithm (whose bisecting decisions are based on SVD, see Chapter 18) is, in contrast to bisecting *K*-means, deterministic and offers comparable clustering quality (Savaresi and Boley 2004).

Unlike *K*-means and EM, most hierarchical clustering algorithms do not have a probabilistic interpretation. Model-based hierarchical clustering (Vaithyanathan and Dom 2000, Kamvar et al. 2002, Castro et al. 2004) is an exception.

The evaluation methodology described in Section 16.3 (page 315) is also applicable to hierarchical clustering. Specialized evaluation measures for hierarchies are discussed by Fowlkes and Mallows (1983), Larsen and Aone (1999) and Sahoo et al. (2006).

The R environment (R Development Core Team 2005) offers good support for hierarchical clustering. The R function `hclust` implements single-link, complete-link, group-average, and centroid clustering; and Ward's method. Another option provided is `median` clustering which represents each cluster by its medoid (cf. k-medoids in Chapter 16, page 324). Support for clustering vectors in high-dimensional spaces is provided by the software package CLUTO (http://glaros.dtc.umn.edu/gkhome/views/cluto).

17.10 Exercises

Exercise 17.1

MINIMUM SPANNING TREE

A single-link clustering can also be computed from the *minimum spanning tree* of a graph. The minimum spanning tree connects the vertices of a graph at the smallest possible cost, where cost is defined as the sum over all edges of the graph. In our case the cost of an edge is the distance between two documents. Show that if $\Delta_{k-1} > \Delta_k > \ldots > \Delta_1$ are the costs of the edges of a minimum spanning tree, then these edges correspond to the $k-1$ merges in constructing a single-link clustering.

Exercise 17.2

Show that complete-link clustering creates the two-cluster clustering depicted in Figure 17.7.

Exercise 17.3

Show that single-link clustering is best-merge persistent and that GAAC and centroid clustering are not best-merge persistent.

Exercise 17.4

Show the equivalence between the process definition of combination similarity (similarity of two clusters that were merged into ω) and the "static" definition of combination similarity on page 350.

Exercise 17.5

Apply group-average clustering to the points in Figures 17.6 and 17.7. Map them onto the surface of the unit sphere in a three-dimensional space to get length-normalized vectors. Is the group-average clustering different from the single-link and complete-link clusterings?

Exercise 17.6

a. Consider running 2-means clustering on a collection with documents from two different languages. What result would you expect?

b. Would you expect the same result when running an HAC algorithm?

Exercise 17.7

Download Reuters-21578. Keep only documents that are in the classes *crude*, *interest*, and *grain*. Discard documents that are members of more than one of these three classes. Compute a (i) single-link, (ii) complete-link, (iii) GAAC, (iv) centroid clustering of the documents. (v) Cut each dendrogram at the second branch from the top to obtain $K = 3$ clusters. Compute the Rand index for each of the 4 clusterings. Which clustering method performs best?

Exercise 17.8

Suppose a run of HAC finds the clustering with $K = 7$ to have the highest value on some pre-chosen goodness measure of clustering. Have we found the highest-value clustering amongst all clusterings with $K = 7$?

Exercise 17.9

Consider the task of producing a single-link clustering of N points on a line:

Show that we only need to compute a total of about N similarities. What is the overall complexity of single-link clustering of points on a line?

Exercise 17.10

Prove that single-link, complete-link, and group-average are monotonic in the sense defined on page 336.

Exercise 17.11

For N points, there are $\leq K^N$ different flat clusterings into K clusters (Section 16.2, page 315). What is the number of different hierarchical clusterings (or dendrograms) of N documents? Are there more flat clusterings or more hierarchical clusterings for given K and N?

Exercise 17.12

For a set of N documents there are up to N^2 distinct similarities between clusters in single-link and complete-link clustering. How many distinct cluster similarities are there in GAAC and centroid clustering?

18 Matrix decompositions and Latent Semantic Indexing

In Chapter 7 we introduced the notion of a *term-document matrix:* an $M \times N$ matrix C, each of whose rows represents a term and each of whose columns represents a document in the collection. Even for a collection of modest size, the term-document matrix C is likely to have several tens of thousand of rows and columns. In this chapter we first develop a class of operations from linear algebra, known as *matrix decomposition*. We then use a special form of matrix decomposition to construct a *low-rank* approximation to the term-document matrix. Next we examine the application of such low-rank approximations to indexing and retrieving documents, a technique referred to as *latent semantic indexing*. While latent semantic indexing has not been established as a significant force in scoring and ranking for information retrieval, it remains an intriguing approach to clustering in a number of domains including for collections of text documents (Section 16.6, page 329). Understanding its full potential remains an area of active research.

Readers who do not require a refresher on linear algebra may skip Section 18.1.

18.1 Linear algebra review

We briefly review some necessary background in linear algebra. Let C be an $M \times N$ matrix with real-valued entries; for a term-document matrix, all entries are in fact non-negative. The *rank* of a matrix is the number of linearly independent rows (or columns) in it; thus, $rank(C) \leq \min\{M, N\}$. A square $r \times r$ matrix all of whose off-diagonal entries are zero is called a *diagonal matrix*; its rank is equal to the number of non-zero diagonal entries. If all the diagonal entries of such a diagonal matrix are 1, it is called the identity matrix of dimension r and represented by I_r.

RANK

For a square $M \times M$ matrix C, the values of λ satisfying

$$C\vec{x} = \lambda\vec{x} \tag{18.1}$$

EIGENVALUES are called the *eigenvalues* of C. The N-vector $\vec{x}$ satisfying (18.1) for an eigenvalue λ is the corresponding *right eigenvector*. The eigenvector corresponding to the eigenvalue of largest magnitude is called the *principal eigenvector.* In a similar fashion, the *left eigenvectors* of C are the M-vectors y such that

$$\vec{y}C = \lambda\vec{y}. \tag{18.2}$$

The number of non-zero eigenvalues of C is rank(C).

Exercise 18.1

What is the rank of the 3×3 diagonal matrix below?

$$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 2 & 1 \end{pmatrix}$$

Exercise 18.2

Show that $\lambda = 2$ is an eigenvalue of

$$C = \begin{pmatrix} 6 & -2 \\ 4 & 0 \end{pmatrix}.$$

Find the corresponding eigenvector.

The eigenvalues of a matrix are found by solving the *characteristic equation*, which is obtained by rewriting (18.1) in the form $(C - \lambda I_M)\vec{x} = 0$. The eigenvalues of Care then the solutions of $|(C - \lambda I_M)| = 0$, where $|S|$ denotes the determinant of a square matrix S. The equation $|(C - \lambda I_M)| = 0$ is an Mth order polynomial equation in λ and can have at most M roots, which are the eigenvalues of C. These eigenvalues can in general be complex, even if all entries of C are real.

We now examine some further properties of eigenvalues and eigenvectors, to set up the central idea of singular value decompositions in Section 18.2 below. First, we look at the relationship between matrix-vector multiplication and eigenvalues. Consider the matrix

$$S = \begin{pmatrix} 30 & 0 & 0 \\ 0 & 20 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Clearly the matrix has rank 3, and therefore has 3 non-zero eigenvalues $\lambda_1 = 30$, $\lambda_2 = 20$ and $\lambda_3 = 1$, with the three corresponding eigenvectors

$$\vec{v_1} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \vec{v_2} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } \vec{v_3} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

For each of the eigenvectors, multiplication by S acts as if we were multiplying the eigenvector by a multiple of the identity matrix; the multiple is different for each eigenvector. Now, consider an arbitrary vector, such as $\vec{v} = \begin{pmatrix} 2 \\ 4 \\ 6 \end{pmatrix}$. We may express $\vec{v}$ as a linear combination of the three eigenvectors of S:

$$\vec{x} = \begin{pmatrix} 2 \\ 4 \\ 6 \end{pmatrix} = 2\vec{x_1} + 4\vec{x_2} + 6\vec{x_3}.$$

Suppose we multiply the arbitrary vector $\vec{v}$ by S:

$$\begin{aligned} S\vec{v} &= S(2\vec{s_1} + 4\vec{x_2} + 6\vec{x_3}) \\ &= 2S\vec{x_1} + 4S\vec{x_2} + 6S\vec{x_3} \\ &= 2\lambda_1\vec{x_1} + 4\lambda_2\vec{x_2} + 6\lambda_3\vec{x_3} \\ &= 60\vec{x_1} + 80\vec{x_2} + 6\vec{x_3}. \end{aligned} \tag{18.3}$$

Even though $\vec{v}$ is an arbitrary vector, the effect of multiplication by S is determined by the eigenvalues and eigenvectors of S. Furthermore, it is intuitively apparent from (18.3) that the product $S\vec{v}$ is relatively unaffected by terms arising from the small eigenvalues of S; in our example, since $\lambda_3 = 1$, the contribution of the third term on the right hand side of (18.3) is small. This suggests that the effect of small eigenvalues (and their eigenvectors) on a matrix-vector product is small. We will carry forward this intuition when studying matrix decompositions and low-rank approximations in Section 18.2. Before doing so, we examine the eigenvectors and eigenvalues of special forms of matrices that will be of particular interest to us.

For a *symmetric* matrix S, the eigenvectors corresponding to distinct eigenvalues are *orthogonal*. Further, if S is both real and symmetric, the eigenvalues are all real.

✎ **Example 18.1:** Consider the real, symmetric matrix

$$S = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}. \tag{18.4}$$

From the characteristic equation $|S - \lambda I| = 0$, we have the quadratic $(2 - \lambda)^2 - 1 = 0$, whose solutions yield the eigenvalues 3 and 1. The corresponding eigenvectors $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ are orthogonal.

18.1.1 Matrix decompositions

In this section we examine ways in which a square matrix can be *factored* into the product of matrices derived from its eigenvectors; we refer to this process as *matrix decomposition*. page 364 This will form the basis of our principal text-analysis technique in Section 18.3. We begin by proving two theorems on the decomposition of a square matrix into the product of three matrices of a special form. The first of these, Theorem 18.1, gives the basic factorization of a square real-valued matrix into three factors. The second, Theorem 18.2, applies to square symmetric matrices and is the basis of the singular value decomposition described in Theorem 18.3.

MATRIX DECOMPOSITION

Theorem 18.1. (Matrix diagonalization theorem) *Let S be a square real-valued $M \times M$ matrix with M linearly independent eigenvectors. Then there exists an* eigen decomposition

EIGEN DECOMPOSITION

$$S = U\Lambda U^{-1}, \tag{18.5}$$

where the columns of U are the eigenvectors of S and Λ is a diagonal matrix whose diagonal entries are the eigenvalues of S in decreasing order

$$\begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \dots & \\ & & & \lambda_M \end{pmatrix}, \lambda_i \geq \lambda_{i+1}. \tag{18.6}$$

If the eigenvalues are distinct, then this decomposition is unique.

To understand how Theorem 18.1 works, we note that U has the eigenvectors of S as columns

$$U = (\vec{u_1}\ \vec{u_2} \cdots \vec{u_M}). \tag{18.7}$$

Then we have

$$\begin{aligned} SU &= S(\vec{u_1}\ \vec{u_2} \cdots \vec{u_M}) \\ &= (\lambda_1\vec{u_1}\ \lambda_2\vec{u_2} \cdots \lambda_M\vec{u_M}) \\ &= (\vec{u_1}\ \vec{u_2} \cdots \vec{u_M}) \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \dots & \\ & & & \lambda_M \end{pmatrix}. \end{aligned}$$

Thus, we have $SU = U\Lambda$, or $S = U\Lambda U^{-1}$.

Exercise 18.3

Compute the unique eigen decomposition of the 2×2 matrix in (18.4).

We next describe how a symmetric square matrix can be decomposed into the product of matrices derived from its eigenvectors. This will pave the way for our development of our main tool for text analysis, the singular value decomposition (Section 18.2).

Theorem 18.2. (Symmetric diagonalization theorem) *Let S be a square, symmetric real-valued $M \times M$ matrix with M linearly independent eigenvectors. Then there exists a* symmetric eigen decomposition

SYMMETRIC EIGEN DECOMPOSITION

$$S = Q\Lambda Q^T, \tag{18.8}$$

where the columns of Q are the orthogonal and normalized (unit length) eigenvectors of S, and Λ is the diagonal matrix whose entries are the eigenvalues of S. Further, all entries of Q are real and we have $Q^{-1} = Q^T$.

We will build on this symmetric eigen decomposition to build low-rank approximations to term-document matrices.

18.2 Term-document matrices and singular value decompositions

The decompositions we have been studying thus far apply to square matrices. However, the matrix we are interested in is the $M \times N$ term-document matrix where (barring a rare coincidence) $M \neq N$. To this end we first describe an extension of the symmetric eigen decomposition known as the *singular value decomposition*. We then show in Section 18.3 how this can be used to construct an approximate version of C. It is beyond the scope of this book to develop a full treatment of the mathematics underlying singular value decompositions; as such, the intuition is that given for symmetric eigen decompositions in Section 18.1.1.

SINGULAR VALUE DECOMPOSITION

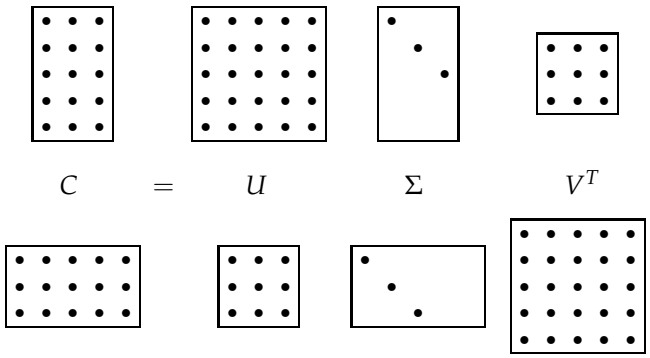
Theorem 18.3. *Let r be the rank of the $M \times N$ matrix C. Then, there is a* singular-value decomposition *(SVD for short) of C of the form*

$$C = U\Sigma V^T, \tag{18.9}$$

where

1. *U is an $M \times M$ matrix whose columns are the orthogonal eigenvectors of CC^T;*
2. *V is an $N \times N$ matrix whose columns are the orthogonal eigenvectors of C^TC, and V^T its transpose;*
3. *The eigenvalues $\lambda_1, \ldots, \lambda_r$ of CC^T are the same as the eigenvalues of C^TC;*
4. *For $1 \leq i \leq r$, let $\sigma_i = \sqrt{\lambda_i}$, with $\lambda_i \geq \lambda_{i+1}$. Then the $M \times N$ matrix Σ is composed by setting $\Sigma_{ii} = \sigma_i$ for $1 \leq i \leq r$, and zero otherwise.*

The values σ_i are referred to as the *singular values* of C.



► **Figure 18.1** Illustration of the singular-value decomposition. In this schematic illustration of (18.9), we see two cases illustrated. In the top half of the figure, we have a matrix C for which $M > N$. The lower half illustrates the case $M < N$.

✎ **Example 18.2:** We now illustrate the singular-value decomposition of a 3×2 matrix of rank 2; the singular values are $\Sigma_{11} = \sqrt{3}$ and $\Sigma_{22} = 1$.

$$C = \begin{pmatrix} 1 & -1 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 2/\sqrt{6} & 0 & 1/\sqrt{3} \\ -1/\sqrt{6} & 1/\sqrt{2} & 1/\sqrt{3} \\ 1/\sqrt{6} & 1/\sqrt{2} & -1/\sqrt{3} \end{pmatrix} \begin{pmatrix} \sqrt{3} & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}. \tag{18.10}$$

As with the matrix decompositions defined in Section 18.1.1, the singular value decomposition of a matrix can be computed by a variety of algorithms, many of which have been publicly available software implementations; pointers to these are given in Section 18.4.

18.3 Low-rank approximations and latent semantic indexing

We next state a matrix approximation problem that at first seems to have little to do with information retrieval. We describe a solution to this matrix problem using singular-value decompositions, then develop its application to information retrieval.

FROBENIUS NORM

Given an $M \times N$ matrix C and a positive integer k, we wish to find an $M \times N$ matrix C_k of rank $\leq k$, so as to minimize the *Frobenius norm* of the matrix difference $X = C - C_k$, defined to be

$$||X||_F = \sqrt{\sum_{i=1}^{M} \sum_{j=1}^{N} X_{ij}^2}. \tag{18.11}$$

Thus, the Frobenius norm of X measures the discrepancy between C_k and C; our goal is to find a matrix C_k that minimizes this discrepancy, while constraining C_k to have rank at most k. If r is the rank of C, clearly $C_r = C$ and the Frobenius norm of the discrepancy is zero in this case. When k is far smaller than r, we refer to C_k as a *low-rank approximation*.

LOW-RANK APPROXIMATION

The singular value decomposition can be used to solve this matrix approximation problem, then derive from it an application to approximating term-document matrices. We invoke the following three-step procedure to this end:

1. Given C, construct its SVD in the form shown in (18.9); thus, $C = U\Sigma V^T$.
2. Derive from Σ the matrix Σ_k formed by replacing by zeros the $r - k$ smallest singular values on the diagonal of Σ.
3. Compute and output $C_k = U\Sigma_k V^T$ as the rank-k approximation to C.

The rank of C_k is at most k: this follows from the fact that Σ_k has at most k non-zero values. Next, we recall the intuition of the example in (18.3): the effect of small eigenvalues on matrix products is small. Thus, it seems plausible that replacing these small eigenvalues by zero will not substantially alter the product, leaving it "close" to C. The following theorem due to Eckart and Young tells us that, in fact, this procedure yields the matrix of rank k with the lowest possible Frobenius error.

Theorem 18.4.

$$\min_{X|\ rank(X)=k} ||C - X||_F = ||C - C_k||_F = \sigma_{k+1}. \tag{18.12}$$

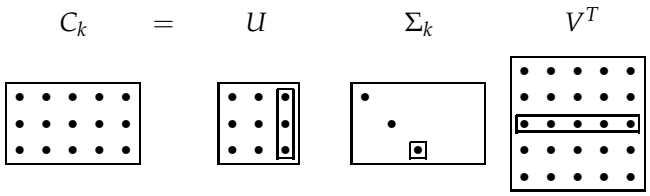
Recalling that the singular values are in decreasing order $\sigma_1 \geq \sigma_2 \geq \cdots$, we learn from Theorem 18.4 that C_k is the best rank-k approximation to C, incurring an error (measured by the Frobenius norm of $C - C_k$) equal to σ_{k+1}. Thus, the larger k is the smaller this error (and in particular, for $k = r$, the error is zero since $\Sigma_r = \Sigma$ and thus $C_r = C$).

To derive further insight into why the process of truncating the smallest $r - k$ singular values in Σ helps generate a rank-k approximation of low error, we examine the form of C_k:

$$C_k = U\Sigma_k V^T \tag{18.13}$$

$$= U \begin{pmatrix} \sigma_1 & 0 & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \sigma_k & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots \end{pmatrix} V^T \tag{18.14}$$

$$= \sum_{i=1}^{k} \sigma_i \vec{u}_i \vec{v}_i^T, \tag{18.15}$$



► **Figure 18.2** Illustration of low rank approximation using the singular-value decomposition. The dashed boxes indicate the matrix entries affected by "zeroing out" the smallest singular values.

where $\vec{u}_i$ and $\vec{v}_i$ are the ith columns of U and V, respectively. Thus, $\vec{u}_i\vec{v}_i^T$ is a rank-1 matrix, so that we have just expressed C_k as the sum of k rank-1 matrices each weighted by a singular value. As i increases, the contribution of the rank-1 matrix $\vec{u}_i\vec{v}_i^T$ is weighted by a sequence of shrinking singular values σ_i.

Exercise 18.4

Compute a rank 1 approximation to the matrix C in Example 18.2, using the SVD as above. What is the Frobenius norm of the error of this approximation?

Exercise 18.5

Consider now the computation in Exercise 18.4. Following the schematic in Figure 18.2, notice that for a rank 1 approximation we have σ_1 being a scalar. Denote by U_1 the first column of U and by V_1 the first column of V. Show that the rank-1 approximation to C can then be written as $U_1\sigma_1V_1^T$.

In fact, Exercise 18.5 can be generalized to rank k approximations: we let U_k and V_k denote the matrix formed by retaining only the first k columns of U and V, respectively. Thus U_k is an $mM \times k$ matrix while V_k^T is a $k \times N$ matrix. Then, we have

$$C_k = U_k\Sigma_k'V_k^T, \tag{18.16}$$

where Σ_k' is the square $k \times k$ submatrix of Σ_k with the singular values $\sigma_1, \ldots, \sigma_k$ on the diagonal. The primary advantage of using (18.16) is to eliminate a lot of redundant columns in U and V, thereby explicitly eliminating multiplication by columns that will contribute zero to the low-rank approximation.

Exercise 18.6

For the matrix C in Example 18.2, write down both Σ_2 and Σ_2'.

Exercise 18.7

Under what conditions is $\Sigma_k = \Sigma_k'$?

Before discussing the approximation of a term-document matrix C by one of lower rank, we first motivate such an approximation. Recall the vector space representation of documents and queries introduced in Chapter 7. This vector space representation enjoys a number of advantages including the uniform treatment of queries and documents as vectors, the induced score computation based on cosine similarity, the ability to weight different terms differently, and its extension beyond document retrieval to such applications as clustering and classification. The vector space representation suffers, however, from its inability to cope with two classic problems arising in natural languages: *synonymy* and *polysemy*. Synonymy refers to a case where two different words (say car and automobile) have the same meaning. Because the vector space representation fails to capture the relationship between synonymous terms such as car and automobile – according each a separate dimension in the vector space – we may have a situation where the computed similarity $\vec{q} \cdot \vec{d}$ between a query $\vec{q}$ (say, car) and a document $\vec{d}$ containing these terms underestimates the true similarity that a user would perceive. Polysemy on the other hand refers to the case where a term such as charge has multiple meanings, so that the computed similarity $\vec{q} \cdot \vec{d}$ overestimates the similarity that a user would perceive. Could we use the co-occurrences of terms (whether, for instance, charge occurs in a document containing steed versus in a document containing electron) to capture the latent semantic associations of terms and alleviate these problems?

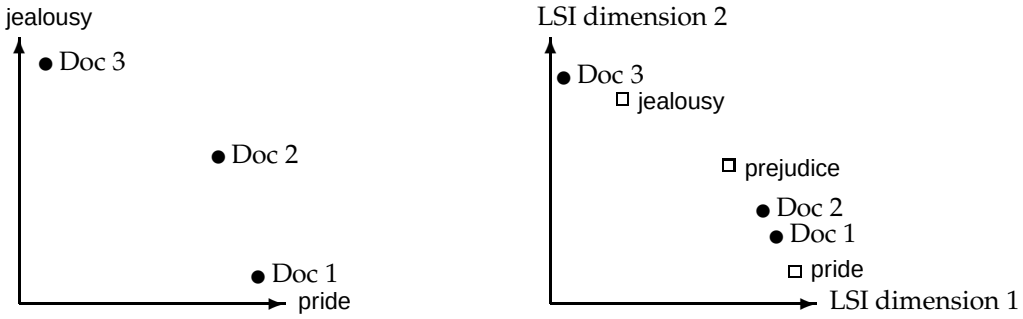
LATENT SEMANTIC INDEXING

Even for a collection of modest size, the term-document matrix C is likely to have several tens of thousand of rows and columns, and a rank in the tens of thousands as well. In *latent semantic indexing* (generally abbreviated *LSI*), we use the SVD to construct a low-rank approximation C_k to the term-document matrix, for a value of k that is far smaller than the original rank of C. In the experimental work cited below, k is generally chosen to be in the low hundreds. We thus map each row/column (respectively corresponding to a term/document) to a k-dimensional space; this space is defined by the k principal eigenvectors (corresponding to the largest eigenvalues) of CC^T and C^TC. Note that the matrix C_k is itself still an $M \times N$ matrix, irrespective of k.

Next, we use the new k-dimensional LSI representation as we did the original representation – to compute similarities between vectors. A query vector $\vec{q}$ is mapped into its representation in the LSI space by the transformation

$$\vec{q}_k = \vec{q}^T U_k \Sigma_k^{-1}. \tag{18.17}$$

Now, we may use cosine similarities as in Chapter 7 to compute the similarity between a query and a document, or between two documents.



► **Figure 18.3** Original and LSI spaces. Only two of many axes are shown in each case.

The fidelity of the approximation of C_k to C leads us to hope that the relative values of cosine similarities are preserved: if a query is close to a document in the original space, it remains relatively close in the k-dimensional space. But this in itself is not sufficiently interesting, especially given that the sparse query vector $\vec{q}$ turns into a dense query vector $\vec{q}_k$ in the low-dimensional space. This has a significant computational cost, when compared with the cost of processing $\vec{q}$ in its native form.

We may view the low-rank approximation of C by C_k as a *constrained optimization* problem: subject to the constraint that C_k have rank at most k, we seek a representation of the terms and documents comprising C with low Frobenius norm for the error $C - C_k$. When forced to squeeze the terms/documents down to a k-dimensional space, the SVD should bring together terms with similar co-occurrences. This intuition suggests, then, that not only should retrieval quality not suffer too much from the dimension reduction, but in fact may *improve*.

Experiments with LSI tend to consistently bear out the following conclusions:

- The computational cost of the SVD is significant; at the time of this writing, we know of no successful experiment with over one million documents. This has been the biggest obstacle to the widespread adoption to LSI.
- As we reduce k, recall tends to increase, as expected.
- Most surprisingly, a value of k in the low hundreds actually *increases* precision on many query benchmarks. This appears to confirm that for a

suitable value of k, LSI addresses some of the challenges of synonymy and polysemy.

The experiments also documented some modes where LSI failed to match the effectiveness of more traditional indexes and query languages. Most notably (and perhaps obviously), LSI shares two basic drawbacks of vector space retrieval: there is no good way of expressing negations (find documents that contain german but not shepherd), or Boolean conditions.

SOFT CLUSTERING

LSI can be viewed as *soft clustering* by interpreting each dimension of the reduced space as a cluster and the value that a document has on that dimension as its fractional membership in that cluster.

18.4 References and further reading

Strang (1986) provides an excellent introductory overview of matrix decompositions including the singular value decomposition. Theorem 18.4 is due to Eckart and Young (1936). The connection between information retrieval and low-rank approximations of the term-document matrix was introduced in Deerwester et al. (1990), with a subsequent survey of results in Berry et al. (1995). Dumais (1993) and Dumais (1995) describe experiments on TREC benchmarks giving evidence that at least on some benchmarks, LSI can produce better precision and recall than standard vector-space retrieval. http://www.cs.utk.edu/~berry/lsi++/ and http://lsi.argreenhouse.com/lsi/LSIpapers.html offer comprehensive pointers to the literature and software of LSI. Hofmann (1999a;b) provides a probabilistic extension of the basic latent semantic indexing technique. Blei et al. (2003) present a latent probabilistic model that is generative and assigns probabilities to documents outside of the training set.

Exercise 18.8

Assume you have a set of documents each of which is in either English or in Spanish. You want to be able to support cross-language retrieval; in other words, users with some information need should be able to issue queries in either English or Spanish, and retrieve documents of either language satisfying the information need. The collection is given in Figure 18.4.

Figure 18.5 gives a glossary relating the Spanish and English words above for your own information. This glossary is NOT available to the retrieval system:

1. Construct below the appropriate term-document matrix C to use for a collection consisting of the above documents. For simplicity, use raw term frequencies rather than normalized tf-idf weights. Make sure to clearly label the dimensions of your matrix.
2. Write down the matrices U_2, Σ_2' and V_2 and from these derive the rank 2 approximation C_2.

DocID	Document text
1	hello
2	open house
3	mi casa
4	hola Profesor
5	hola y bienvenido
6	hello and welcome

► **Figure 18.4** Documents for Exercise 18.8.

Spanish	English
mi	my
casa	house
hola	hello
profesor	professor
y	and
bienvenido	welcome

► **Figure 18.5** Glossary for Exercise 18.8.

3. State succinctly what the (i, j) entry in the matrix $C^T C$ represents.
4. State succinctly what the (i, j) entry in the matrix $C_2^T C_2$ represents, and why it differs from that in $C^T C$.

19 *Web search basics*

Thus far in this book, we have considered search engines for content whose authorship is of relatively high quality; furthermore, the users of such engines tended to be relatively skilled users. In this and the following two chapters, we consider web search engines. Sections 19.1–19.3 provide some background and history to help the reader appreciate the forces that conspire to make the web chaotic, fast-changing and (from the standpoint of information retrieval) very different from the "traditional" collections studied thus far in this book. Sections 19.5 and 19.6 deal with estimating the number of documents indexed by web search engines, and the elimination of duplicate documents in web indexes, respectively. These two sections serve as background material for the following two chapters.

19.1 Background and history

The web is unprecedented in many ways: unprecedented in scale, unprecedented in the almost-complete lack of coordination in its creation, and unprecedented in the diversity of backgrounds and motives of its participants. Each of these contributes to making web search different – and generally far harder – than searching "traditional" documents.

The invention of hypertext, envisioned by Vannevar Bush in the 1940's and realized in working systems in the 1970's, significantly precedes the formation of the World Wide Web (which we will simply refer to as the web), in the 1990's. Web usage has shown tremendous growth to the point where it now claims a good fraction of humanity as participants, by relying on a simple, open client-server design: (1) the server communicates with the client via a protocol (the *http* or hypertext transfer protocol) that is lightweight and simple, asynchronously carrying a variety of payloads (text, images and – over time – richer media such as audio and video files) encoded in a simple markup language called *HTML* (for hypertext markup language); (2) the client – generally a *browser*, an application within a graphical user environ-

HTTP

HTML

ment – can ignore what it does not understand. Each of these seemingly innocuous features has contributed enormously to the growth of the web, so it is worthwhile to examine them further.

URL

The basic operation is as follows: a client (such as a browser) sends an *http request* to a *web server*. The browser specifies a *URL* (for *Universal Resource Locator*) such as `http://www.stanford.edu/home/atoz/contact.html`. In this example URL, the string `http` refers to the protocol to be used for transmitting the data. The string `www.stanford.edu` is known as the *domain* (sometimes the *top-level domain*) and specifies the root of a hierarchy of web pages (typically mirroring a filesystem hierarchy underlying the web server). In this example, `/home/atoz/contact.html` is a path in this hierarchy with a file `contact.html` that contains the information to be returned by the web server at `www.stanford.edu` in response to this request. The HTML-encoded file `contact.html` holds the hyperlinks and the content (in this instance, contact information for Stanford University), as well as formatting rules for rendering this content in a browser. Such an http request thus allows us to fetch the content of a page, something that will prove to be useful to us for crawling and indexing documents (Chapter 20).

The designers of the first browsers made it easy to view the HTML markup tags on the content of a URL. This simple convenience allowed new users to create their own HTML content without extensive training and experience; rather, they learned from example content that they liked. As they did so, a second feature of browsers supported the rapid proliferation of web content creation and usage: browsers ignored what they did not understand. This did not, as one might fear, lead to the creation of numerous incompatible dialects of HTML. What it did promote was amateur content creators who could freely experiment with and learn from their newly created web pages without fear that a simple syntax error would "bring the system down". Publishing on the web became a mass activity that was not limited to a few trained programmers, but rather open to tens and eventually hundreds of millions of individuals. For most users and for most information needs, the web quickly became the best way to supply and consume information on everything from rare ailments to subway schedules.

The mass publishing of information on the web is essentially useless unless this wealth of information can be discovered and consumed by other users. Early attempts at making web information "discoverable" fell into two broad categories: (1) full-text index search engines such as Altavista, Excite and Infoseek and (2) taxonomies populated with web pages in categories, such as Yahoo! The former presented the user with a keyword search interface supported by inverted indexes and ranking mechanisms building on those introduced in earlier chapters. The latter allowed the user to browse through a hierarchical tree of category labels. While this is at first blush a convenient and intuitive metaphor for finding web pages, it has a number

of drawbacks: first, classifying web pages into taxonomy tree nodes is for the most part a manual editorial process, which is difficult to scale with the size of the web. Arguably, we only need to have "high-quality" web pages in the taxonomy, with only the best web pages for each category. However, just discovering these and classifying them accurately and consistently into the taxonomy entails significant human effort. Further, in order for a user to effectively discover web pages classified into the nodes of the taxonomy tree, the user's idea of what sub-tree(s) to seek for a particular topic should match that of the editors performing the classification. This quickly becomes challenging as the size of the taxonomy grows; the Yahoo! taxonomy tree surpassed 1000 distinct nodes fairly early on. Given these challenges, the popularity of taxonomies declined over time, even though variants (such as About.com and the Open Directory Project) sprang up with subject-matter experts collecting and annotating web pages for each category.

The first generation of web search engines transported classical search techniques such as those in the preceding chapters to the web domain, focusing on the challenge of scale. The earliest web search engines had to contend with indexes containing millions of documents, which was a few orders of magnitude larger than any prior information retrieval system in the public domain. Indexing, query serving and ranking at this scale required the harnessing together of tens of machines to create highly available systems, again at scales not witnessed hitherto in a consumer-facing search application. The first generation of web search engines was largely successfully at solving these challenges while continually indexing a significant fraction of the web, all the while serving queries with sub-second response times. However, the quality and relevance of web search results left much to be desired owing to the idiosyncracies of content creation on the web. This necessitated the invention of new ranking and spam-fighting techniques in order to ensure the quality of the search results.

19.2 Web characteristics

The essential feature that led to the explosive growth of the web – decentralized content publishing with essentially no central control of authorship – turned out to be the biggest challenge for web search engines in their quest to index and retrieve this content. Web page authors created content in dozens of (natural) languages and thousands of dialects, thus demanding many different forms of stemming and other linguistic operations. Because publishing was now open to tens of millions, web pages exhibited heterogeneity at a daunting scale, in many crucial aspects. First, content-creation was no longer the privy of editorially-trained writers; while this represented a tremendous democratization of content creation, it also resulted in a tremendous varia-

tion in grammar and style (and in many cases, no recognizable grammar or style). Indeed, web publishing in a sense unleashed the best and worst of desktop publishing on a planetary scale, so that pages quickly became riddled with wild variations in colors, fonts and structure. Some web pages, including the professionally created home pages of some large corporations, consisted entirely of images (which, when clicked, led to richer textual content) – and therefore, no indexable text.

What about the substance of the text in web pages? The democratization of content creation on the web meant a new level of granularity in *opinion* on virtually any subject. This meant that the web contained truth, lies, contradictions and suppositions on a grand scale. This gives rise to the question: which web pages does one trust? In a simplistic approach, one might argue that some publishers are trustworthy and others not – begging the question of how a search engine is to assign such a measure of trust to each website or web page. In Chapter 21 we will examine approaches to understanding this question. More subtly, there may be no universal, user-independent notion of trust; a web page whose contents are trustworthy to one user may not be so to another. In traditional (non-web) publishing this is not an issue: users self-select sources they find trustworthy. Thus one reader may find the reporting of *The New York Times* to be reliable, while another may prefer *The Wall Street Journal*. But when a search engine is the only viable means for a user to become aware of (let alone select) most content, this challenge becomes significant.

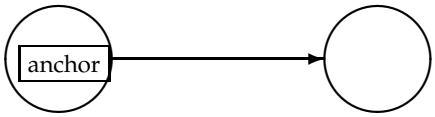
While the question "how big is the web?" has no easy answer (see Section 19.5), the question "how many web pages are in a search engine's index" is more precise, although, even this question has issues. By the end of 1995, Altavista reported that it had crawled and indexed approximately 30 million *static web pages*. Static web pages are those whose content does not vary from one request for that page to the next. For this purpose, a professor who manually updates his home page every week is considered to have a static web page, but an airport's flight status page is considered to be dynamic. Dynamic pages are typically mechanically generated and one sign of such a page is that the URL has the character "?" in it. Since the number of static web pages was believed to be doubling every few months in 1995, engines such as Altavista had to constantly add hardware and bandwidth for crawling and indexing web pages.

STATIC WEB PAGES

19.2.1 The web graph

We can view the static web consisting of static HTML pages together with the hyperlinks between them as a directed graph in which each web page is a node and each hyperlink a directed edge.

Figure 19.1 shows two nodes A and B from the web graph, each corre-



► **Figure 19.1** Two nodes of the web graph joined by a link.

sponding to a web page, with a hyperlink from A to B. We refer to the set of all such nodes and directed edges as the web graph. Figure 19.1 also shows that (as is the case with most links on web pages) there is some text surrounding the origin of the hyperlink on page A. This text is generally encapsulated in the `href` tag that encodes the hyperlink in the HTML code of page A, and is referred to as *anchor text*. As one might suspect, this directed graph is not *strongly connected*: there are pairs of pages such that one cannot proceed from one page of the pair to the other by following hyperlinks. We refer to the hyperlinks into a page as *in-links* and those out of a page as *out-links*. The number of in-links to a page (also known as its *in-degree*) has averaged from roughly 8 to 15, in a range of studies. We similarly define the out-degree of a web page to be the number of links out of it. There is ample evidence that these links are not randomly distributed; for one thing, the distribution of the number of links into a web page does not follow the Poisson distribution one would expect if every web page were to pick the destinations of its links uniformly at random. Rather, this distribution is widely reported to be a *power law*, in which the total number of web pages with in-degree i is proportional to $1/i^{\alpha}$; the value of α typically reported by studies is 2.1.[1]

ANCHOR TEXT

IN-LINKS

OUT-LINKS

POWER LAW

Exercise 19.1

If the number of pages with in-degree i is proportional to $1/i^{2.1}$, write down the probability that a randomly chosen web page has in-degree 1.

Exercise 19.2

If the number of pages with in-degree i is proportional to $1/i^{2.1}$, what is the average in-degree of a web page?

Exercise 19.3

If the number of pages with in-degree i is proportional to $1/i^{2.1}$, then as the largest in-degree goes to infinity, does the fraction of pages with in-degree i grow, stay the

1. Cf. Zipf's law of the distribution of words in text in Chapter 5 (page 84), which is a power law with $\alpha = 1$.

same, or diminish? How would your answer change for values of the exponent other than 2.1?

Exercise 19.4

The average in-degree of all nodes in a snapshot of the web graph is 9. What can we say about the average out-degree of all nodes in this snapshot?

19.2.2 Spam

Early in the history of web search, it became clear that web search engines were an important means for connecting advertisers to prospective buyers. A user searching for maui golf real estate is not merely seeking news or entertainment on the subject of housing on golf courses on the island of Maui, but instead likely to be seeking to purchase such a property. Sellers of such property and their agents, therefore, have a strong incentive to create web pages that rank highly on such a query. In a search engine whose scoring was based on term frequencies, a web page with numerous repetitions of maui golf real estate would rank highly. This led to the first generation of *spam*, which (in the context of web search) is the manipulation of web page content for the purpose of appearing high up in search results for selected keywords. To avoid irritating users with these repetitions, sophisticated *spammers* resorted to such tricks as rendering these repeated terms in the same color as the background. Despite these words being consequently invisible to the human user, a search engine indexer would parse the invisible words out of the HTML representation of the web page and index these words as being present in the page.

SPAM

At its root, spam stems from the heterogeneity of motives in content creation on the web. In particular, many web content creators have commercial motives and therefore stand to gain from manipulating search engine results. You might argue that this is no different from a company that uses large fonts to list its phone numbers in the yellow pages; but this generally costs the company more and is thus a fairer mechanism. A more apt analogy, perhaps, is the use of company names beginning with a long string of A's to be listed early in a yellow pages category. In fact, the yellow pages' model of companies paying for larger/darker fonts has been replicated in web search: in many engines, it is possible to pay to have one's web page included in the engine's search index – a model known as *paid inclusion*. Different engines have different policies on whether to allow paid inclusion, and whether such a payment has any effect on ranking in search results.

PAID INCLUSION

Search engines soon became sophisticated enough in their spam detection to screen out an unusually large number of repetitions of particular keywords. Spammers responded with a richer set of spam techniques, the best known of which we now describe. The first of these techniques is *cloaking*: the spammer's web server returns different pages depending on whether

the http request comes from a web search engine's crawler, or from a human user's browser. The former causes the web page to be indexed by the search engine under misleading keywords. When the user searches for these keywords and elects to view the page, he receives a web page that has altogether different content than that indexed by the engine. Such deception of search indexers is unknown in the traditional world of information retrieval; it stems from the fact that the web is partly collaborative but also partly competitive.

A *doorway page* contains text and metadata carefully chosen to rank highly on selected search keywords. When a browser requests the doorway page, it is redirected to a page containing content of a more commercial nature. More complex spamming techniques involve manipulation of the metadata related to a page including (for reasons we will see in Chapter 21) the links into a web page. Given that spamming is inherently an economically motivated activity, there has sprung around it an industry of *Search Engine Optimizers*, or SEO's to provide consultancy services for clients who seek to have their web pages rank highly on selected keywords. Web search engines frown on this business of attempting to decipher and adapt to their proprietary ranking techniques and indeed announce policies on forms of SEO behavior they do not tolerate (and have been known to shut down search requests from certain SEO's for violation of these). Inevitably, the parrying between such SEO's (who gradually infer features of each web engine's ranking methods) and the web search engines (who adapt in response) is an unending struggle; indeed, the research sub-area of *adversarial information retrieval* has sprung up around this battle. One potent technique for addressing spammers that fabricate the textual content of their web pages is the exploitation of the link structure of the web – a technique known as *link analysis*. The first web search engine to apply link analysis (to be detailed in Chapter 21) was Google, although all web search engines currently make use of it (and correspondingly, spammers now invest considerable effort in subverting it).

SEARCH ENGINE OPTIMIZERS

ADVERSARIAL INFORMATION RETRIEVAL

19.3 Advertising as the economic model

Early in the history of the web, companies used graphical banner advertisements on web pages at popular websites (news and entertainment sites such as MSN, America Online, Yahoo! and CNN). The primary purpose of these advertisements was *branding*: to convey to the viewer a positive feeling about the brand of the company placing the advertisement. Typically these advertisements were priced on a *cost per mil* (*CPM*) basis: the cost to the company of having its banner advertisement displayed 1000 times. Some websites struck contracts with their advertisers in which an advertisement was priced not by the number of times it is displayed (also known as *impressions*), but

CPM

rather by the number of times it was *clicked on* by the user. This pricing model is known as the *cost per click* (*CPC*) model. In such cases, clicking on the advertisement leads the user to a web page set up by the advertiser, where the user is induced to make a purchase. Here the goal of the advertisement is not so much brand promotion as to induce a transaction. This distinction between brand and transaction-oriented advertising was already widely recognized in the context of conventional media such as broadcast and print. The interactivity of the web allowed the CPC billing model – clicks could be metered and monitored by the website and billed to the advertiser.

CPC

However, the user at the news/entertainment website is typically not there with an intent to make a purchase, as much as to consume news and entertainment. How could a company better target its audience? Companies do in fact achieve some measure of focus by carefully selecting the websites on which they advertised. For instance, a company selling golf clubs might wish to advertise on a web page containing sports news and even better on a web pages that discuss golf news, but perhaps not on a web page announcing recent breakthroughs on biochemistry.

Demographic focusing of web advertising was already in use in the late 1990's, when web search engines were growing in usage (and therefore constantly in need of capital expenditures for hardware and bandwidth). The challenge for web search companies was to create a revenue stream that outweighed these expenditures. The pioneer in this direction was a company named Goto, which changed its name to Overture prior to eventual acquisition by Yahoo! Goto was not, in the traditional sense, a search engine; rather, for every query term q it accepted *bids* from companies who wanted their web page shown on the query q. In response to the query q, Goto would return the pages of all advertisers who bid for q, ordered by their bids. Furthermore, when the user clicked on one of the returned results, the corresponding advertiser would make a payment to Goto (in the initial implementation, this payment equalled the advertiser's bid for q).

Several aspects of Goto's model are worth highlighting. First, a user typing the query q into Goto's search interface was actively expressing an interest and intent related to the query q. For instance, a user typing `golf clubs` is more likely to be imminently purchasing a set than one who is simply browsing news on golf. Second, Goto only got compensated when a user actually expressed interest in an advertisement – as evinced by the user clicking the advertisement. Taken together, these created a powerful mechanism by which to connect advertisers to consumers, quickly raising the annual revenues of Goto/Overture into hundreds of millions of dollars. This style of search engine came to be known variously as *sponsored search* or *paid placement*.

SPONSORED SEARCH
PAID PLACEMENT

Given these two kinds of search engines – the "pure" engines such as Google and Altavista, versus the sponsored search engines – the logical next step was to combine them into a single user experience. Current search en-

gines follow precisely this model: they provide pure search results (generally known as *algorithmic search* results) as the primary response to a user's search, together with sponsored search results displayed separately and distinctively to the right of the algorithmic results. Retrieving sponsored search results and ranking them in response to a query has now become considerably more sophisticated than the simple Goto scheme; the process entails a blending of ideas from information retrieval and microeconomics, and is beyond the scope of this book. From the standpoint of advertisers, understanding how search engines do this ranking and how to allocate marketing campaign budgets to different sponsored search engines has become a profession known as *search engine marketing* (SEM).

ALGORITHMIC SEARCH

SEARCH ENGINE MARKETING

The inherently economic motives underlying sponsored search give rise to attempts by some participants to subvert the system to their advantage. This can take many forms, one of which is known as *click spam*. There is currently no universally accepted definition of click spam. It refers (as the name suggests) to clicks on sponsored search results that are not from bona fide search users. For instance, a devious advertiser may attempt to exhaust the advertising budget of a competitor by clicking repeatedly (through the use of a robotic click generator) on that competitor's sponsored search advertisements. Search engines face the challenge of discerning which of the clicks they observe are part of a pattern of click spam, to avoid charging their advertiser clients for such clicks.

CLICK SPAM

Exercise 19.5

The Goto method ranked advertisements matching a query by *bid*: the highest-bidding advertiser got the top position, the second-highest the next, and so on. What can go wrong with this when the highest-bidding advertiser places an advertisement that is irrelevant to the query? Why might an advertiser with an irrelevant advertisement bid high in this manner?

Exercise 19.6

Suppose that, in addition to bids, we had for each advertiser their *click-through rate*: the ratio of the historical number of times users click on their advertisement to the number of times the advertisement was shown. Suggest a modification of the Goto scheme that exploits this data to avoid the problem in Exercise 19.5 above.

19.4 The search user experience

It is crucial that we understand the users of web search as well. This is again a significant change from traditional information retrieval, where users were typically professionals with at least some training in the art of phrasing queries over a well-authored collection whose style and structure they understood well. In contrast, web search users tend to not know (or care) about the heterogeneity of web content, the syntax of query languages and the art of phrasing queries; indeed, a mainstream tool (as web search has come to become) should not place such onerous demands on billions of people. A

range of studies has concluded that the average number of keywords in a web search is somewhere between 2 and 3. Syntax operators (Boolean connectives, wildcards, etc.) are seldom used, again a result of the composition of the audience – "normal" people, not information scientists.

It is clear that the more user traffic a web search engine can attract, the more revenue it stands to earn from sponsored search. How do search engines differentiate themselves and grow their traffic? Here Google identified two principles that helped it grow at the expense of its competitors: (1) a focus on relevance, specifically precision rather than recall in the first few results; (2) a user experience that is lightweight, meaning that both the search query page and the search results page are uncluttered and almost entirely textual, with very few graphical elements. The effect of the first was simply to save users time in locating the information they sought; more on this below. The effect of the second is to provide a user experience that is extremely responsive, or at any rate not bottlenecked by the time to load the search query or results page.

19.4.1 User query needs

There appear to be three broad categories into which common web search queries can be grouped: (i) informational, (ii) navigational and (iii) transactional. We now explain these categories; it should be clear that some queries will fall in more than one of these categories, while others will fall outside them.

INFORMATIONAL QUERIES

Informational queries seek general information on a broad topic, such as leukemia or Provence. There is typically not a single web page that contains all the information sought; indeed, users with informational queries typically try to assimilate information from multiple web pages.

NAVIGATIONAL QUERIES

Navigational queries seek the website or home page of a single entity that the user has in mind, say Lufthansa airlines. In such cases, the user's expectation is that the very first search result should be the home page of Lufthansa.

TRANSACTIONAL QUERY

A *transactional query* is one that is a prelude to the user performing a transaction on the web – such as purchasing a product, downloading a file or making a reservation. In such cases, the engine should return results listing services that provide form interfaces for such transactions.

Discerning which of these categories a query falls into can be challenging. The category not only governs the algorithmic search results, but the suitability of the query for sponsored search results (since the query may reveal an intent to purchase). For navigational queries, some have argued that the engine should return only a single result or even the target web page directly. Nevertheless, web search engines have historically engaged in a battle of bragging rights over which one indexes more web pages. Does the user really care? Perhaps not, but the media does highlight measurements

(often statistically indefensible) of the sizes of various search engines. Users are influenced by these reports and thus, search engines do have to pay attention to how their index sizes compare to competitors'. For informational (and to a lesser extent, transactional) queries, the user does care about the comprehensiveness of the engine.

19.5 Index size and estimation

To a first approximation, comprehensiveness grows with index size, although it does matter which specific pages an engine indexes – some pages are more informative than others. It is also difficult to reason about the fraction of the web indexed by an engine, because there is an infinite number of dynamic web pages; for instance, `http://www.yahoo.com/any_string` returns a valid HTML page rather than an error, politely informing the user that there is no such page at Yahoo! Such a "soft 404 error" is only one example of many ways in which web servers can generate an infinite number of valid web pages. Indeed, some of these are malicious spider traps devised to cause a search engine's crawler (the component that systematically fetches web pages for the engine's index, described in Chapter 20) to stay within a spammer's website and index many pages from that site.

We could ask the following better-defined question: given two search engines, what are the relative sizes of their indexes? Even this question turns out to be imprecise, because:

1. In response to queries a search engine can return web pages whose contents it has not (fully or even partially) indexed. For one thing, engines generally index only the first few thousand words in a web page. In some cases, an engine is aware of a page p that is *linked to* by pages it has indexed, but has not indexed p itself. As we will see in Chapter 21, it is still possible to meaningfully return p in search results.

2. Search engines generally organize their indexes in various tiers and partitions, not all of which are examined on every search. For instance, a web page deep inside a website may be indexed but not retrieved on general web searches; it is however retrieved as a result on a search specific to that website.

Thus, search engine indexes include multiple classes of indexed pages, so that there is no single measure of index size. These issues notwithstanding, a number of techniques have been devised for crude estimates of the ratio of the index sizes of two search engines, E_1 and E_2. The basic hypothesis underlying these techniques is that each engine indexes a fraction of the web chosen independently and uniformly at random. This involves some questionable assumptions: first, that there is a finite size for the web from which

each engine chooses a subset, and second, that each engine chooses an independent, uniformly chosen subset. As will be clear from the discussion of crawling in Chapter 20, this is far from true. However, if we begin with these assumptions, then we can invoke a classical estimation technique known as the *capture-recapture method*.

CAPTURE-RECAPTURE METHOD

Suppose that we could pick a random page from the index of E_1 and test whether it is in E_2's index and symmetrically, test whether a random page from E_2 is in E_1. These experiments give us fractions x and y such that our estimate is that a fraction x of the pages in E_1 are in E_2, while a fraction y of the pages in E_2 are in E_1. Then, letting $|E_i|$ denote the size of the index of engine E_i, we have

$$x|E_1| \approx y|E_2|,$$

from which we have the form we will use

$$\frac{|E_1|}{|E_2|} \approx \frac{y}{x}. \tag{19.1}$$

If our assumption about E_1 and E_2 being independent and uniform random subsets of the web were true, and our sampling process unbiased, then Equation (19.1) should give us an unbiased estimator for $|E_1|/|E_2|$. We distinguish between two scenarios here. Either the measurement is performed by someone with access to the index of one of the engines (say an employee of E_1), or the measurement is performed by an independent party with no access to the innards of either engine. In the former case, we can simply pick a random document from one index. The latter case is more challenging; we begin with the sampling process by which we pick a random page from one engine *from outside the engine*, then describe the checking process by which we verify whether the random page is present in the other engine.

To implement the sampling phase, we might generate a random page from the entire (idealized, finite) web and test it for presence in each engine. Unfortunately, picking a web page uniformly at random is a difficult problem. We briefly outline several attempts to achieve such a sample, pointing out the biases inherent to each; following this we describe in some detail one technique that much research has built on.

1. *Random searches:* Begin with a search log of web searches; send a random search from this log to E_1 and a random page from the results. Since such logs are not widely available outside a search engine, one implementation is to trap all search queries going out of a work group (say scientists in a research center) that agrees to have all its searches logged. This approach has a number of issues, including the bias from the types of searches made public by the work group. Further, a random document from the results of such a random search to E_1 is not the same as a random document from E_1.

2. *Random IP addresses:* A second approach is to generate random IP addresses and send a request to a web server residing at the random address, collecting all pages at that server. The biases here include the fact that many hosts might share one IP (due to a practice known as virtual hosting) or not accept http requests from the host where the experiment is conducted. Further, this technique is more likely to hit one of the many sites with few pages, skewing the document probabilities; we may be able to correct for this effect if we understand the distribution of pages on a website.

3. *Random walks:* If the web graph were a strongly connected directed graph, we could run a random walk starting at an arbitrary web page. This walk would converge to a steady state distribution (see Chapter 21, Section 21.2.1 for more background material on this), from which we could in principle pick a web page with a fixed probability. This method, too has a number of biases. First, the web is not strongly connected so that, even with various corrective rules, it is difficult to argue that we can reach a steady state distribution starting from any page. Second, the time it takes for the random walk to settle into this steady state is unknown and could exceed the length of the experiment.

Clearly each of these approaches is far from perfect. We now describe a fourth sampling approach, *random queries*. This approach is noteworthy for two reasons: it has been successfully built upon for a series of increasingly refined estimates, and conversely it has turned out to be the approach most likely to be misinterpreted and carelessly implemented, leading to misleading measurements. The idea is to pick a page (almost) uniformly at random from an engine's index by posing a random query to it. It should be clear that picking a set of random terms from (say) Webster's dictionary is not a good way of implementing this idea. For one thing, not all dictionary terms occur equally often, so this approach will not result in documents being chosen uniformly at random from the engine. For another, there are a great many terms in web documents that do not occur in a standard dictionary such as Webster's. To address the problem of dictionary terms not in a standard dictionary, we begin by amassing a sample web dictionary. This could be done by crawling a limited portion of the web, or by crawling a manually-assembled representative subset of the web such as Yahoo! (as was done in the earliest experiments with this method). Consider a conjunctive query with two or more randomly chosen words from this dictionary.

The probability of the event that a page is in the results set of such a random conjunctive query induces a distribution over all pages in the union of the two engines. Then, we estimate $|E_1|/|E_2|$ by taking the ratio of the corresponding induced distributions. We can improve the estimate by repeating the experiment a large number of times.

Operationally, we proceed as follows: we use a random conjunctive query on E_1 and pick from the top 100 returned results a page p at random. We then test p for presence in E_2 by choosing 6-8 low-frequency terms in p and using them in a conjunctive query for E_2. Both the sampling process and the testing process have a number of issues.

1. Our sample is biased towards longer documents.
2. Picking from the top 100 results of E_1 induces a bias from the ranking algorithm of E_1. Picking from all the results of E_1 makes the experiment slower. This is particularly so because most web search engines put up defenses against excessive robotic querying.
3. During the checking phase, a number of additional biases are introduced: for instance, E_2 may not handle 8-word conjunctive queries properly.
4. Either E_1 or E_2 may refuse to respond to the test queries, treating them as robotic spam rather than as bona fide queries.
5. There could be operational problems like connection time-outs.

A sequence of research has built on this basic paradigm to eliminate some of these issues; there is no perfect solution yet, but the level of sophistication in statistics for understanding the biases is increasing.

Exercise 19.7

Two web search engines A and B each generate a large number of pages uniformly at random from their indexes. 30% of A's pages are present in B's index, while 50% of B's pages are present in A's index. What is the number of pages in A's index relative to B's?

19.6 Near-duplicates and shingling

One aspect we have ignored in the discussion of index size in Section 19.6 is *duplication*: the web contains multiple copies of the same content. By some estimates, as many as 40% of the pages on the web are duplicates of other pages. Many of these are legitimate copies; for instance, certain information repositories are mirrored simply to provide redundancy and access reliability. Search engines try to avoid indexing multiple copies of the same content, to keep down storage and processing overheads.

The simplest approach to detecting duplicates is to compute, for each web page, a *fingerprint* that is a succinct (say 64-bit) digest of the sequence of characters on that page. Then, whenever the fingerprints of two web pages are equal, we test whether the pages themselves are equal and if so declare one of them to be a duplicate copy of the other. This simplistic approach fails

to capture a crucial and widespread phenomenon on the web: *near duplication*. In many cases, the contents of one web page are identical to those of another except for a few characters – say, a notation showing the date and time at which the page was last modified. Even in such cases, we want to be able to declare the two pages to be close enough that we only index one copy. Short of exhaustively comparing all pairs of web pages, an infeasible task at the scale of billions of pages, how can we detect and filter out such near duplicates?

Exercise 19.8

Web search engines A and B each crawl a random subset of the same size of the web. Some of the pages crawled are duplicates – exact textual copies of each other at different URLs. Assume that duplicates are distributed uniformly amongst the pages crawled by A and B. Further, assume that a duplicate is a page that has exactly two copies – no pages have more than two copies. A indexes pages without duplicate elimination whereas B indexes only one copy of each duplicate page. The two random subsets have the same size before duplicate elimination. If, 45% of A's indexed URLs are present in B's index, while 50% of B's indexed URLs are present in A's index, what fraction of the web consists of pages that do not have a duplicate?

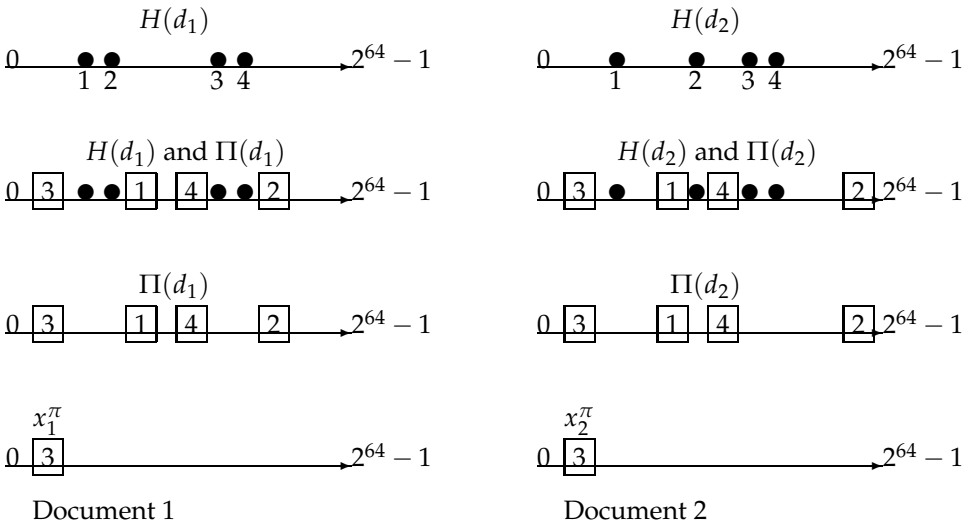
19.6.1 Shingling

SHINGLING

We now describe a solution to the problem of detecting near-duplicate web pages. The answer lies in a technique known as *shingling*. Given a positive integer k and a sequence of terms in a document d, define the k-shingles of d to be the set of all consecutive sequences of k terms in d. As an example, consider the following text: a rose is a rose is a rose. The 4-shingles for this text ($k = 4$ is a typical value used in the detection of near-duplicate web pages) are a rose is a, rose is a rose and is a rose is. The first two of these shingles each occur twice in the text. Intuitively, two documents are near duplicates if the sets of shingles generated from them are nearly the same. We now make this intuition precise, then develop a method for efficiently computing and comparing the sets of shingles for all web pages.

Let $S(d_j)$ denote the set of shingles of document d_j. Recall the Jaccard coefficient (Chapter 3, page 55), which measures the degree of overlap between the sets $S(d_1)$ and $S(d_2)$ as $|S(d_1) \cap S(d_2)|/|S(d_1) \cup S(d_2)|$; denote this by $J(S(d_1), S(d_2))$. Our test for near duplication between d_1 and d_2 is to compute this Jaccard coefficient; if it exceeds a preset threshold (say, 0.9), we declare them near duplicates and eliminate one from indexing. However, this does not appear to have simplified matters: we still have to compute Jaccard coefficients pairwise.

To avoid this, we use a form of hashing. First, we map every shingle into a hash value over a large space, say 64 bits. For $j = 1, 2$, let $H(d_j)$ be the corresponding set of 64-bit hash values derived from $S(d_j)$. We now invoke the following trick to detect document pairs whose sets $H()$ have large Jaccard overlaps. Let π be a random permutation from the 64-bit integers to the



► **Figure 19.2** Illustration of shingle sketches. We see two documents going through four stages of shingle sketch computation. In the first step (top row), we apply a 64-bit hash to each shingle from each document to obtain $H(d_1)$ and $H(d_2)$ (circles). Next, we apply a random permutation Π to permute $H(d_1)$ and $H(d_2)$, obtaining $\Pi(d_1)$ and $\Pi(d_2)$ (squares). The third row shows only $\Pi(d_1)$ and $\Pi(d_2)$, while the bottom row shows the minimum values x_1^π and x_2^π for each document.

64-bit integers. Denote by $\Pi(d_j)$ the set of permuted hash values in $H(d_j)$; thus for each $h \in H(d_j)$, there is a corresponding value $\pi(h) \in \Pi(d_j)$.

Let x_j^π be the smallest integer in $\Pi(d_j)$. Then

Theorem 19.1.

$$J(S(d_1), S(d_2)) = Pr[x_1^\pi = x_2^\pi].$$

Proof. We give the proof in a slightly more general setting: consider a family of sets whose elements are drawn from a common universe. View the sets as columns of a matrix A, with one row for each element in the universe. The element $a_{ij} = 1$ if element i is present in the set S_j that the jth column represents.

Let Π be a random permutation of the rows of A; denote by $\Pi(S_j)$ the column that results from applying Π to the jth column. Finally, let x_j^π be the index of the first row in which the column $\Pi(S_j)$ has a 1. We then prove that for any two columns j_1, j_2,

$$\Pr[x_{j_1}^\pi = x_{j_2}^\pi] = J(S_{j_1}, S_{j_2}).$$

S_{j_1}	S_{j_2}
0	1
1	0
1	1
0	0
1	1
0	1

► **Figure 19.3** Two sets S_{j_1} and S_{j_2}; their Jaccard coefficient is 2/5.

If we can prove this, the theorem follows.

Consider two columns j_1, j_2 as shown in Figure 19.3, which shows that the ordered pairs of entries of S_{j_1} and S_{j_2} partition the rows into four types: those with 0's in both of these columns, those with a 0 in S_{j_1} and a 1 in S_{j_2}, those with a 1in S_{j_1} and a 0in S_{j_2}, and finally those with 1's in both of these columns. Indeed, the first four rows of Figure 19.3 exemplify all of these four types of rows. Denote by C_{00} the number of rows of the first of these types, C_{01} the second, C_{10} the third and C_{11} the fourth. Then,

$$J(S_{j_1}, S_{j_2}) = \frac{C_{11}}{C_{01} + C_{10} + C_{11}}. \tag{19.2}$$

To complete the proof by showing that the right-hand side of (19.2) equals $\Pr[x^\pi_{j_1} = x^\pi_{j_2}]$, consider scanning columns j_1, j_2 in increasing row index until the first non-zero entry is found in either column. Because Π is a random permutation, the probability that this smallest row has a 1 in both columns is exactly the right-hand side of (19.2). □

Thus, our test for the Jaccard coefficient of the shingle sets is probabilistic: we compare the computed values x^π_i from different documents. If a pair coincides, we have candidate near duplicates. Repeat the test independently for 200 random permutations π (a choice suggested in the literature). Call the set of these 200 values of x^π_i the *sketch* $\psi(d_i)$ of d_i. We can then estimate the Jaccard coefficient for any pair of documents d_i, d_j to be $|\psi_i \cap \psi_j|/200$; if this exceeds a preset threshold, we declare that d_i and d_j are similar.

How can we quickly compute $|\psi_i \cap \psi_j|/200$ for all pairs i, j? Indeed, how do we represent all pairs of documents that are similar, without incurring a blowup that is quadratic in the number of documents? First, we use fingerprints to remove all but one copy of *identical* documents. We may also remove common HTML tags and integers from the shingle computation, to eliminate shingles that occur very commonly in documents without telling us anything about duplication. Next we use a *union-find* algorithm to create

clusters that contain documents that are similar. To do this, we must accomplish a crucial step: going from the set of sketches to the set of pairs i, j such that d_i and d_j are similar.

To this end, we compute the number of shingles common for any pair of documents whose sketches have any members in common. We begin with the list of sorted $< x_i^\pi, d_i >$ pairs and for each x_i^π, generate all pairs i, j for which x_i^π is present in both their sketches. We then accumulate these into counts for each pair i, j with non-zero sketch overlap; by applying the preset threshold, we know which pairs i, j have heavily overlapping sketches. For instance, if the preset threshold were 80%, we would need the merged count to be at least 160. As we identify such pairs, we run the union-find to group documents into near-duplicate "syntactic clusters". This is essentially a variant of the single-link clustering algorithm introduced in Section 17.2 (page 340).

One final trick cuts down the space needed in the computation of $|\psi_i \cap \psi_j|/200$ for pairs i, j, which in principle could still demand space quadratic in the number of documents. To remove from consideration those pairs i, j whose sketches have few shingles in common, we preprocess the sketch for each document as follows: sort the x_i^π in the sketch, then shingle this sorted sequence to generate a set of *super-shingles* for each document. If two documents have a super-shingle in common, we proceed to compute the precise value of $|\psi_i \cap \psi_j|/200$. This again is a heuristic but can be highly effective in cutting down the number of i, j pairs for which we accumulate the sketch overlap counts.

Exercise 19.9

Instead of using the process depicted in Figure 19.2, consider instead the following process for estimating the Jaccard coefficient of the overlap between two sets S_1 and S_2. We pick a random subset of the elements of the universe from which S_1 and S_2 are drawn; this corresponds to picking a random subset of the rows of the matrix A in the proof. We exhaustively compute the Jaccard coefficient of these random subsets. Why is this estimate an unbiased estimator of the Jaccard coefficient for S_1 and S_2?

Exercise 19.10

Explain why this estimator would be very difficult to use in practice.

19.7 References and further reading

Bush (1945) foreshadowed the web when he described an information management system that he called *memex*. Berners-Lee et al. (1992) describes one of the earliest incarnations of the web. Kumar et al. (2000) and Broder et al. (2000) provide comprehensive studies of the web as a graph. The use of anchor text was first described in McBryan (1994). The taxonomy of web queries in Section 19.4 is due to Broder (2002).

The estimation of web search index sizes has a long history of development covered by Bharat and Broder (1998), Lawrence and Giles (1998), Rusmevichientong et al. (2001), Lawrence and Giles (1999), Henzinger et al. (2000a), Henzinger et al. (2000b), Bar-Yossef and Gurevich (2006). Shingling was introduced by Broder et al. (1997) and used for detecting websites (rather than simply pages) that are identical by Bharat et al. (2000).

20 *Web crawling and indexes*

20.1 Overview

Web crawling is the process by which we gather pages from the web, for the primary purpose of indexing them and supporting a search engine. The objective of crawling is to quickly and efficiently gather as many useful web pages as possible, together with the link structure that interconnects them. In Chapter 19 we studied the complexities of the web stemming from its creation by millions of un-coordinated individuals. In this chapter we study the resulting difficulties for crawling the web.

The goal of this chapter is not to describe how to build the crawler for a full-scale commercial search engine. We focus instead on a range of issues that are generic to crawling from the student project scale to substantial research projects. We begin by listing desiderata for web crawlers, and then discuss in Section 20.2 how each of these issues is addressed. We list the desiderata for web crawlers in two categories: features that web crawlers *must* provide, followed by features they *should* provide. The remainder of this chapter describes the architecture and some implementation details for a distributed web crawler that satisfies these features.

20.1.1 Features a crawler *must* provide

Robustness: The web contains servers that create *spider traps*, which are generators of web pages that mislead crawlers into getting stuck fetching an infinite number of pages in a particular domain. Crawlers must be designed to be resilient to such traps. Not all such traps are malicious; some are the inadvertent side-effect of faulty website development.

Politeness: Web servers have both implicit and explicit policies regulating the rate at which a crawler can visit them. These politeness policies must be respected.

20.1.2 Features a crawler *should* provide

Distributed: The crawler should have the ability to execute in a distributed fashion across multiple machines.

Scalable: The crawler architecture should permit scaling up the crawl rate by adding extra machines and bandwidth.

Performance and efficiency: The crawl system should make maximum use of various system resources including processor, storage and network bandwidth.

Quality: Given that significant fractions of the web are of poor utility in terms of serving user query needs, the crawler should be biased towards fetching "useful" pages first.

Freshness: In many applications, the crawler should operate in continuous mode: it should obtain fresh copies of previously fetched pages. A search engine crawler, for instance, can thus ensure that the search engine's index contains a fairly faithful representation of each indexed web page. For such continuous crawling, a crawler should be able to crawl a page with a frequency that approximates the rate of change of that page.

Extensible: Crawlers should be designed to be extensible in many ways – to cope with new data formats, new fetch protocols, and so on. This demands that the crawler architecture be modular.

20.2 Crawling

The basic operation of any hypertext crawler (whether for a web, an intranet or other hypertext document collection) is as follows. The crawler begins with one or more URLs that constitute a *seed set*. It picks a URL from this seed set, then fetches the web page at that URL. The fetched page is then parsed, to extract both the text and the links from the page (each of which points to another URL). The extracted text is fed to a text indexer (described in Chapters 4 and 5). The extracted links (URLs) are then added to a *URL frontier*, which at all times consists of URLs whose corresponding pages have yet to be fetched by the crawler. Initially, the URL frontier contains the seed set; as pages are fetched, the corresponding URLs are deleted from the URL frontier. The entire process may be viewed as traversing the web graph (see Chapter 19).

This seemingly simple recursive traversal of the web graph is complicated by the many demands on a practical web crawling system: the crawler has to be distributed, scalable, efficient, polite, robust and extensible while fetching

pages of high quality. We examine the effects of each of these issues. Our
MERCATOR treatment follows the design of the *Mercator* crawler that has formed the basis of a number of research and commercial crawlers. As a reference point, fetching a billion pages (a small fraction of the static web at present) in a month-long crawl requires fetching several hundred pages each second. We will see how to use a multi-threaded design to address several bottlenecks in the overall crawler system in order to attain this fetch rate.

20.2.1 Crawler architecture

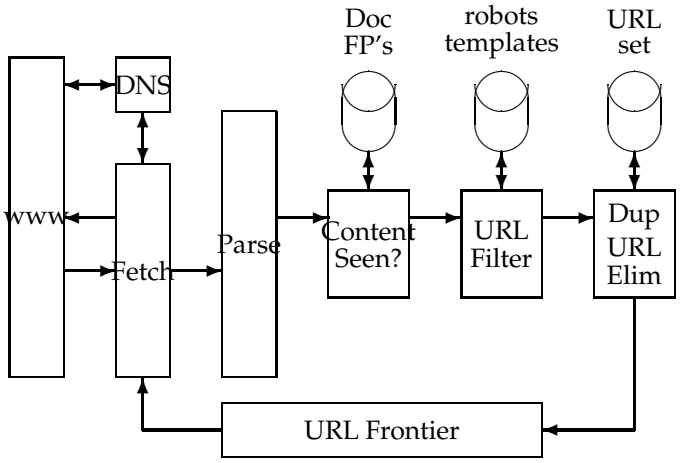
The simple scheme outlined above for crawling demands several modules that fit together as shown in Figure 20.1.

1. The URL frontier, containing URLs yet to be fetched in the current crawl (in the case of continuous crawling, a URL may have been fetched previously but is back in the frontier for re-fetching). We describe this further in Section 20.2.3.
2. A *DNS resolution* module that determines the web server from which to obtain a URL to be fetched. We describe this further in Section 20.2.2.
3. A fetch module that retrieves the web page at a URL.
4. A parsing module that extracts the set of links from a fetched web page.
5. A duplicate elimination module that determines whether an extracted link is already in the URL frontier or has recently been fetched.

Crawling is performed by anywhere from one to potentially hundreds of threads, each of which loops through the logical cycle in Figure 20.1. These threads may be run in a single process, or be partitioned amongst multiple processes running at different nodes of a distributed system. We begin by assuming that the URL frontier is in place and non-empty and defer our description of the implementation of the URL frontier to Section 20.2.3.

A crawler thread begins by taking a URL from the frontier and fetching the web page at that URL, generally using the http protocol. The fetched page is then written into a temporary store, from which a number of operations are performed on it. Next, the page is parsed and the text as well as the links in it are extracted. The text (with any tag information – e.g., terms in boldface) is passed on to the indexer. Link information including anchor text is also passed on to the indexer for use in ranking in ways described in Chapter 21. In addition, each extracted link goes through a series of tests to determine whether the link should be added to the URL frontier.

First, the thread tests whether a web page with the same content has already been seen at another URL. The simplest implementation for this would



► **Figure 20.1** The basic crawler architecture.

use a simple fingerprint such as a checksum (placed in a store labeled "Doc FP's" in Figure 20.1). A more sophisticated test would use shingles instead of fingerprints, as described in Chapter 19.

Next, a *URL filter* is used to determine whether the extracted URL should be excluded from the frontier based on one of several tests. For instance, the crawl may seek to exclude certain domains (say, all .com URLs) – in this case the test would simply filter out the URL if it were from the .com domain. A similar test could be inclusive rather than exclusive. Many hosts on the web place certain portions of their websites off-limits to crawling, under a standard known as the *Robots Exclusion Protocol*. This is done by placing a file with the name robots.txt at the root of the URL hierarchy at the site. Here is an example robots.txt file that specifies that no robot should visit any URL starting with /yoursite/temp/, except for the robot called "searchengine".

ROBOTS EXCLUSION PROTOCOL

```
User-agent: *
Disallow: /yoursite/temp/

User-agent: searchengine
Disallow:
```

The robots.txt file must be fetched from a website in order to test whether the URL in consideration passes its restrictions and can therefore be added to the URL frontier. Rather than fetch it afresh for testing on each URL to be

added to the frontier, a cache can be used to obtain a recently fetched copy of the file for the host, especially since many of the links extracted from a page fall within the host from which the page was fetched. Thus, by performing the filtering during the link extraction process, we would have especially high locality in the stream of hosts that we need to test for robots.txt files, leading to high cache hit rates. Unfortunately, this runs afoul of webmasters' politeness expectations. A URL (particularly one referring to a low-quality or rarely changing document) may be in the frontier for days or even weeks. If we were to perform the robots filtering *before* adding such a URL to the frontier, its robots.txt file could have changed by the time the URL is dequeued from the frontier and fetched. We must consequently perform robots-filtering immediately before attempting to fetch a web page. As it turns out, maintaining a cache of robots.txt files is still highly effective; there is sufficient locality even in the stream of URLs dequeued from the URL frontier.

URL NORMALIZATION

At this point all URLs are *normalized* in the following sense: often the HTML encoding of a link from a web page p indicates the target of that link relative to the page p. Thus, there is a relative link encoded thus in the HTML of the page en.wikipedia.org/wiki/Main_Page:

```
<a href="/wiki/Wikipedia:General_disclaimer" title="Wikipedia:General
disclaimer">Disclaimers</a>
```

points to the URL http://en.wikipedia.org/wiki/Wikipedia:General_disclaimer.

Finally, the URL is checked for duplicate elimination: if the URL is already in the frontier or (in the case of a non-continuous crawl) already crawled, we do not add it to the frontier. When the URL is added to the frontier, it is assigned a priority based on which it is eventually removed from the frontier for fetching. The details of this priority queuing are in Section 20.2.3.

Certain housekeeping tasks are typically performed by a dedicated thread. The background thread is quiescent except that it wakes up once every few seconds to log crawl progress statistics (URLs crawled, frontier size, etc.), decide whether to terminate the crawl, or (once every few hours of crawling) checkpoint the crawl. In checkpointing, a snapshot of the crawler's state (say, the URL frontier) is committed to disk. In the event of a catastrophic crawler failure, the crawl is restarted from the most recent checkpoint.

Distributing the crawler

We have mentioned that the threads in a crawler could run under different processes, each at a different node of a distributed crawling system. Such distribution is essential for scaling; it can also be of use in a geographically distributed crawler system where each node crawls hosts "near" it. Partitioning the hosts being crawled amongst the crawler nodes can be done by

a hash function, or by some more specifically tailored policy. For instance, we may locate a crawler node in Europe to focus on European domains, although this is not dependable for several reasons – the routes that packets take through the internet do not always reflect geographic proximity, and in any case the domain of a host does not always reflect its physical location.

How do the various nodes of a distributed crawler communicate and share URLs? The idea is to replicate the flow of Figure 20.1 at each node, with one essential difference: following the URL filter, we use a *host splitter* to despatch each surviving URL to the crawler node responsible for the URL; thus the set of hosts being crawled is partitioned among the nodes. This modified flow is shown in Figure 20.2. The output of the host splitter goes into the Duplicate URL Eliminator block of each other node in the distributed system.

The "Content Seen?" module in the distributed architecture of Figure 20.2 is, however, complicated by several factors:

1. Unlike the URL frontier and the duplicate elimination module, content fingerprints/shingles cannot be partitioned based on host name. There is nothing preventing the same (or highly similar) content from appearing on different web servers. Consequently, the sets of fingerprints/shingles must be partitioned across the nodes based on some property of the fingerprint/shingle (say by taking the fingerprint modulo the number of nodes). The result of this locality-mismatch is that most set membership tests result in a remote procedure call (although it is possible to batch lookup requests).

2. There is very little locality in the stream of document fingerprints/shingles. Thus, caching popular content fingerprints does not help (since there are no popular fingerprints).

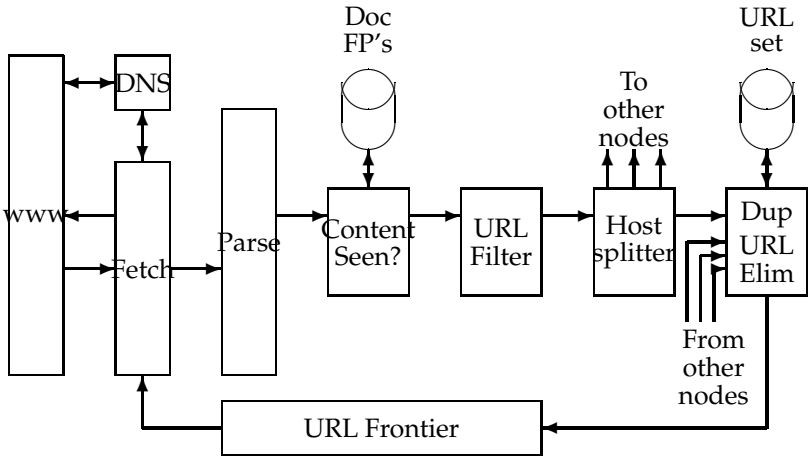
3. Documents change over time and so, in the context of continuous crawling, we must be able to delete their outdated fingerprints/shingles from the content-seen set(s). In order to do so, it is necessary to save the content fingerprint/shingle of the document in the URL frontier, along with the URL itself.

Exercise 20.1

Why is it better to partition hosts (rather than individual URLs) between the nodes of a distributed crawl system?

Exercise 20.2

Why should the host splitter precede the Duplicate URL Eliminator?



► **Figure 20.2** Distributing the basic crawl architecture.

20.2.2 DNS resolution

IP ADDRESS

DNS RESOLUTION

DNS SERVER

Each web server (and indeed any host connected to the internet) has a unique *IP address*: a sequence of four bytes generally represented as four integers separated by dots; for instance 207.142.131.248 is the numerical IP address associated with the host www.wikipedia.org. Given a URL such as www.wikipedia.org in textual form, translating it to an IP address (in this case, 207.142.131.248) is a process known as *DNS resolution* or DNS lookup; here DNS stands for *Domain Name Service*. During DNS resolution, the program that wishes to perform this translation (in our case, a component of the web crawler) contacts a *DNS server* that returns the translated IP address. (In practice the entire translation may not occur at a single DNS server; rather, the DNS server contacted initially may recursively call upon other DNS servers to complete the translation.) For a more complex URL such as en.wikipedia.org/wiki/Domain_Name_System, the crawler component responsible for DNS resolution strips out the host name – in this case en.wikipedia.org – and looks up the IP address for the host en.wikipedia.org.

DNS resolution is a well-known bottleneck in web crawling. Due to the distributed nature of the Domain Name Service, DNS resolution may entail multiple requests and round-trips across the internet, requiring seconds and sometimes even longer. Right away, this puts in jeopardy our goal of fetching several hundred documents a second. A standard remedy is to introduce

caching: URLs for which we have recently performed DNS lookups are likely to be found in the DNS cache, avoiding the need to go to the DNS servers on the internet. However, obeying politeness constraints (see Section 20.2.3) limits the rate of cache hits.

There is another important difficulty in DNS resolution; the lookup implementations in standard libraries (likely to be used by anyone developing a crawler) are generally synchronous. This means that once a request is made to the Domain Name Service, other crawler threads at that node are blocked until the first request is completed. To circumvent this, most web crawlers implement their own DNS resolver as a component of the crawler. Thread t executing the resolver code sends a message to the DNS server and then performs a timed wait: it resumes either when being signaled by another thread or when a set time quantum expires. A single, separate DNS thread listens on the standard DNS port (port 53) for incoming response packets from the name service. Upon receiving a response, it signals the appropriate crawler thread (in this case, t) and hands it the response packet if t has not yet resumed because its time quantum has expired. A crawler thread that resumes because its wait time quantum has expired retries for a fixed number of attempts, sending out a new message to the DNS server and performing a timed wait each time; the designers of Mercator recommend of the order of five attempts. The time quantum of the wait increases exponentially with each of these attempts; Mercator started with one second and ended with roughly 90 seconds, in consideration of the fact that there are host names that take tens of seconds to resolve.

20.2.3 The URL frontier

Fundamentally, the URL frontier at a node is given a URL by its crawl process (or by the host splitter of another crawl process). It maintains the URLs in the frontier and regurgitates them in some order whenever a crawler thread seeks a URL. Two important considerations govern the order in which URLs are returned by the frontier. First, high-quality pages that change frequently should be prioritized for frequent crawling. Thus, the priority of a page should be a function of both its change rate its quality (using some reasonable quality estimate). The combination is necessary because a large number of spam pages change completely on every fetch.

The second consideration is politeness: we must avoid repeated fetch requests to a host within a short time span. The likelihood of this is exacerbated because of a form of locality of reference: many URLs link to other URLs at the same host. As a result, a URL frontier implemented as a simple priority queue might result in a burst of fetch requests to a host. This might occur even if we were to constrain the crawler so that at most one thread could fetch from any single host at any time. A common heuristic is to insert a

gap between successive fetch requests to a host that is an order of magnitude larger than the time taken for the most recent fetch from that host.

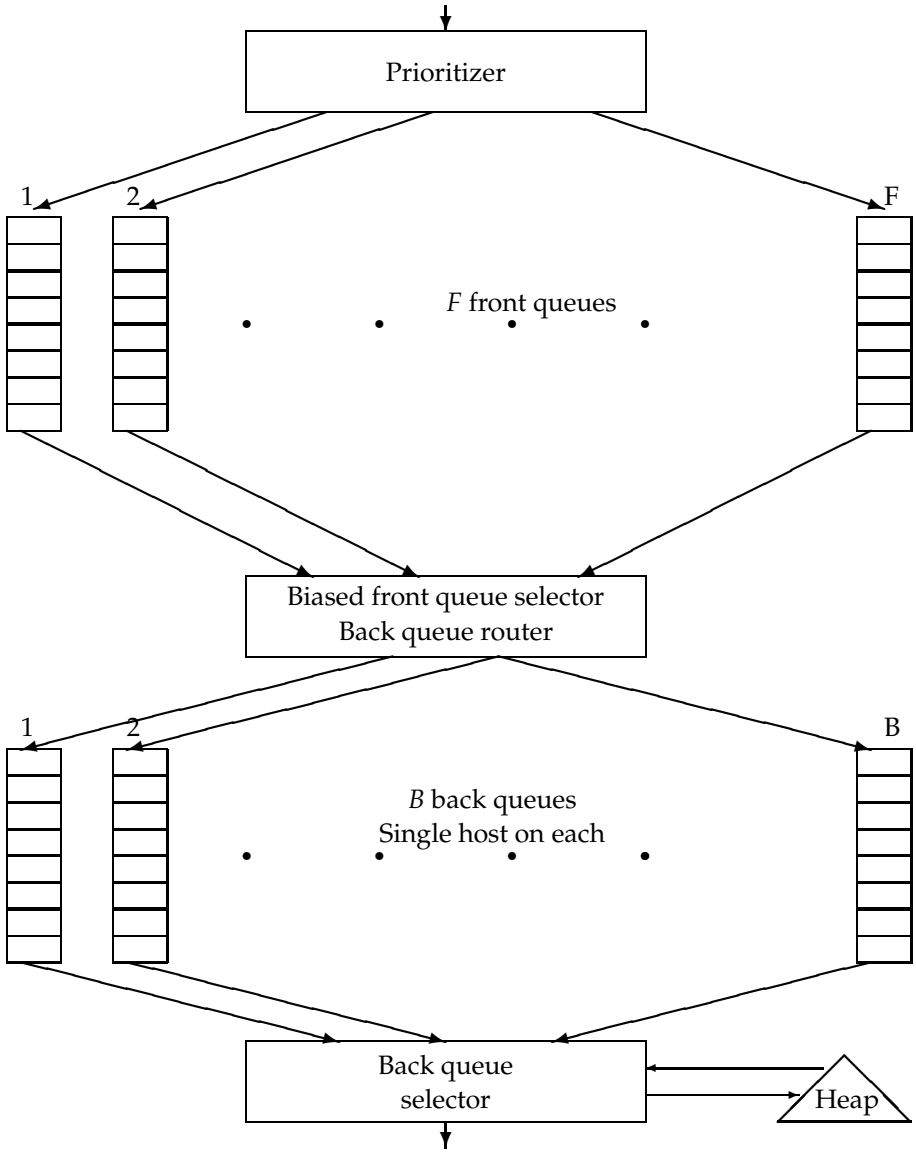
Figure 20.3 shows a polite and prioritizing implementation of a URL frontier. Its goals are to ensure that (i) only one connection be open at a time to any host; (ii) a waiting time of a few seconds occurs between successive requests to a host and (iii) high-priority pages are crawled preferentially.

The two major sub-modules are a set of F *front queues* in the upper portion of the figure, and a set of *back queues* in the lower part; all of these are FIFO queues. The front queues implement the prioritization, while the back queues implement politeness. In the flow of a URL added to the frontier as it makes its way through the front and back queues, a *prioritizer* first assigns to the URL an integer priority i between 1 and F based on its fetch history (taking into account the rate at which the web page at this URL has changed between previous crawls). For instance, a document that has exhibited frequent change would be assigned a higher priority. Other heuristics could be application-dependent and explicit – for instance, URLs from news services may always be assigned the highest priority. The URL is now appended to the ith of the front queues.

Each of the B back queues maintains the following invariants: (i) it is non-empty while the crawl is in progress and (ii) it only contains URLs from a single host. An auxiliary table T (Figure 20.4) is used to maintain the mapping from hosts to back queues. Whenever a back-queue is empty and is being re-filled from a front-queue, table T must be updated accordingly.

In addition, we maintain a heap with one entry for each back queue, the entry being the earliest time t_e at which the host corresponding to that queue can be contacted again.

A crawler thread requesting a URL from the frontier extracts the root of this heap and (if necessary) waits until the corresponding time entry t_e. It then takes the URL u at the head of the back queue q corresponding to the extracted heap root, and proceeds to fetch the URL u. After fetching u, the calling thread checks whether q is empty. If so, it picks a front queue and extracts from its head a URL v. The choice of front queue is biased (usually by a random process) towards queues of higher priority, ensuring that URLs of high priority flow more quickly into the back queues. We examine v to check whether there is already a back queue holding URLs from its host. If so, v is added to that queue and we reach back to the front queues to find another candidate URL for insertion into the now-empty queue q. This process continues until q is non-empty again. In any case, the thread inserts a heap entry for q with a new earliest time t_e based on the properties of the URL in q that was last fetched (such as when its host was last contacted as well as the time taken for the last fetch), then continues with its processing. For instance, the new entry t_e could be the current time plus ten times the last fetch time.



► **Figure 20.3** The URL frontier. URL's extracted from already crawled pages flow in at the top of the figure. A crawl thread requesting a URL extracts it from the bottom of the figure. En route, a URL flows through one of several *front queues* that manage its priority for crawling, followed by one of several *back queues* that manage the crawler's politeness.

Host	Back queue
stanford.edu	23
microsoft.com	47
acm.org	12

► **Figure 20.4** Example of an auxiliary hosts-to-back queues table.

The number of front queues, together with the policy of assigning priorities and picking queues, determines the priority properties we wish to build into the system. The number of back queues governs the extent to which we can keep all crawl threads busy while respecting politeness. The designers of Mercator recommend a rough rule of three times as many back queues as crawler threads.

On a web-scale crawl, the URL frontier grows to the point where it demands more memory at a node than is available. The solution is to let most of the URL frontier reside on disk. A portion of each queue is kept in memory, with more brought in from disk as it is drained in memory.

Exercise 20.3

In the preceding discussion we encountered two recommended "hard constants" – the increment on t_e being `ten` times the last fetch time, and the number back queues being `three` times the number of crawl threads. How are these two constants related?

20.3 Distributing indexes

In Section 4.4 we described distributed indexing. We now consider the distribution of the index across a large cluster of machines for supporting querying. Two obvious alternative index implementations suggest themselves: *partitioning by terms*, also known as global index organization, and *partitioning by documents*, also know as local index organization. In the former, the dictionary of index terms is partitioned into subsets, each subset residing at a set of nodes. Along with the terms at a node, we keep the postings for those terms. A query is routed to the nodes corresponding to its query terms. In principle, this allows greater concurrency since a stream of queries with different query terms would hit different sets of machines.

TERM PARTITIONING
DOCUMENT PARTITIONING

In practice, partitioning indexes by dictionary terms turns out to be unwieldy. Multi-word queries require the sending of long postings lists between sets of nodes for merging, and the cost of this outweighs the greater concurrency. Load balancing the partitioning is governed not by an a priori analysis of relative term frequencies, but rather by the distribution of query terms and their co-occurrences. Achieving good partitions is a function of

the co-occurrences of query terms and entails the clustering of terms to optimize objectives that are not yet fully understood. Finally, this strategy makes implementation of dynamic indexing more difficult.

A more common implementation is to partition by documents: each node contains the index for a subset of all documents. Each query is distributed to all nodes, with the results from various nodes being merged before presentation to the user. This strategy trades more local disk seeks for less inter-node communication. One difficulty in this approach is that global statistics used in scoring – such as idf – must be computed across the entire document collection even though the index at any single node only contains a subset of the documents. These are computed by distributed "background" processes that periodically refresh the node indexes with fresh global statistics.

How do we decide the partition of documents to nodes? Based on our development of the crawler architecture in Section 20.2.1, one simple approach would be to assign all pages from a host to a single node. This partitioning could follow the partitioning of hosts to crawler nodes. A danger of such partitioning is that on many queries, a preponderance of the results would come from documents at a small number of hosts (and hence a small number of index nodes).

A hash of each URL into the space of index nodes results in a more uniform distribution of query-time computation across nodes. At query time, the query is broadcast to each of the nodes, with the top k results from each node being merged to find the top k documents for the query. A common implementation heuristic is to partition the document collection into indexes of documents that are more likely to score highly on most queries (using, for instance, techniques in Chapter 21) and low-scoring indexes with the remaining documents. We only search the low-scoring indexes when there are too few matches in the high-scoring indexes.

20.4 Connectivity servers

CONNECTIVITY SERVER
CONNECTIVITY QUERIES

For reasons to become clearer in Chapter 21, web search engines require a *connectivity server* that supports fast *connectivity queries* on the web graph. Typical connectivity queries are *which URLs link to a given URL?* and *which URLs does a given URL link to?* To this end, we wish to store mappings in memory from URL to outlinks, and from URL to inlinks. Applications include crawl control, web graph analysis, connectivity, crawl optimization and *link analysis* (to be covered in Chapter 21).

Consider a web with four billion pages, each with ten links to other pages. In the simplest form, we would require 32 bits or 4 bytes to specify each end (source and destination) of each link, requiring a total of

$$4 \times 10^9 \times 10 \times 8 = 3.2 \times 10^{11}$$

bytes of memory. Some basic properties of the web graph can be exploited to use well under 10% of this memory requirement. At first sight, we appear to have a data compression problem – which is amenable to a variety of standard solutions. However, our goal is not to simply compress the web graph to fit into memory; we must do so in a way that supports connectivity queries.

We assume that each web page is represented by a unique integer; the specific scheme used to assign these integers is described below. We build an *adjacency table* that resembles an inverted index: it has a row for each web page, with the different rows ordered by the corresponding integers. The row for any page p contains a sorted list of integers, each corresponding to a web page that links to p. This table permits us to respond to queries of the form *which pages link to p?* In similar fashion we build a table whose entries are the pages linked to by p.

This table representation cuts the space taken by the naive representation (in which we explicitly represent each link by its two end points, each a 32-bit integer) by 50%. Our description below will focus on the table for the links *from* each page; it should be clear that the techniques apply just as well to the table of links to each page. To further reduce the storage for the table, we exploit several ideas:

1. Similarity between lists: Many rows of the table have many entries in common. Thus, if we explicitly represent one version of several similar rows, the remainder can be succinctly expressed in terms of the prototypical row.

2. Locality: many links from a page go to "nearby" pages – pages on the same host, for instance. This suggests that in encoding the destination of a link, we can often use small integers and thereby save space.

3. We use gap encodings in sorted lists: rather than store the destination of each link, we store the offset from the previous entry in the row.

We now develop each of these techniques.

In a *lexicographic* ordering of all URLs, we treat each URL as an alphanumeric string and sort these strings. For instance, a segment of this sorted order may look like the following:

```
www.stanford.edu/alchemy
www.stanford.edu/biology
www.stanford.edu/biology/plant
www.stanford.edu/biology/plant/copyright
www.stanford.edu/biology/plant/people
www.stanford.edu/chemistry
```

```
1, 2, 4, 8, 16, 32, 64
1, 4, 9, 16, 25, 36, 49, 64
1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144
1, 4, 8, 16, 25, 36, 49, 64
```

► **Figure 20.5** A four-row segment of the table of links.

For a lexicographic sort to truly model web locality, the domain name part of the URL should be inverted, so that www.stanford.edu becomes edu.stanford.www, but this is not necessary here since we are mainly concerned with links local to a single host.

To each URL, we assign its position in this ordering as the unique identifying integer. Figure 20.5 shows an example of such a numbering and the resulting table. In this example sequence, `www.stanford.edu/biology` is assigned the integer 2 since it is second in the sequence.

We next exploit a property that stems from the way most websites are structured to get similarity and locality. Most websites have a template with a set of links from each page in the site to a fixed set of pages on the site (such as its copyright notice, terms of use, and so on). In this case, the rows corresponding to pages in a website will have many table entries in common. Moreover, under the lexicographic ordering of URLs, it is very likely that the pages from a website appear as contiguous rows in the table.

We adopt the following strategy: we walk down the table, encoding each table row in terms of the seven preceding rows. In the example of Figure 20.5, we could encode the fourth row as "the same as the row at offset 2 (meaning, two rows earlier in the table), with 9 replaced by 8". This requires the specification of the offset, the integer(s) dropped (in this case 9) and the integer(s) added (in this case 8). The use of only the seven preceding rows has two advantages: (i) the offset can be expressed with only 3 bits; this choice is optimized empirically and (ii) fixing the maximum offset to a small value like seven avoids having to perform an expensive search among many candidate prototypes in terms of which to express the current row.

What if none of the preceding seven rows is a good prototype for expressing the current row? This would happen, for instance, at each boundary between different websites as we walk down the rows of the table. In this case we simply express the row as starting from the empty set and "adding in" each integer in that row. By using gap encodings to store the gaps (rather than the actual integers) in each row, and encoding these gaps tightly based on the distribution of their values, we obtain further space reduction. In experiments mentioned in Section 20.5, the series of techniques outlined here appears to use as few as 3 bits per link, on average – a dramatic reduction

from the 64 required in the naive representation.

While these ideas give us a representation of sizeable web graphs that comfortably fit in memory, we still need to support connectivity queries. What is entailed in retrieving from this representation the set of links from a page? First, we need an index from a hash of the URL to its row number in the table. Next, we need to reconstruct these entries, which may be encoded in terms of entries in other rows. This entails following the offsets to reconstruct these other rows – a process that in principle could lead through many levels of indirection. In practice however, this does not happen very often. A heuristic for controlling this can be introduced into the construction of the table: when examining the preceding seven rows as candidates from which to model the current row, we demand a threshold of similarity between the current row and the candidate prototype. This threshold must be chosen with care. If the threshold is set too high, we seldom use prototypes and express many rows afresh. If the threshold is too low, most rows get expressed in terms of prototypes, so that at query time the reconstruction of a row leads to many levels of indirection through preceding prototypes.

Exercise 20.4

We noted that expressing a row in terms of one of seven preceding rows allowed us to use no more than three bits to specify which of the preceding rows we are using as prototype. Why seven and not eight preceding rows? *(Hint: consider the case when none of the preceding seven rows is a good prototype.)*

Exercise 20.5

We noted that for the above scheme, decoding the links incident on a URL could result in many levels of indirection. Construct an example in which the number of levels of indirection grows linearly with the number of URL's.

20.5 References and further reading

The first web crawler appears to be Matthew Gray's Wanderer, written in the spring of 1993. The Mercator crawler is due to Najork and Heydon (Najork and Heydon 2001; 2002); the treatment in this chapter follows their work. Other classic early descriptions of web crawling include Burner (1997), Brin and Page (1998), Cho et al. (1998) and the creators of the Webbase system at Stanford (Hirai et al. 2000). Cho and Garcia-Molina (2002) give a taxonomy and comparative study of different modes of communication between the nodes of a distributed crawler. The Robots Exclusion Protocol standard is described at http://www.robotstxt.org/wc/exclusion.html. Boldi et al. (2002) and Shkapenyuk and Suel (2002) provide more recent details of implementing large-scale distributed web crawlers.

Our discussion of DNS resolution (Section 20.2.2) uses the current convention for internet addresses, known as IPv4 (for Internet Protocol version 4) – each IP address is a sequence of four bytes. In the future, the convention for

addresses (collectively known as the internet *address space*) is likely to use a new standard known as IPv6 (http://www.ipv6.org/).

Tomasic and Garcia-Molina (1993) and Jeong and Omiecinski (1995) are key early papers evaluating term partitioning versus document partitioning for distributed indexes. Document partitioning is found to be superior, at least when the distribution of terms is skewed, as it typically is in practice. This result has generally been confirmed in more recent work (MacFarlane et al. 2000). But the outcome depends on the details of the distributed system; at least one thread of work has reached the opposite conclusion (Ribeiro-Neto and Barbosa 1998, Badue et al. 2001). Barroso et al. (2003) describe the distribution methods used at Google. The first implementation of a connectivity server was described by Bharat et al. (1998). The scheme discussed in this chapter, currently believed to be the best published scheme (achieving as few as 3 bits per link for encoding), is described in a series of papers by Boldi and Vigna (2004b;a).

21 *Link analysis*

The analysis of hyperlinks and the graph structure of the web has been instrumental in the development of web search. In this chapter we focus on the use of hyperlinks for ranking web search results. Such link analysis is one of many factors considered by web search engines in computing a composite score for a web page on any given query. We begin by reviewing some basics of the web as a graph in Section 21.1, then proceed to the technical development of the elements of link analysis for ranking.

Link analysis for web search has intellectual antecedents in the field of citation analysis, aspects of which overlap with an area known as bibliometrics. These disciplines seek to quantify the influence of scholarly articles by analyzing the pattern of citations amongst them. Much as citations are a form by which a scholarly article confers authority on other articles, link analysis on the web views hyperlinks from a web page to another as a form of conferral of authority. Clearly, not every citation or hyperlink implies such authority conferral; for this reason, simply measuring the quality of a web page by the number of in-links (citations) is not robust enough. For instance, one may contrive to set up multiple web pages pointing to a target web page, with the intent of artificially boosting the latter's tally of in-links. Nevertheless, the phenomenon of citation is prevalent and dependable enough that it is feasible for web search engines to derive useful signals for ranking from more sophisticated link analysis.

21.1 The web as a graph

Recall the notion of the web graph from Section 19.2.1. Our study of link analysis builds on two intuitions:

1. The hyperlink from A to B connotes a conferral of authority on page B, by the creator of page A.

2. The anchor text describes the page B.

We begin by examining the second intuition, before proceeding to the first.

21.1.1 Anchor text and the web graph

The following fragment of HTML code from a web page shows a hyperlink pointing to the home page of the Journal of the ACM:

```
<a href="http://www.acm.org/jacm/">Journal of the ACM.</a>
```

In this case, the link points to the page `http://www.acm.org/jacm/` and the anchor text is *Journal of the ACM.* Clearly, in this example the anchor is descriptive of the target page. But then the target page (B = `http://www.acm.org/jacm/`) itself contains the same description as well as considerable additional information on the journal. So what use is the anchor text?

The web is full of instances where the page B does not provide an accurate description of itself. In many cases this is a matter of how the publishers of page B choose to present themselves; this is especially common with corporate web pages, where a web presence is a marketing statement. For example, at the time of the writing of this book the home page of the IBM corporation (`http://www.ibm.com`) did not contain the term computer anywhere in its HTML code, despite the fact that IBM is widely viewed as the world's largest computer maker. Similarly, the HTML code for the home page of Yahoo! (`http://www.yahoo.com`) does not at this time contain the word portal.

Thus, there is often a gap between how a web page presents itself and how many users of the web (and web search engines) would describe – and therefore search for – that web page. This represents an important gap that cannot be bridged by conventional inverted indexes, namely, web searchers need not use the same terms to describe a page they seek as the target page itself. In addition, many web pages are rich in graphics and images, and/or embed their text in these images; in such cases, the HTML parsing performed when crawling such web pages will not extract text that is useful for indexing these pages.

In such cases, the fact that the anchors of many hyperlinks pointing to `http://www.ibm.com` include the word computer can be exploited by web search engines. For instance, the anchor text terms can be included as terms under which to index the target web page. Thus, the postings for the term computer would include the document `http://www.ibm.com` and that for the term portal would include the document `http://www.yahoo.com`, using a special indicator to show that these terms occur as anchor (rather than in-page) text. As with in-page terms, anchor text terms are generally weighted based on frequency, with a penalty for terms that occur very often (the most common terms in anchor text across the web are Click and here).

The use of anchor text has some interesting side-effects. Searching for big blue on most web search engines returns the home page of the IBM corporation as the top hit; this is consistent with the popular nickname that many people use to refer to IBM. On the other hand, there have been (and continue to be) many instances where derogatory anchor text such as evil empire leads to somewhat unexpected results on querying for these terms on web search engines. This phenomenon has been exploited in orchestrated campaigns against specific sites. More generally, orchestrated anchor text may be viewed as a form of spamming, since a website can create misleading anchor text pointing to itself, to boost its ranking on selected query terms – the inverse of derogatory anchor text. Detecting and combating such systematic abuse of anchor text is another form of spam detection that web search engines perform.

Exercise 21.1

Is it always possible to follow directed edges (hyperlinks) in the web graph from any node (web page) to any other? Why or why not?

Exercise 21.2

Find an instance of misleading anchor-text on the web.

Exercise 21.3

Given the collection of anchor-text phrases for a web page x, suggest a heuristic for one term or phrase from this collection that is most descriptive of x.

Exercise 21.4

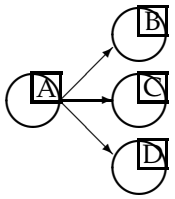
Does your heuristic in the previous exercise take into account a single domain D repeating anchor text for x from multiple pages in D?

21.2 Pagerank

PAGERANK

Our first technique for using links in the web graph for ranking assigns to every node in the web graph a numerical score between 0 and 1, known as its *pagerank*. The pagerank of a node will depend on the link structure of the web graph. Given a query, a web search engine constructs a composite score for each web page that combines a text-based score such as cosine similarity (Chapter 7) together with the pagerank score. This composite score is used to provide a ranked list of results for the query.

Consider a random surfer who begins at a web page (a node of the web graph) and executes a random walk on the web: at each of a succession of time steps, the surfer proceeds from the page A he is at to a randomly chosen web page that A hyperlinks to. Figure 21.1 shows the surfer at a node A, out of which there are three hyperlinks to nodes B, C and D; the surfer proceeds at the next time step to one of these three nodes, each being chosen with probability 1/3.



► **Figure 21.1** The random surfer at node A proceeds with probability 1/3 to each of B, C and D.

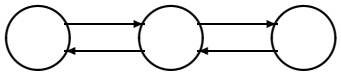
As the surfer proceeds in this fashion from node to node in his random walk, he visits some nodes more often than others; intuitively, these are nodes with many links coming in from other frequently visited nodes. What if the current location of the surfer, the node A, has no outgoing links? To address this we introduce an additional operation for our random surfer: the TELEPORT *teleport* operation. Instead of the surfer always moving from a node to other nodes it links to, in the teleport operation the surfer jumps from a node to any other node in the web graph, chosen uniformly at random. In other words, if n is the total number of nodes in the web graph, the teleport operation takes the surfer to each node with probability $1/n$. Thus, the surfer could teleport back to his present position (with probability $1/n$).

In assigning a pagerank score to each node of the web graph, we use the teleport operation in two ways:

1. When at a node with no outgoing links, the surfer invokes the teleport operation.

2. At any other node (that does have outgoing links), the surfer invokes the teleport operation with probability $0 < \alpha < 1$ and the standard random walk (follow an outgoing link chosen uniformly at random as in Figure 21.1) with probability $1 - \alpha$, where α is a fixed parameter chosen in advance. Typically, α might be 0.1.

In Section 21.2.1, we will use the theory of Markov chains to argue that when the surfer follows this combined process (random walk plus teleport) he visits each node v of the web graph a fixed fraction of the time $\pi(v)$ that depends on (1) the structure of the web graph and (2) the value of α. We call this value $\pi(v)$ the pagerank of v and will show how to compute this value in Section 21.2.2.



► **Figure 21.2** A simple Markov chain with three states; the numbers on the links indicate the transition probabilities.

21.2.1 Markov chains

A Markov chain is a *discrete-time stochastic process:* a process that occurs in a series of time-steps, at each of which a random choice is made. A Markov chain consists of N *states*; we re-use the symbol N here because in fact each web page will correspond to a state in the Markov chain we will formulate.

A Markov chain is characterized by an $n \times n$ *transition probability matrix* P each of whose entries is in the interval $[0, 1]$; the entries in each row of P add up to 1. The Markov chain is said to be in one of the n states at any given time-step; then, the entry P_{ij} tells us the probability that the state at the next time-step is j, conditioned on the current state being i. Each entry P_{ij} is known as a transition probability. It is clear then that

$$P_{ij} \in [0, 1], \forall i, j$$

and

$$\sum_{j=1}^{n} P_{ij} = 1, \forall i.$$

Fundamentally, the distribution of next states for a Markov chain depends only on the current state, and not on how the Markov chain arrived at the current state. Figure 21.2 shows a simple Markov chain with three states.

PROBABILITY VECTOR

A *probability vector* is a vector all of whose entries are in the interval $[0, 1]$, and the entries add up to 1. An n-dimensional probability vector each of whose components corresponds to one of the n states of a Markov chain can be viewed as a probability distribution over its states.

We can view a random surfer on the web graph as a Markov chain, with one state for each web page and each transition probability representing the probability of moving from one web page to another. The teleport operation contributes to these transition probabilities. We can readily derive this Markov chain from the adjacency matrix of the web graph, which encodes

the hyperlinks (edges) between web pages. We can depict the probability distribution of the surfer's position at any time step by a probability vector $\vec{x}$. At $t = 0$ the surfer may begin at a state whose corresponding entry in $\vec{x}$ is 1 while all others are zero. By definition, the surfer's distribution at $t = 1$ is given by the probability vector $\vec{x}P$; at $t = 2$ by $(\vec{x}P)P = \vec{x}P^2$, and so on. We can thus compute a priori the surfer's distribution over the states at any time, given only the initial distribution and the transition probability matrix P.

If a Markov chain is allowed to run for many time steps, each state is visited at a (different) frequency that depends on the structure of the Markov chain. In our running analogy, the surfer visits certain web pages (say, popular news home pages) more often than other pages. We now make this intuition precise, establishing conditions under which such a steady-state visit frequency exists. Following this, we set the pagerank of each node v to this steady-state visit frequency and show how it can be computed.

ERGODIC MARKOV CHAIN

Definition: A Markov chain is said to be *ergodic* if the following two conditions hold.

1. For any two states i, j, there is an integer $k \geq 2$ such that we have a sequence of k states $s_1 = i, s_2, \ldots, s_k = j$ such that $\forall 1 \leq \ell \leq k-1$, the transition probability $P_{s_\ell, s_{\ell+1}} > 0$.
2. There exists a time T_0 such that for all states j in the Markov chain, for all choices of the state i in which it is started at time step $t = 0$ and for all $t > T_0$, the probability of being in state j at time t is > 0.

Theorem 21.1. *For any ergodic Markov chain, there is a unique steady-state probability distribution over the states, $\vec{\pi}$, such that if $N(i,t)$ is the number of visits to state i in t steps, then*

$$\lim_{t \to \infty} \frac{N(i,t)}{t} = \pi(i),$$

where $\pi(i) > 0$ is the steady-state probability for state i.

It follows from Theorem 21.1 that the random walk with teleporting results in a unique distribution of steady-state probabilities over the states of the induced Markov chain. This steady-state probability for a state is the pagerank of the corresponding web page.

Exercise 21.5

Write down the transition probability matrix for the example in Figure 21.2.

Exercise 21.6

Consider a web graph with three nodes 1, 2 and 3. The links are as follows: $1 \to 2, 3 \to 2, 2 \to 1, 2 \to 3$. Write down the transition probability matrices for the surfer's walk with teleporting, for the following three values of the teleport probability: (a) $\alpha = 0$; (b) $\alpha = 0.5$ and (c) $\alpha = 1$.

Exercise 21.7

A user of a browser can, in addition to clicking a hyperlink on the page x he is currently browsing, use the *back button* to go back to the page from which he arrived at x. Can such a user of back buttons be modeled as a Markov chain?

Exercise 21.8

Can one model the use of back buttons by a Markov chain that has a state for every hyperlink on the web, since a back button generally takes the user backwards on a link?

Exercise 21.9

What is the effect of repeated invocations of the back button?

Exercise 21.10

Consider a Markov chain with three states A, B and C, and transition probabilities as follows. From state A, the next state is B with probability 1. From B, the next state is either A with probability p_A, or state C with probability $1 - p_A$. From C the next state is A with probability 1. For what values of $p_A \in [0, 1]$ is this Markov chain ergodic?

Exercise 21.11

Show that for any directed graph, the Markov chain induced by a random walk with the teleport operation is ergodic.

Exercise 21.12

Show that the pagerank of every page is at least α/n. What does this imply about the difference in pagerank values (over the various pages) as α becomes close to 1?

21.2.2 The Pagerank computation

How do we compute these pagerank values? Recall the definition of a left eigenvector from Equation 18.2 in Chapter 18; the left eigenvectors of the transition probability matrix P are N-vectors $\vec{\pi}$ such that

$$\vec{\pi} P = \lambda \vec{\pi}. \tag{21.1}$$

The N entries in the eigenvector $\vec{\pi}$ are the steady-state probabilities of the random walk with teleporting, and thus the pagerank values for the corresponding web pages. Indeed, we may interpret Equation 21.1 as telling us that if $\vec{\pi}$ is the probability distribution of the surfer across the web pages, he remains in the distribution $\vec{\pi}$ – thus, $\vec{\pi}$ is the steady-state distribution. If we were to compute the dominant left eigenvector of the matrix P – the one with eigenvalue 1 – we would have computed the pagerank values.

There are many algorithms available for computing left eigenvectors; the references at the end of Chapter 18 and the present chapter are a guide to these. We give here a rather elementary method, sometimes known as *power iteration*. If $\vec{x}$ is the initial distribution over the states, then the distribution at time t is $\vec{x}P^t$. As t grows large, we would expect that the distribution $\vec{x}P^t$ is

very similar to the distribution $\vec{x}P^{t+1}$, since for large t we would expect the Markov chain to attain its steady state. By Theorem 21.1 this is independent of the initial distribution $\vec{x}$. The power iteration method is simply to simulate the surfer's walk: begin at a state and run the walk for a large number of steps t, keeping track of the visit frequencies at each of the states. After a large number of steps t, these frequencies "settle down" so that the variation in the computed frequencies is below some predetermined threshold. We declare these to be the computed pagerank values.

We consider the web graph in Exercise 21.6 with $\alpha = 0.5$. The transition probability matrix of the surfer's walk with teleporting is then

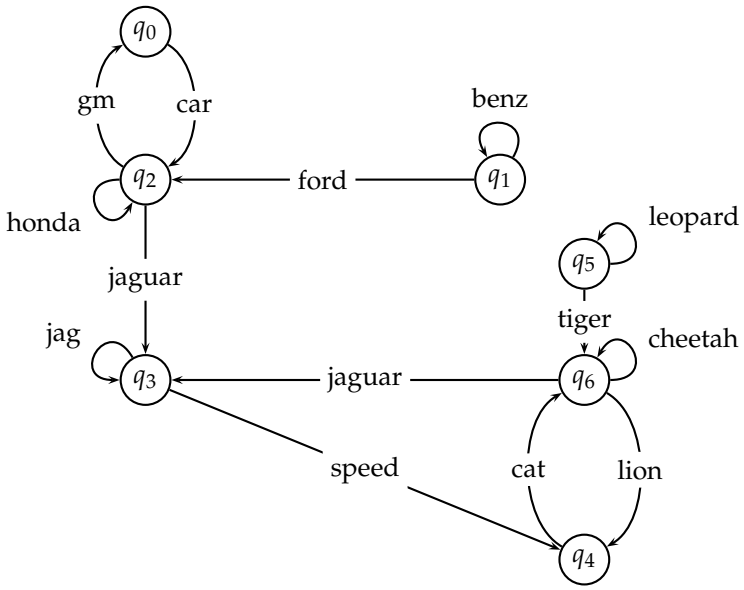
$$P = \begin{pmatrix} 1/6 & 2/3 & 1/6 \\ 5/12 & 1/6 & 5/12 \\ 1/6 & 2/3 & 1/6 \end{pmatrix}. \tag{21.2}$$

Imagine that the surfer starts in state 1, corresponding to the initial probability distribution vector $\vec{x} = (1\ 0\ 0)$. Then, after one step the distribution is

$$\vec{x}P = \begin{pmatrix} 1/6 & 2/3 & 1/6 \end{pmatrix}. \tag{21.3}$$

After two steps the distribution $\vec{x}P^2$ is $\vec{x} = (1/3 \quad 1/3 \quad 1/3)$, after three steps $\vec{x} = (7/24 \quad 5/12 \quad 7/24)$. Continuing for several steps, we see that the distribution converges to the steady state of $\vec{x} = (5/18 \quad 4/9 \quad 5/18)$. In this simple example, we may directly calculate this steady-state probability distribution by observing the symmetry of the Markov chain: states 1 and 3 are symmetric, as evident from the fact that the first and third rows of the transition probability matrix in Equation (21.2) are identical. Postulating, then, that they both have the same steady-state probability and denoting this probability by p, we know that the steady-state distribution is of the form $\vec{\pi} = (p\ (1-2p)\ p)$. Now, using the identity $\vec{\pi} = \vec{\pi}P$, we solve a simple linear equation to obtain $p = 5/18$ and consequently, $\vec{\pi} = (5/18\ 4/9\ 5/18)$.

Note that the pagerank values of pages (and the implicit ordering amongst them) are independent of any query a user might pose; pagerank is thus a query-independent measure of the absolute quality of each web page. On the other hand, the relative ordering of pages should, intuitively, depend on the query being served. For this reason, search engines use absolute quality measures such as pagerank as just one of many factors in scoring a web page on a query.



► **Figure 21.3** A small web graph. Arcs are annotated with the word that occurs in the anchor text of the corresponding link.

✎ **Example 21.1:** Consider the graph in Figure 21.3. For a teleportation rate of 0.14 its stochastic transition matrix is:

$$\begin{array}{ccccccc}
0.02 & 0.02 & 0.88 & 0.02 & 0.02 & 0.02 & 0.02 \\
0.02 & 0.45 & 0.45 & 0.02 & 0.02 & 0.02 & 0.02 \\
0.31 & 0.02 & 0.31 & 0.31 & 0.02 & 0.02 & 0.02 \\
0.02 & 0.02 & 0.02 & 0.45 & 0.45 & 0.02 & 0.02 \\
0.02 & 0.02 & 0.02 & 0.02 & 0.02 & 0.02 & 0.88 \\
0.02 & 0.02 & 0.02 & 0.02 & 0.02 & 0.45 & 0.45 \\
0.02 & 0.02 & 0.02 & 0.31 & 0.31 & 0.02 & 0.31
\end{array}$$

The pagerank vector of this matrix is:

$$\vec{x} = (0.05 \quad 0.04 \quad 0.11 \quad 0.25 \quad 0.21 \quad 0.04 \quad 0.31)$$

q_2, q_3, q_4 and q_6 are the nodes with at least two inlinks. Of these, q_2 has the lowest pagerank since activity is draining out of the top part of the graph – the walker can only return there through teleportation.

21.2.3 Topic-specific Pagerank

Thus far, we have discussed the pagerank computation with a teleport operation in which the surfer jumps to a random web page chosen uniformly at random. We now consider teleporting to a random web page chosen *non-uniformly*. For example, a sports aficionado might expect pages on sports to be ranked higher than non-sports pages. Let us imagine that the sports pages are "near" one another in the web graph. Then, a random surfer who frequently finds himself on random sports pages is likely (in the course of the random walk) to spend most of his time at sports pages, so that the steady-state distribution of sports pages is boosted.

Suppose our random surfer, endowed with a teleport operation as before, teleports to *a random web page on the topic of sports* instead of teleporting to a uniformly chosen random web page. We will not focus on how we collect all web pages on the topic of sports; in fact, we only need a non-zero subset S of sports-related web pages. This may be obtained, for instance, from a manually built directory of sports pages such as the open directory project (http://www.dmoz.org/) or that of Yahoo!

Provided the set S of sports-related pages is non-empty, it follows that there is a non-empty set of web pages $Y \supseteq S$ over which the random walk has a steady-state distribution; let us denote this *sports pagerank* distribution by $\vec{\pi}_s$. For web pages not in Y, we set the pagerank values to zero. We call $\vec{\pi}_s$ the *topic-specific pagerank* for sports.

TOPIC-SPECIFIC PAGERANK

We do not demand that teleporting takes the random surfer to a uniformly chosen sports page; the distribution over teleporting targets S could in fact be arbitrary.

In like manner we can envision topic-specific pagerank distributions for each of several topics such as science, religion, politics and so on. Each of these distributions assigns to each web page a pagerank value in the interval $[0, 1)$. For a user interested in only a single topic from among these topics, we may invoke the corresponding pagerank distribution when scoring and ranking search results. This gives us the potential of considering settings in which the search engine knows what topics a user is interested in. This may arise from users who either explicitly register their interests, or through the system learning by observing the user's behavior and page access patterns over time.

Within this realm where a user's topics of interest are known to the engine, the above discussion leads to a pagerank distribution that is tailored to a single topic. But if, for instance, a user is known to have a mixture of interests from multiple topics, it is no longer clear how to adapt these methods. For instance, a user may have an interest mixture (or *profile*) that is 60% sports and 40% politics; can we compute a *personalized pagerank* for this user? At first glance, this appears daunting: how could we possibly compute a different

PERSONALIZED PAGERANK

pagerank distribution for each user profile (with, potentially, infinitely many possible profiles)? First, note that a user with this mixture of interests could teleport as follows: determine first whether to teleport to the set S of known sports pages, or to the set of known politics pages. This choice is made at random, choosing sports pages 60% of the time and politics pages 40% of the time. Once we choose that a particular teleport step is to (say) a random sports page, we choose a web page in S uniformly at random to teleport to. This in turn leads to an ergodic Markov chain with a steady-state distribution that is personalized to this user's preferences over topics (see Exercise 21.16).

While this idea has intuitive appeal, its implementation appears cumbersome: it seems to demand that for each user, we compute a transition probability matrix and compute its steady-state distribution. We are rescued by the fact that the evolution of the probability distribution over the states of a Markov chain is governed by a linear system. In Exercise 21.16 we show that it is not necessary to compute a pagerank vector for every distinct combination of user interests over topics; the personalized pagerank vector for any user can be expressed as a linear combination of the underlying topic-specific pageranks. For instance, the personalized pagerank vector for the user whose interests are 60% sports and 40% politics can be computed as

$$0.6\vec{\pi}_s + 0.4\vec{\pi}_p, \tag{21.4}$$

where $\vec{\pi}_s$ and $\vec{\pi}_p$ are the topic-specific pagerank vectors for sports and for politics, respectively.

Exercise 21.13

How does the set Y relate to S?

Exercise 21.14

Is the set Y always the set of all web pages? Why or why not?

Exercise 21.15

Is the sports pagerank of any page in S at least as large as its pagerank?

Exercise 21.16

Consider a setting where we have two topic-specific pagerank values for each web page: a sports pagerank $\vec{\pi}_s$, and a politics pagerank $\vec{\pi}_p$. Let α be the (common) teleportation probability used in computing both sets of topic-specific pageranks. For $q \in [0,1]$, consider a user whose interest profile is divided between a fraction q in sports and a fraction $1-q$ in politics. Show that the user's personalized pagerank is the steady state distribution of a random walk in which – on a teleport step – the walk teleports to a sports page with probability q and to a politics page with probability $1-q$.

Exercise 21.17

Show that the Markov chain corresponding to this walk is ergodic and hence the user's personalized pagerank can be obtained by computing the steady state distribution of this Markov chain.

Exercise 21.18

Show that in this steady state distribution, the steady state probability for any web page x equals $q\pi_s(x) + (1-q)\pi_p(x)$.

21.3 Hubs and Authorities

HUB SCORE
AUTHORITY SCORE

We now develop a scheme in which every web page is assigned *two* scores, one called its *hub score* and the other its *authority score*. The idea is that for any query, we compute not one but two ranked lists of results – one ranking induced by the hub scores and the other by the authority scores.

This approach stems from a particular insight into the creation of web pages, reasoning that there are two primary kinds of web pages useful as results for *broad-topic searches*. By a broad topic search we mean an informational query such as "I wish to learn about leukemia". There are authoritative sources of information on the topic; in this case, the National Cancer Institute's page on leukemia would be such a page. We will call such pages *authorities*; in the computation we are about to describe, they are the pages that will emerge with high authority scores.

On the other hand, there are many pages on the web that are hand-compiled lists of links to authoritative web pages on a specific topic. These *hub* pages are not in themselves authoritative sources of topic-specific information, but rather compilations that someone with an interest in the topic has spent time putting together. The approach we will take, then, is to use these hub pages to discover the authority pages. In the computation we now develop, these hub pages are the pages that will emerge with high hub scores.

A good hub page is one that points to many good authorities. A good authority page is one that is pointed to by many good hub pages. We thus appear to have a circular definition of hubs and authorities; we will turn this into an iterative computation. Suppose that we have a subset of the web graph, that is, a subset of all web pages together with the hyperlinks amongst them. We will iteratively compute a hub score and an authority score for every web page in this subset, deferring the discussion of how we pick this subset until Section 21.3.1.

For a web page x, a node in our chosen subset of the web graph, we use $h(x)$ to denote its hub score and $a(x)$ its authority score. Initially, we set $h(x) = a(x) = 1$ for all nodes x. We also denote by $x \mapsto y$ the existence of a hyperlink from x to y. The core of the iterative algorithm is a pair of updates to the hub and authority scores of all pages given by Equation 21.5, which capture the intuitive notions that good hubs point to good authorities and that good authorities are pointed to by good hubs.

$$\begin{aligned} h(x) &\leftarrow \sum_{x \mapsto y} a(y) \\ a(x) &\leftarrow \sum_{y \mapsto x} h(y). \end{aligned} \tag{21.5}$$

Thus, the first line of (21.5) sets the hub score of page x to the authority scores of the pages it links to. In other words, if x links to pages with high authority scores, its hub score increases. The second line plays the reverse role; if page x is linked to by good hubs, its authority score increases.

What happens as we perform these updates iteratively, recomputing hub scores for all nodes, then new authority scores based on these recomputed hub scores, and so on? Let us recast the equations (21.5) into matrix-vector form. Let $\vec{h}$ and $\vec{a}$ denote the vectors of all hub and all authority scores respectively, for the pages in our subset of the web graph. Let A denote the *adjacency matrix* of the subset of the web graph that we are dealing with: A is a square matrix with one row and one column for each web page at hand. The entry A_{ij} is 1 if there is a hyperlink from page i to page j, and 0 otherwise. Then, we may write (21.5)

$$\begin{aligned} \vec{h} &\leftarrow A\vec{a} \\ \vec{a} &\leftarrow A^T\vec{h}, \end{aligned} \tag{21.6}$$

where A^T denotes the transpose of the matrix A. Now the right hand side of each line of (21.6) is a vector that is the left hand side of the other line of (21.6). Substituting these into one another, we may rewrite (21.6) as

$$\begin{aligned} \vec{h} &\leftarrow AA^T\vec{h} \\ \vec{a} &\leftarrow A^TA\vec{a}. \end{aligned} \tag{21.7}$$

Now, (21.7) bears an uncanny resemblance to a pair of eigenvector equations (Section 18.1); indeed, if we replace the $\leftarrow$ symbols by $=$ symbols and introduce the (unknown) eigenvalue, the first line of (21.7) becomes the equation for the eigenvectors of AA^T, while the second becomes the equation for the eigenvectors of A^TA:

$$\begin{aligned} \vec{h} &= \lambda_h AA^T\vec{h} \\ \vec{a} &= \lambda_a A^TA\vec{a}. \end{aligned} \tag{21.8}$$

Here we have used λ_h to denote the eigenvalue of AA^T and λ_a to denote the eigenvalue of A^TA.

This leads to some key consequences:

1. The iterative updates in (21.5) (or equivalently, (21.6)), if scaled by the appropriate eigenvalues, are equivalent to the power iteration method for computing the eigenvectors of AA^T and A^TA. Thus, the iteratively computed entries of $\vec{h}$ and $\vec{a}$ settle into unique steady state values determined by the entries of A and hence the link structure of the graph.

2. In computing these eigenvector entries, we are not restricted to using the power iteration method; indeed, we could use any fast method for computing the eigenvectors of a matrix.

The resulting computation thus takes the following form:

1. Assemble the target subset of web pages, form the graph induced by their hyperlinks and compute AA^T and A^TA.

2. Compute the principal eigenvectors of AA^T and A^TA to form the vector of hub scores $\vec{h}$ and authority scores $\vec{a}$.

3. Output the top-scoring hubs and the top-scoring authorities.

✎ **Example 21.2:** Assuming the query jaguar and double-weighting of links whose anchors contain the query word, the matrix A for Figure 21.3 is as follows:

$$\begin{matrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 2 & 1 & 0 & 1 \end{matrix}$$

The hub and authority vectors are:

$$\vec{h} = (0.03 \quad 0.04 \quad 0.33 \quad 0.18 \quad 0.04 \quad 0.04 \quad 0.35)$$

$$\vec{a} = (0.10 \quad 0.01 \quad 0.12 \quad 0.47 \quad 0.16 \quad 0.01 \quad 0.13)$$

Here, q_3 is the main authority – two hubs (q_2 and q_6) are pointing to it via highly weighted jaguar links.

Since the iterative updates captured the intuition of good hubs and good authorities, the high-scoring pages we output would give us good hubs and authorities from the target subset of web pages. We now turn to the remaining detail: how do we gather a target subset of web pages around a topic such as leukemia?

Exercise 21.19

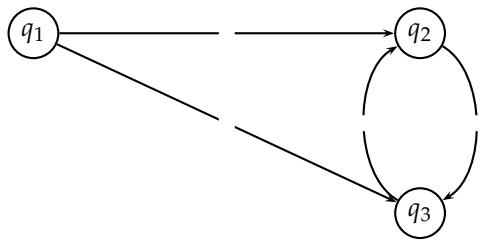
If all the hub and authority scores are initialized to 1, what is the hub/authority score of a node after one iteration?

Exercise 21.20

How would you interpret the entries of the matrices AA^T and A^TA?

Exercise 21.21

What are the principal eigenvalues of AA^T and A^TA?



► **Figure 21.4** Web graph for Exercise 21.22.

Exercise 21.22

Consider the web graph in Figure 21.4. Compute pagerank, hub and authority scores for each of the three pages. Also give the relative ordering of the 3 nodes for each of these scores, indicating any ties.

Pagerank: Assume that at each step of the pagerank random walk, we teleport to a random page with probability 0.1, with a uniform distribution over which particular page we teleport to.

Hubs/Authorities: Normalize the hub (authority) scores so that the maximum hub (authority) score is 1.

Hint 1: Using symmetries to simplify and solving with linear equations might be easier than using iterative methods.

Hint 2: For partial credit, provide at least the relative ordering (indicating any ties) of the three nodes for each of the three scoring measures.

21.3.1 Choosing the subset of the web

In assembling a subset of web pages around a topic such as leukemia, we must cope with the fact that good authority pages may not contain the specific query term leukemia. This is especially true, as noted in Section 21.1.1, when an authority page is using its web page to project a certain marketing presence. For instance, many pages on the IBM website are authoritative sources of information on computer hardware, even though these pages may

not contain the term computer or hardware. However, a hub compiling computer hardware resources is likely to use these terms and also link to the relevant pages on the IBM website.

Building on these observations, the following procedure has been suggested for compiling the subset of the web for which to compute hub and authority scores.

1. Given a query (say leukemia), use a text index to get all pages containing leukemia. Call this the *root set* of pages.
2. Build the *base set* of pages, to include the root set as well as any page that either links to a page in the root set, or is linked to by a page in the root set.

We then use the base set for computing hub and authority scores. The base set is constructed in this manner for three reasons:

1. A good authority page may not contain the query text (such as computer hardware).
2. If the text query manages to capture a good hub page P_h in the root set, then the inclusion of all pages linked to by any page in the root set will capture all the good authorities linked to by P_h in the base set.
3. Conversely, if the text query manages to capture a good authority page P_a in the root set, then the inclusion of pages points to P_a will bring other good hubs into the base set. In other words, the "expansion" of the root set into the best set enriches the common pool of good hubs and authorities.

HITS

This algorithm is known as *HITS*, which is an acronym for *Hyperlink-Induced Topic Search*. Running HITS across a variety of queries reveals some interesting insights about link analysis. Frequently, the documents that emerge as top hubs and authorities include languages other than the language of the query. These pages were presumably drawn into the base set, following the assembly of the root set. Thus, some elements of *cross-language retrieval* (where a query in one language retrieves documents in another) are evident here; interestingly, this cross-language effect resulted purely from link analysis, with no linguistic translation taking place.

We conclude this section with some notes on implementing this algorithm. The root set consists of all pages matching the text query; in fact, implementations (see the references below) suggest that it suffices to use some 200 or so web pages for the root set, rather than all pages matching the text query. Any algorithm for computing eigenvectors may be used for computing the hub/authority score vector. In fact, we need not compute the exact values of these scores; it suffices to know the relative values of the scores so that we

may identify the top hubs and authorities. To this end, it is possible that a small number of iterations of the power iteration method yield the relative ordering of the top hubs and authorities. Experiments have suggested that in practice, some five iterations of (21.5) yield fairly good results; moreover, since the link structure of the web graph is fairly sparse (the average web page links to about ten others), we do not perform these as matrix-vector products but rather as additive weight propagations along the hyperlinks.

21.4 References and further reading

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The HITS algorithm is due to Kleinberg (1999). Chakrabarti et al. (1998) developed variants that weighted links in the iterative computation based on the presence of query terms in the pages being linked and compared these to results from several web search engines. Bharat and Henzinger (1998) further developed these and other heuristics, showing that certain combinations outperformed the basic HITS algorithm. Borodin et al. (2001) provides a systematic study of several variants of the HITS algorithm. Ng et al. (2001) introduces a notion of *stability* for link analysis, arguing that small changes to link topology should not lead to significant changes in the ranked list of results for a query. Numerous other variants of HITS have been developed by a number of authors, the best know of which is perhaps SALSA (Lempel and Moran 2000).

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