Heuristics for Combinatorial Optimization

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Exact and heuristic methods

- **Exact methods**: devised to provide a provably optimal solution
- **Heuristic methods**: provides "good" solution with *no optimality guarantee*
- Try to devise an exact approach, first!
  - search for an efficient algorithm (e.g. shortest path-like problem)
  - MILP model + MILP solver
  - exploit some special property
  - suitable (re)formulation of the problem
  - search for (scientific) literature
  - ...
- ... otherwise, heuristics! (*eurìskein = to find*)
  - example: optimal transportation-network configuration ("hard" congestion models)
  - limited available time

When do we use heuristics?

- Sometime cannot be used, since an optimal solution is mandatory!
- NP-hard problem $\not\Rightarrow$ heuristics! (e.g., MILP solver are now able to solve some of them!)
- Use of heuristic to provide a "good" solution in a "reasonable" amount of time. Some appropriate cases:
  - limited amount of time to provide a solution (running time)
  - limited amount of time or resources to develop a solution algorithm
  - just estimates of the problem parameters are available
  - quick scenario evaluation in interactive Decision Support Systems
  - *real time* system

One (among many) possible classification

Specific heuristics

- exploits special features of the problem at hand
- may encode the current "manual" solution, good practice
- may be "the first reasonable algorithm come to our mind"

General heuristic approaches

- constructive heuristics
- meta-heuristics (algorithmic schemes)
- approximation algorithms
- iper-heuristics
- ...

C. Blum and A. Roli, "Metaheuristics in Combinatorial Optimization: Overview and Conceptual Comparison", ACM Computer Surveys 35:3, 2003 (p. 268-308)

K. S orensen, "Metaheuristics – the metaphor exposed", International Transactions in Operational Research (22), 2015 (p. 3-18)

Constructive heuristics

- Build a solution incrementally selecting a subset of alternatives
- Expansion criterion (no backtracking)

Greedy algorithms (strictly local optimality in the expansion criterion)

Initialize solution S;
While (there are choice to make)
add to S the *most convenient* element [1]

- Widespread use: simulate practice; simple implementation; small running times ($\sim$ linear); embedded as sub-procedure (e.g. in B&B)
- Sorting elements by **Dispatching rules**: static or dynamic scores
- Randomization (randomized scores, random among the best n etc.)
- Primal / dual heuristics

[1] Taking feasibility constraints into account, e.g., by excluding elements that make the solution unfeasible

Example: greedy algorithm KP/0-1

Item j with w_j and p_j; capacity W; select items maximizing profit!

1. Sort object according to ascending $\frac{p_j}{w_j}$.
2. Initialize: $S := \emptyset$, $\bar{W} := W$, $z := 0$
3. **for** $j = 1, \ldots, n$ **do**
4.   **if** $(w_j \leq \bar{W})$ **then**
5. $S := S \cup \{j\}$, $\bar{W} := \bar{W} - w_j$, $z := z + p_j$.
6.   **endif**
7. **endfor**

- Static dispatching rule

Example: Greedy algorithm for the Set Covering Problem

SCP: given set M and $\mathcal{M} \subset 2^M$, c_j, $j \in \mathcal{M}$;
select a min cost combination of subsets in $\mathcal{M}$ whose union is M

1. Initialize: $S := \emptyset$, $\bar{M} := \emptyset$, $z := 0$
2. if $\bar{M} = M$ ($\Leftrightarrow$ all elements are covered), STOP;
3. compute the set $j \notin S$ minimizing the ratio $\dfrac{c_j}{\sum_{i \in M \setminus \bar{M}} a_{ij}}$;
4. set $S := S \cup \{j\}$, $\bar{M} := \bar{M} \cup \{i : a_{ij} = 1\}$, $z := z + c_j$ and go to 2.

- Dynamic dispatching rule

Algorithms embedding exact methods: an example (SCP)

$$\min \sum_{j \in \mathcal{M}} c_j x_j$$

$$s.t. \sum_{j \in \mathcal{M}} a_{ij} x_j \geq 1 \quad \forall\, i \in M$$

$$x_j \in \{0,1\} \quad \forall\, j \in \mathcal{M}$$

1. Initialize: $S := \emptyset$, $\bar{M} := \emptyset$, $z := 0$
2. se $\bar{M} = M$ ($\Leftrightarrow$ tall elements are covered), STOP;
3. solve *linear programming relaxation* of SCP (with $x_j = 1$ ($j \in S$), and let x^* be the corresponding optimal solution;
4. let $j = \arg\max_{j \notin S} x_j^*$;
5. set $S := S \cup \{j\}$, $\bar{M} := \bar{M} \cup \{i : a_{ij} = 1\}$, $z := z + c_j$ and go to 2.

Algorithms embedding exact solution methods: in general

- Expansion criterion based on solving a sub-problem to optimality (once or at each expansion)
- Example: best (locally optimal!) element to add by MILP;
- Example: locally good element to add by LP relaxation of MILP;
- normally longer running times but better final solution
- "Less greedy": solving the sub-problem involves all (remaining) decisions variables (global optimality)

Simplifying exact procedures: some examples

- Run Cplex on a MILP model for a limited amount of time
- simplify an enumeration scheme (select only a limited subset of alternatives)

  Beam search
- partial breath-first visit ot the enumeration tree

  compute a score for each node (likelihood it leads to an optimal leave)

  at each level select the k best-score nodes and branch them
- let: n levels, b branches per node, k beam size

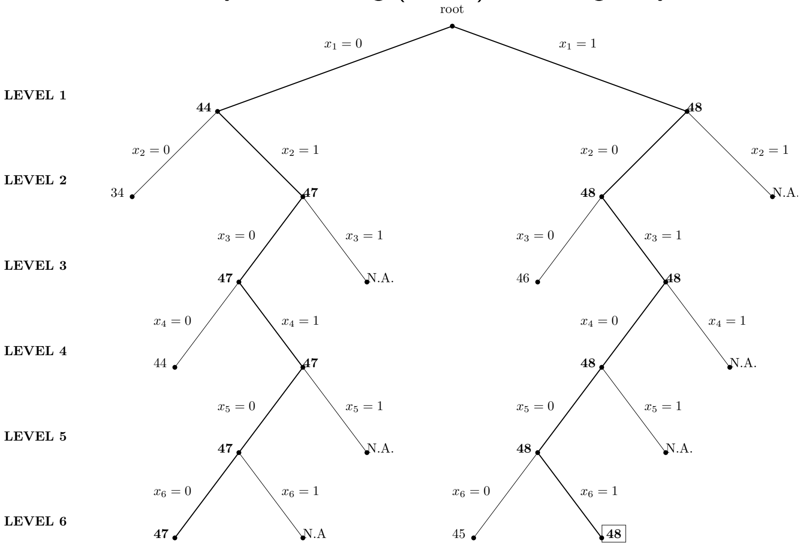
  $n \cdot k$ nodes in the final tree

  $n \cdot b \cdot k$ score evaluations

  calibrate k so that specific time limits are met
- variant (with some backtrack): recovery beam search

Beam search for KP-0/1

$n = 6$ items; binary branchining ($b = 2$); $k = 2$; greedy evaluation of nodes



Neighbourhood Search and Local Search

Neghbourhood of a solution $s \in X$ is $N : s \to N(s)$, $N(s) \subseteq X$

Basic LS scheme:

1. Determine an initial solution x;
2. **while** $(\exists\, x' \in N(x) : f(x') < f(x))$ **do** $\{$
3. $\quad x := x'$
4. $\}$
5. **return**(x) (x is a **local optimum***)

***Notice:** "combinatorial convexity" depends on x **and** on $N(x)$

LS components

- a method to find an **initial solution**;
- a **solution representation**, which is the base for the following elements;
- the application that, starting from a solution, generates the **neighbourhood** (moves);
- the function that **evaluates** solutions;
- a neighbourhood **exploration strategy**.

Initial solution

- random
- from current practice
- (fast) heuristics
- randomized heuristics
- ...
- no theoretical preference: better initial solutions may lead to worst local optima
- random or randomized + multistart

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Solution representation

- **Encodes** the features of the solutions
- Very important: impact on the following design steps (related to how we imagine the solutions and the solution space to be explored!)
- Example: KP-0/1

  list of loaded items

  characteristic (binary) vector

  ordered item sequence
- **Decoding** may be needed
- Example: KP-0/1

  list and vector representation: immediate decoding

  ordered sequence: a solution is derived by loading items in the given order up to saturating the knapsack

Neighbourhood (moves)

Neighbour solutions by *moves* that perturb x (neighbourhood *centre*)

Example KP/0-1: (i) insertion; (ii) swap one in/out; (iii) ...

- **Neighbourhood size**: number of neighbour solutions
- **Evaluation complexity**: should be quick! possibly incremental evaluation
- **Neighbourhood complexity**: time to explore (evaluate) all the neighbour solutions of a the current one (efficiency!)
- **Neighbourhood strength**: ability to produce good local optima (notice: local optima depend also on the neighbourhood definition)

  little perturbations, small size, fast evaluation, less strong .vs. large perturbation, large size, slow evaluation, larger improving power
- **Connection** feature is desirable

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Neighbourhood: KP/0-1 example

- Insertion neighbourhood has $O(n)$ size; Swap neigh. has $O(n^2)$ size
- A stronger neigh. by allowing also double-swap moves, size $O(n^4)$
- An insertion or a swap move can be incrementally evaluated in $O(1)$
- Overall neigh. complexity: insertion $O(n)$, swap $O(n^2)$
- Insertion neigh. or Swap neigh. are not connected.
  Insertion+removing neigh. is connected

Neighbourhood definition: solution representation is important!

- Insertion, swapping, removing moves are based on list or vector representation!
- Difficult to implement (and imagine) them on the ordered-sequence representation
- For the ordered-sequence representation, moves that perturb the order are more natural. e.g.swapping position:
  - from $1-2-3-4-5-6-7$ to $1-6-3-4-5-2-7$ (swap 2 and 6) or $5-2-3-4-1-6-7$ (swap 1 and 5)
  - size is $O(n^2)$, connected (with respect to maximal solutions)
  - neigh. evaluation in $O(n)$ (no fully-incremental evaluation)
  - overall complexity $O(n^3)$

Solution evaluation function

- Evaluation is used to compare neighbours to each other and select the best one
- Normally, the objective function
- May include some extra-feature (e.g. weighted sum)
- May include penalty terms (e.g. infeasibility level)
  - In KP/0-1, let X be the subset of loaded items
  - $\tilde{f}(X) = \alpha \sum_{i \in X} p_i - \beta \max\left\{0, \sum_{i \in X} w_i - W\right\} \qquad (\alpha, \beta > 0)$
  - activate "removing" move in a connected "insertion+removing" neighbourhood

Exploration strategies

Which improving neighbour solution to select?

- **Stepest descent** strategy: the best neighbour (all evaluated!)
- **First improvement** strategy: the first improving neighbour. Sorting matters! (heuristic, random)

Possible variants:

- **random** choice among the best k neighbours
- **store** interesting second-best neighbours and use them as recovery starting points for LS

Sample application to TSP

- First question: is LS justified? Exact approaches exists, not suitable for large instances and small running times. Notice that TSP is NP-Hard
- Notation and assumptions:

  $G = (V, A)$ (undirected)

  G is complete

  $|V| = n$

  cost c_{ij} (may be $= c_{ji}$ in the symmetric case)

- Define all the elements of LS

LS for TSP: initial solution by Nearest Neighbour heuristic

1. select node $i_0 \in V$; $cost = 0$, $Cycle = \{i_0\}$, $i = i_0$.
2. select $j = \arg \min_{j \in V \setminus Cycle} \{c_{ij}\}$
3. set $Cycle = Cycle \cup \{j\}$; $cost = cost + c_{ij}$
4. set $i = j$
5. if still nodes to be visited, go to 2
6. $Cycle = Cycle \cup \{i_0\}$; $cost = cost + c_{ii_0}$

- $O(n^2)$ (or better): simple but not effective (too greedy, last choices are critical)
- repeat with different i_0
- randomize Step 2

LS for TSP: Nearest/Farthest Insertion

1. Choose the two nearest/farthest nodes i and j an build the initial cycle $C = i - j - i$
2. select the node $r = \arg\min_{v \in V \setminus C} / \max_{v \in V \setminus C} \{c_{vj} : j \in C\}$
3. modify C by inserting r between pairs of consecutive nodes i and j in the current cycle such that $c_{ir} + c_{rj} - c_{ij}$ is minimized
4. if still nodes to be visited, go to 2.

- $O(n^3)$: rather effective (farthest version better, more balanced cycles)
- may randomize initial pair and/or r selection

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LS for TSP: Best Insertion

1. Choose the nearest nodes i and j: $C = i - j - i$, $cost = c_{ij} + c_{ji}$
2. select the node $r = \arg\min_{i \in V \setminus C} \{c_{ir} + c_{rj} - c_{ij} : i, j \text{ consecutive in } C\}$
3. modify C by inserting r between nodes i and j minimizing $c_{ir} + c_{rj} - c_{ij}$
4. if still nodes to be visited, go to 2.

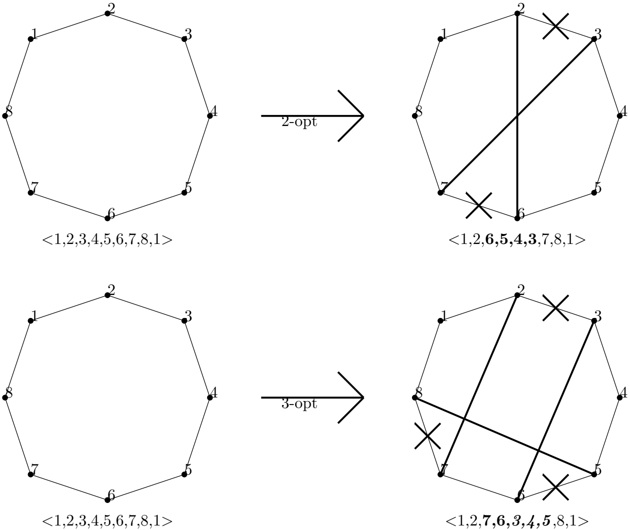
- $O(n^3)$: rather effective (lest than farthest/nearest insertion)
- may randomize initial pair and/or r selection

LS for TSP: Solution Representation

- **arc representation**: arcs in the solution, e.g. as a binary adjacency matrix
- **adjacency representation**: a vector of n elements between 1 and n (representing nodes), $v[i]$ reports the node to be visited after node i
- **path representation**: ordered sequence of the n nodes (a solution is a node permutation!)

LS for TSP: *k*-opt neighbourhoods

Concept: replace *k* arcs in with *k* arcs out [Lin and Kernighan, 1973]



LS for TSP: *k*-opt neighbourhoods

- In terms of path representation, 2-opt is a substring reversal
- Example: $< 1, 2, 3, 4, 5, 6, 7, 8, 1 > \longrightarrow < 1, 2, 6, 5, 4, 3, 7, 8, 1 >$
- 2-opt size: $\frac{(n-1)(n-2)}{2} = O(n^2)$
- k-opt size: $O(n^k)$
- Neighbour evaluation: incremental for the symmetric case, $O(1)$
- 2-opt move evaluation: reversing sequence between i and j in the sequence $< 1 \ldots h, i, \ldots, j, l, \ldots, 1 >$

$$C_{new} = C_{old} - c_{hi} - c_{jl} + c_{hj} + c_{il}$$

- which k? $k = 2$ good, $k = 3$ fair improvement, $k = 4$ little improvement

LS for TSP: evaluation function and exploration strategy

No specific reason to adopt special choices:

- Neighbours evaluated by the objective function (cost of the related cycle)
- Steepest descent (or first improvement)

Neighbourhood search and Trajectory methods

- LS trades-off simplicity/efficiency and effectiveness, but it gets stuck in local optima
- Need to escape from local optima (only convexity implies global optimality)
  - Random multistart (random initial solutions)
  - Variable neighbourhood (change neighbourhood if local optimum)
  - Randomized exploration strategy (e.g. random among best k neigh)
  - Backtrack (memory and recovery of unexplored promising neighbours)
  - ...
- *Neighbourhood search* or *Trajectory methods*: a walk trough the solution space, recording the best visited solution

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Avoiding loops

- A walk escaping local optima may worsen the current solution and fall into loops
- In order to avoid loops:

- (only improving solutions are accepted = LS)
- randomized exploration
  - alternative random ways
  - does not exploit information on the problem (structure)
  - e.g. Simulated Annealing
- memory of visited solutions
  - store visited solution and do not accept them
  - structure can be exploited
  - e.g. Tabu Search

- Notice. Visiting a same solution is allowed: we just need to avoid choosing the same neighbour

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Simulated Annealing [Kirkpatrick, 1983]

- Metaphore: annealing process of glass, metal. Alternate warming/cooling to obtain "optimal" molecular structure
- (One possible) search scheme:

Determine an initial solution x
intialize: best solution $x^* \leftarrow x$ and iteration $k = 0$
repeat
  $k \leftarrow k + 1$
  generate a (random) neighbour y
  if y is better **than** x^*, then $x^* \leftarrow y$
  $Loss = \min\{0, f(y) - f(x)\}$ (minimization problems)[2]
  compute $p = exp\left(-\frac{Loss}{T(k)}\right)$
  accept y *with* **probability** p
  if accepted, $x \leftarrow y$
until (no further neighbours of x, or max trials)
return x^*

[2] $Loss = \min\{0, f(x) - f(y)\}$ (maximization problems)

SA: cooling schedule

- Parameter $T(k)$: temperature, *cooling schedule*
- $T(\mathit{first}) > T(\mathit{last})$: the probability of accepting not improving solutions is decreasing over time
- Example of cooling schedule:

- initial T (maximum)
- number of iterations at constant T
- T decrement
- minimum T

+ (one of) the first NS metaphors
+ provably converges to the global optimum (under strong assumptions)
+ simple to implement

— there are better (on-the-field) NS metaheuristics!

Tabu Search [Fred Glover, 1989]

- **Memory** is used to avoid cycling: store *information on visited solutions* (allows exploiting structure of the problem)
- Basic idea: store visited solutions and **exclude them (= make tabu)** from neighbourhoods
- Implementation by storing **Tabu List** of the **last** t **solutions**

$$T(k) := \{x^{k-1}, x^{k-2}, \ldots, x^{k-t}\}$$

  at iteration k, avoid cycles of length $\leq t$
- t is a parameter to be calibrated
- From $N(x)$ to $N(x, k)$

Storing "information" instead of solutions

- Tabu List (may) store *information* on the last t solutions
- E.g., often *moves* are stored instead of solutions because of
  - *efficiency* (checking equality between full solutions may take long time and slow down the search)
  - *storage* capacity (storing full solution information may take large memory)
- Example: TSP, 2-opt. TL stores the last t pairs of arcs added (to avoid arcs or involved nodes)
- Notice. Visiting a same solution is allowed: we just need to avoid choosing the same neighbour (recall $N(x,k) \neq N(x,l)$)
- t (tabu tenior) has to be calibrated:
  - too small: TS may cycle
  - too large: too many tabu neighbours

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Aspiration criteria

- By storing “information”, unvisited solutions may be declared as tabu
- If a tabu neighbour solution satisfies one or more **aspiration criteria**, tabu list is *overruled*
- Aspiration criterion: a solution is “interesting”, e.g. the solution is the best found so far (not visited before!)

Stopping criteria

- (A solution is found satisfying an optimality certificate, if available...)
- Maximum number of iterations, or time limit
- Maximum number of NOT IMPROVING iterations
- Empty neighbourhood and no overruling
  - perhaps t is too long
  - perhaps visit non-feasible solutions (e.g. COP with many constraints): modifying the evaluation function, alternate dual and primal search

TS basic scheme

Determine an **initial** solution x; $k := 0$, $T(k) = \emptyset$, $x^* = x$;

repeat

let $y = \arg\text{best}\big(\{\tilde{f}(y), y \in N(x,k)\} \cup$
$\{y \in N(x) \setminus N(x,k) \mid y$ satisfies aspiration$\}\big)$

compute $T(k+1)$ from $T(k)$ by inserting y (or move $x \mapsto y$, or information) and, if $|T(k)| \geq t$, removing the elder solution (or move or information)

if $f(y)$ improves $f(x^*)$, let $x^* := y$;

$x = y$, $k{+}{+}$

until (stopping criteria)

return (x^*).

Same basic elements as LS (+ tabu list, aspiration, stop)

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Intensification and diversification phases

- **Intensification** explores more solutions in a small portion of the solution space: solutions with similar features
- **Diversification** moves the search towards unexplored regions of the search space: solutions with different features
- the basic TS scheme may be improved by **alternating** intensification and diversification, to find and exploit new promising regions and, hence, new (and possibly better) local optima
- **memory** may play a role (store information on visited solutions, e.g. to allow avoiding the same features during diversification)

Intesification and diversification can be applied to **any** metaheuristics (not only to TS)

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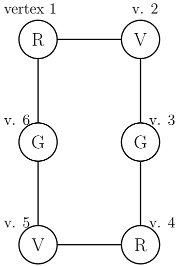
Intensification

- enumerate (implicitly) all the solutions in a (small) region where good solutions have been found (e.g. fix some variables in a MILP model and run a solver)
- use a more detailed neighbourhood (e.g. allowing many possible moves)
- relax aspiration criteria
- modify evaluation function to penalize far away solutions

Diversification

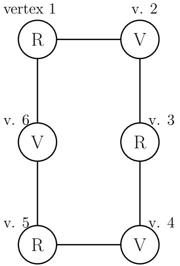
- use "larger" neighbourhoods (e.g. k-opt $\rightarrow$ $(k+1)$-opt in TSP, until a better solution is found)
  - if more neighbourhoods are used, they rely on independent tabu lists
- modify the evaluation function to promote far away solutions
- use the last local minimum to build a far-away ("complementary") solution to start a new intensification
- use a long term memory to store the "more visited" features and penalize them in the evaluation function
  - as a quick-and-dirty approximation, use a dynamic tabu list length t: t is short during intensification and long during diversification (we may start with small $t = t_0$ and increment it as long as we do not find improving solutions, until a maximum t is reached or an improvement resets $t = t_0$ for a new intensification)

Example: Tabu Search for Graph Coloring



1	2	3	4	5	6
R	V	G	R	V	G

$f = 3$



1	2	3	4	5	6
R	V	R	V	R	V

$f = 2$

- move: change the color of one node at a time (no new color). 12 neighbours: VVGRVG, GVGRVG, RRGRVG, RGGRVG, RVRRVG etc. **none feasible!**
- objective function to evaluate: little variations (**plateau!**)

$\tilde{f}$ that penalizes non-feasibilities, includes (weighted sum) other features, **but ...**

Too many constraints: change perspective!

Given a k-coloring, search for a $k-1$-coloring

- Initial solution: delete *one* color by changing it in *one* of the others
- Evaluation $\tilde{f}$: number of *monochromatic edges* (minimize non-feasibilities)
- Move: as before, change the color of one vertex
- **Granular TS**: consider only nodes belonging to monochromatic edges
- Tabu list: last t pairs (v, r) (vertx v kept color r)

- if $\tilde{f} = 0$, new feasible solution with $k-1$ colors: set $k = k-1$ and start again!

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Population based heuristics

At each iteration

- a set[3] of solutions (**population**) is maintained
- some solutions are recombined[4] to obtain new solutions (among which a better one, hopefully)

Several paradigms (often just the metaphor changes!)

- Evolutionary Computation (Genetic algorithms)
- Scatter Search and path relinking
- Ant Colony Optmization
- Swarm Optmization
- etc.

General purpose (soft computing) and easy to implement (more than effective!)

[3] In trajectory/based metaheuristics, a single

[4] In trajectory/based metaheuristics, perturbation, move

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Genetic Algorithms [Hollande, 1975]

Survival of the fittest (evolution)	⇜⇝	Optimization
Individual	⇜⇝	Solution
Fitness	⇜⇝	Objective function

Encode solutions *of the specific problem*.

Create an initial set of solutions (*initial population**).

Repeat

- *Select** pairs (or groups) of solutions (parent).
- *Recombine** parents to generate new solutions (offspring).
- Evaluate the *fitness** of the new solutions
- *Replace** the population, using the new solutions.

Until (*stopping criterion*)

Return the best generated solution.

*** Genetic Operators**

Encoding: *chromosome*, sequence of *genes*

- KP 0/1: binary vector, n genes $= 0 \ / \ 1$

1	0	0	1	1	0	0	0	1	0

- TSP: path representation: n genes $=$ cities

3	2	6	1	8	0	4	7	1	5

- Normally, each gene is related to one of the decision variables of the Combinatorial Optimization Problem (COP)

- Encoding is important and affect following design steps (like solution representation in neighbourhood search)

- **Decoding** to transform a chromosome (or individual) into a solution of the COP (in the cases above it is straightforward)

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Encoding: *chromosome*, sequence of *genes*

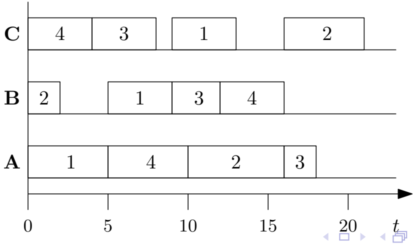
- Job shop scheduling: $n * m$ genes = jobs (decoding!!!)

Job	machine , t_{ij}		
1	A , 5	B , 4	C , 4
2	B , 2	A , 6	C , 5
3	C , 4	B , 2	A , 2
4	C , 4	A , 5	B , 4

Encoding:

4	2	1	1	3	4	2	3	1	2	3	4

Decoding:



Genetic operators

- **Initial population**: random + *some* heuristic/local search
  - random $\rightarrow$ diversification (very important!!!)
  - heuristic (randomized) $\rightarrow$ faster convergence (not too many heuristic solutions, otherwise fast convergence to local optimum)
- **Fitness**: (variants of the) objective function (see Neighbourhood Search)

Genetic operators: Selection

- **Selection**: larger fitness $\rightsquigarrow$ larger *probability* to be selected
- Notice: even worse individual should be selected with small probability to (*avoid premature convergence!*): they may contain good features (genes), even if their overall fitness is poor
- Mode 1: select one t-uple of individuals to be combined at a time
- Mode 2: select a subset of individuals to form a *mating pool*, and combine all the individual in the mating pool.

Genetic operators: Selection schemes

- p_i: probability of selecting individual i; f_i: fitness of i

In general, compute p_i such that the higher f_i, the higher p_i

- **Montecarlo**: p_i is proportional to f_i

  $p_i = f_i \,/\, \sum_{k=1}^{N} f_k$ f_i: fitness of i

  Super-individuals may be selected too often
- **Linear ranking**: sort individual by increasing fitness and σ_i is the position of i, set $p_i = \dfrac{2\sigma_i}{N(N+1)}$
- *n*-**tournament**: select a small subset of individuals uniformly in the population, then select the best individual in the subset

Genetic operators: recombination [crossover]

- From $n \geq 1$ *parents*, obtain *m offspring* **different but similar**
- offspring inherits genes (features) from one of the parents at random

- Uniform (probability normally depends on the parent fitness)

1	0	0	1	1	0	0	0	1	0	parent 1 (fitness 8)
0	0	1	0	1	0	1	1	0	1	parent 2 (fitness 5)
1	0	0	0	1	0	0	1	0	0	offspring

- *k*-cut-point: "adjacent genes represents correlated features"

cut point (between genes 3 and 4) — cut point (between genes 8 and 9)

*	*	*	*	*	*	*	*	*	*	parent 1
+	+	+	+	+	+	+	+	+	+	parent 2
*	*	*	+	+	+	+	+	*	*	offspring 1
+	+	+	*	*	*	*	*	+	+	offspring 2

Mutation

After or during crossover, some genes are randomly changed

- Against *genetic drift*: **one** gene takes the same value in all the individuals of the population (loss of genetic diversity)
- Effects and side effects (sometimes we want them!):
  - (re)introduce genetic diversity
  - slow population convergence (normally we change very few genes with very small probability)
  - can be used to obtain diversification (more genes with more probability: simple way to diversify, not the best one)

Integrating Local Search

Local search may be used to improve offspring (simulate children education)

- Replace an individual with the related local minimum
- May lead to premature convergence
- Efficiency may degrade!
  - simple, fast LS
  - apply to a selected subset of individuals
  - more sophisticated NS only at the end, as post-optimization

Crossover, mutation and non-fesible offspring

Crossover/mutation operators may generate unfeasible offspring. We can:

- Reject unfeasible offspring
- Penalize (modified fitness)
- Repair (during the decoding)
- Design specific operators guaranteeing feasibility. E.g. for *TSP*:
  - **Order crossover** (similar, since reciprocal order is maintained)

1	4	9	2	6	8	3	0	5	7	parent 1
0	2	1	5	3	9	4	7	6	8	parent 2
1	4	9	2	3	6	8	0	5	7	offspring 1
0	2	1	4	9	3	5	7	6	8	offspring 2

  - Mutation by substring reversal (= 2-opt)

1	4	**9**	2	6	**8**	3	0	5	7
⟶			⟵					⟶	
1	4	**8**	6	2	**9**	3	0	5	7

Generational Replacement

Generational replacement: old individuals are replaced by offspring

- **Steady state**: a few individuals (likely the *worst* ones) are replaced
- **Elitism**: a few individuals (likely the *best* ones) are kept
- **Best individuals**: generate R new individuals from N old ones; keep the best N among the $N + R$

Population management: keep the population diversified, whilst obtaining (at least one) better and better solution

- Acceptance criteria for new individuals (e.g. fitness)
- Diversity threshold (e.g. Hamming distance)
- Variable threshold to alternate *intensification* and *diversification*

Stopping criteria

- Time limit
- Number of (not improving) iterations (=generations)
- Population convergence: all individuals are similar to each other (pathology: not well designed or calibrated)

Observations

- Advantages: general, robust, adaptability (just an encoding and a fitness function!)
- Disadvantages: many parameters! (you may save time in developing the code but spend it in calibration)
- Overstatement: *complexity comes back to the user*, that should find the optimal combination of the parameters.
  Normally, the designer should provide the user with a method able to directly find the optimal combination of decision variables. In fact, the algorithm designer should also provide the user with the **parameter calibration**!

- Genetic algorithms are in the class of *weak methods* or *soft computing* (exploit little or no knowledge of the specific problem)

Validating optimization algorithms

Some criteria:

- (Design and implementation time / cost)
- Efficiency (running times)
- Effectiveness (quality of the provided solutions)
- *Reliability*, if stochastic (every run provide a good solution)

Evaluation/validation techniques:

- **Computational experiments**. Steps
  - desing and implementation of the optimization algorithm
  - benchmark selection (real, literature, ad-hoc): "many" instances
  - parameter calibration (before -not during- test)
  - test (notice: multiple [e.g. 10] running if stochastic)
  - statistics (including reliability) and comparison with alternative
- Probabilistic analysis (more theoretical, e.g. probability of optimum)
- Worst case analysis (performance guarantee, often too pessimistic)

Parameter calibration (or estimation)

- **Pre-deployment** activity (designer should do, not the user!)
- Estimation valid for *every* instance (for evaluation purposes)
- Standard technique:
  - select an instance **sub**set (= training set)
  - extensive test on the training set
  - take **interaction** among parameters into account
  - stochastic components make the calibration harder
- Advanced techniques:
  - Black box optimization
  - Automatic estimation (e.g. *i-race* package)
  - Adaptivity

Warning: metaheuristc principles .vs. metaphores

Many (good) metaheuristics are inspired by (good) metaphores

Recent literature proposed *a true tsunami of "novel" metaheuristic methods, most of them based on a metaphor of some natural or man-made process*: the behavior of any species (bees, wasps, monkeys, apes, birds etc.), the flow of water, musicians playing together etc.

Actually, the basic principles are often not novel, but the same as for trajectory or population based methods

Good or new metaphores do not necessarily lead to good or new metaheuristics!

Golden Rule

An algorithm is good if it provides good results (validation!), and not if it is described by a suggestive metaphor. *See Sörensen, 2015*

Hybrid metaheuristics: very brief introduction!

Integration between different techniques, at different levels (components, concepts, etc.). Examples:

- population based + trajectory methods (find good regions + intensification)
- tabu search + simulated annealing
- **Matheuristics** (hot research topic, thesis avaialble!)
  - mathematical programming driven constructive heuristics
  - exact methods to find the best move in large neighbourhoods
  - heuristics to help exact methods (e.g. primal and dual bounds)
  - Rounding heuristics
  - Local branching
  - ...
- **Data driven optimization** (hot research topic, thesis avaialble!)
  - Artificial Intelligence to detect or learn promising region or search direction
  - Machine Learning to set optimization model parameters
  - ...
- ...