Supervised Learning

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Outline

- When and why do we need to learn? (DONE!)
  - Examples of applications
  - Common tasks in ML
- How can we learn? (TODAY)
  - Hypothesis space
  - Learning (searching) algorithm
  - Examples of hypothesis spaces
  - Examples of algorithms
- but above all... Can we actually learn? (NEXT TIME)
  - VC-dimension
  - A learning bound

Supervised Learning

Formalization and terminology

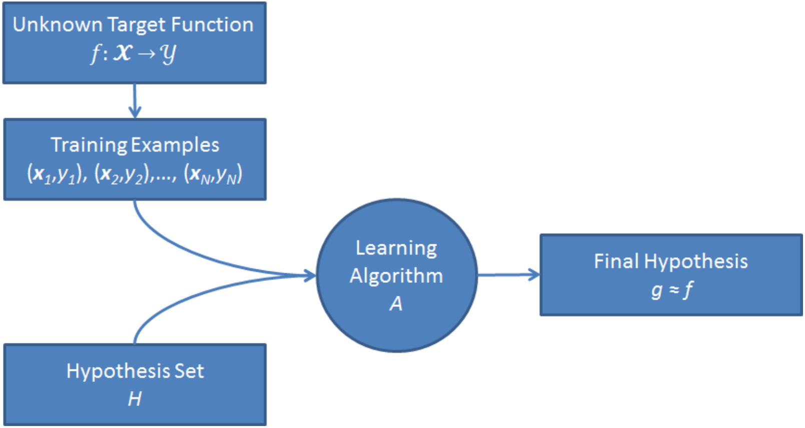
- Input: $\mathbf{x} \in \mathcal{X}$ (e.g. email representation)
- Output: $y \in \mathcal{Y}$ (e.g. spam/no_spam)
  - classification: $\mathcal{Y} \equiv \{-1, +1\}$
  - multi-class classification: $\mathcal{Y} \equiv \{1, \ldots, m\}$
  - regression: $\mathcal{Y} \equiv \mathbb{R}$
- Oracle (two alternatives):
  - Target function $f : \mathcal{X} \rightarrow \mathcal{Y}$ deterministic (ideal and unknown!)
  - Probability distributions $P(\mathbf{x}), P(y|\mathbf{x})$ stochastic version (still unknown!)
- Data: $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ (e.g. historical records)

- Select an hypothesis $g : \mathcal{X} \rightarrow \mathcal{Y}$ from a set $\mathcal{H}$ using training data

Supervised Learning in action

- A series of pairs $(\mathbf{x}_i, y_i)$, called training set, is available. These pairs are supposed generated according to a probability function $P(\mathbf{x}, y) = P(\mathbf{x})P(y|\mathbf{x})$
- A 'plausible' hypothesis $g : \mathcal{X} \rightarrow \mathcal{Y}$ is selected from a set $\mathcal{H}$ using training data
- The error on training data is called empirical error/risk
- The expected error on given pairs $(\mathbf{x}, y)$ drawn according to $P(\mathbf{x}, y)$ is called ideal error/risk
- The selected hypothesis g should generalize well: correct predictions should be done for new unseen examples drawn according to $P(\mathbf{x}, y)$, i.e. minimizing the ideal risk.

Supervised Learning: the learning setting


Unknown Target Function
$f: \mathcal{X} \rightarrow \mathcal{Y}$
Training Examples
$(\mathbf{x}_1,y_1), (\mathbf{x}_2,y_2),\ldots, (\mathbf{x}_N,y_N)$
Learning Algorithm
A
Final Hypothesis
$g \approx f$
Hypothesis Set
H

Learning Puzzles

x	y
1	2
2	4
3	6
5	10
4	?

x	y
10101	+1
11011	+1
01100	-1
00110	-1
01110	?

Are these impossible tasks?

YES

Does this mean learning is an impossible task?

NO

The fundamental assumption in ML

ML Assumption

There is a stochastic process which explains observed data. We do not know the details about it but we know it is there!

e.g. the social behavior is not purely random!

The aim of Machine Learning is to build good (or useful) approximations of this process (reverse engineering).

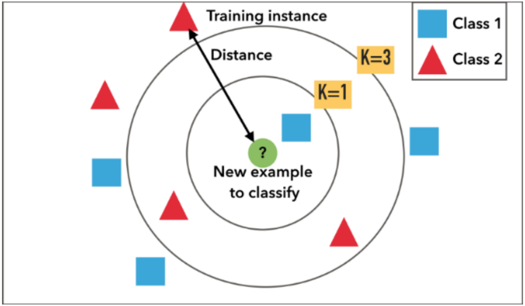
The Inductive Bias

Machine Learning is not magic!!

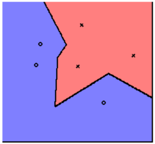
For learning to be feasible, further assumptions have to be made about the 'complexity' of the unknown target function and the hypothesis space.

- The hypothesis space cannot contain all possible formulas or functions
- The assumptions we make about the type of function to approximate is called inductive bias
- In particular, it consists of:
    - The hypothesis set: definition of the space $\mathcal{H}$
    - The learning algorithm, how the space $\mathcal{H}$ is explored

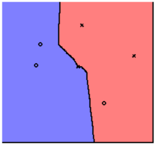
Example: K-Neirest-Neighbor (kNN)



knn (K=1): l2 Distance



knn (K=3): l2 Distance

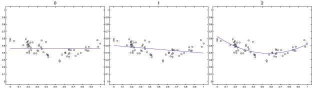


- Nearby instances should have the same label
- Complexity is tuned by the K parameter

Example: Polynomial Regression

Let's take another simple example:

- Training data $\mathcal{S} = \{(x_1, y_1), \dots, (x_n, y_n)\}, x \in \mathbb{R}, y \in \mathbb{R}$
- We want to find a polynomial curve that approximates the examples above, that is a function of type:
  $h_{\mathbf{w}}(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_p x^p,\ p \in \mathbb{N}$



- $\text{error}_S(h_{\mathbf{w}}) = \frac{1}{n} \sum_{i=1}^{n} (h_{\mathbf{w}}(x_i) - y_i)^2$ (empirical error)
- $\text{TEST} = \{(x_{n+1}, y_{n+1}), \dots, (x_N, y_N)\}$ (for estimating the ideal error)

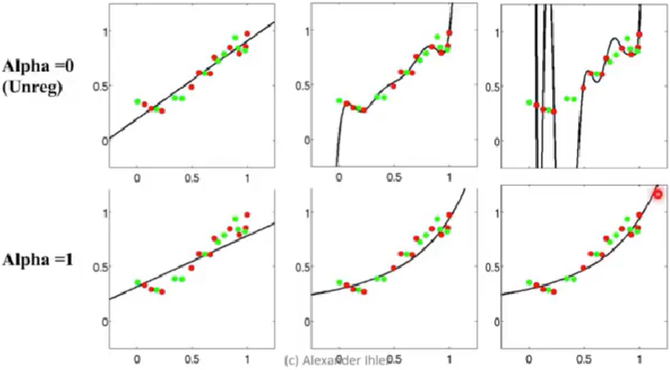
Questions:

- How can we choose p? ($\mathcal{H}$ definition)
- How can we choose w's? ($\mathcal{H}$ search)

Example: Polynomial Regression

- Given a p, the problem becomes:
- $[\mathbf{X}]_i = [1, x_i, x_i^2, \ldots, x_i^p]$ (i-th row of the matrix $\mathbf{X}$)
- $[\mathbf{y}]_i = y_i$ (i-th row of the vector $\mathbf{y}$)
- TRAIN: Solve $\min_{\mathbf{w}} \frac{1}{n}||\mathbf{y} - \mathbf{X}\mathbf{w}||^2 + \alpha||\mathbf{w}||^2$ by using the *ridge regression* method:
- $\mathbf{w} = (\mathbf{X}^\top \mathbf{X} + \alpha \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$

The effect of α

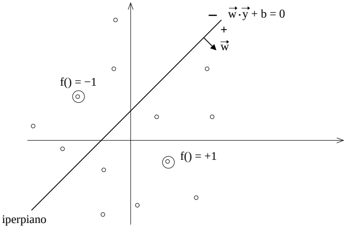


(c) Alexander Ihler

Hypothesis Space: Example 1

Hyperplanes in $\mathbb{R}^2$

- Instance space: points in the plane $\mathcal{X} = \{y | y \in \mathbb{R}^2\}$
- Hypothesis space: dichotomies induced by hyperplanes in $\mathbb{R}^2$, that is $\mathcal{H} = \{f_{\mathbf{w},b}(y) = \text{sign}(\mathbf{w} \cdot y + b), \mathbf{w} \in \mathbb{R}^2, b \in \mathbb{R}\}$

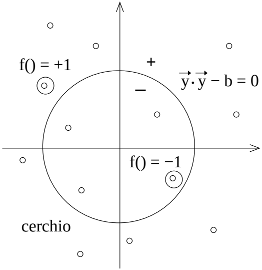


What changes in $\mathbb{R}^n$?

Hypothesis Space: Example 2

Circles in $\mathbb{R}^2$

- Instance space: points in the plane $\mathcal{X} = \{y | y \in \mathbb{R}^2\}$
- Hypothesis space: dichotomies induced by circles centered at the origin in $\mathbb{R}^2$, that is $\mathcal{H} = \{f_b(y) = \text{sign}(||y||^2 - b), b \in \mathbb{R}\}$

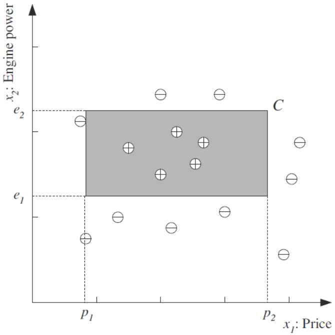


What changes in $\mathbb{R}^n$?

Hypothesis Space: Example 3

Rectangles in $\mathbb{R}^2$

- Instance space: points in the plane $\mathcal{X} = \{(p, e) | (p, e) \in \mathbb{R}^2\}$
- Hypothesis space: dichotomies induced by rectangles in $\mathbb{R}^2$, that is $\mathcal{H} = \{f_\theta(y) = [p_1 \leq p \leq p_2 \cap e_1 \leq e \leq e_2], \theta = \{p_1, p_2, e_1, e_2\}\}$ where $[z] = +1$ if $z =$ True, -1 otherwise.



What changes in $\mathbb{R}^n$

Hypothesis Space: Example 4

Conjunction of m positive literals

- Instance space: strings of m bits, $\mathcal{X} = \{s | s \in \{0,1\}^m\}$
- Hypothesis space: all the logic sentences involving positive literals $l_1, \ldots, l_m$ (l_1 is true if the first bit is 1, l_2 is true if the second bit is 1, etc.) and just containing the operator $\wedge$ (**and**)

$$\mathcal{H} = \{f_{\{i_1,\ldots,i_j\}}(s) | f_{\{i_1,\ldots,i_j\}}(s) \equiv l_{i_1} \wedge l_{i_2} \wedge \cdots \wedge l_{i_j}, \{i_1, \ldots, i_j\} \subseteq \{1, \ldots, m\}\}$$

E.g. $m = 3$, $X = \{0,1\}^3$
Examples of instances: $s_1 = 101$, $s_2 = 001$, $s_3 = 100$, $s_4 = 111$
Examples of hypotheses: $h_1 \equiv l_2$, $h_2 \equiv l_1 \wedge l_2$, $h_3 \equiv true$, $h_4 \equiv l_1 \wedge l_3$, $h_5 \equiv l_1 \wedge l_2 \wedge l_3$
h_1, h_2, and h_5 are false for s_1, s_2 and s_3 and true for s_4; h_3 is true for any instance; h_4 is true for s_1 and s_4 but false for s_2 and s_3

Hypothesis Space: Example 4

Conjunction of m positive literals

- Question 1: how many and which are the distinct hypotheses for $m = 3$?
  - Ans.(which): true, l_1, l_2, l_3, $l_1 \wedge l_2$, $l_1 \wedge l_3$, $l_2 \wedge l_3$, $l_1 \wedge l_2 \wedge l_3$
  - Ans.(how many): 8
- Question 2: how many distinct hypotheses there are as a function of m?
  - Ans.: 2^m, in fact for each possible bit of the input string the corresponding literal may occur or not in the logic formula, so:

$$\underbrace{2 \cdot 2 \cdot 2 \cdots 2}_{m \text{ times}} = 2^m$$

Recap

Notions

- Target function: deterministic vs. stochastic
- Training/empirical error
- Test error vs. ideal error
- Inductive Bias implementation

Exercises

- Think about some possible binary classification, multi-class classification and regression tasks. What hypothesis spaces can be considered?
- Implement polynomial regression using the Ridge Regression method available in scikit-learn, see `sklearn.linear_model.Ridge()` and look at the behavior of the solution when changing the parameter α