Combinatorial problems and Search

FIT4012 Advanced topics in computational science

This material is based on slides provided with the book 'Stochastic Local Search: Foundations and Applications' by Holger H. Hoos and Thomas Stützle (Morgan Kaufmann, 2004) - see www.sls-book.net for further information.

Overview

- Combinatorial Problems
- Computational Complexity
- Stochastic Local Search

Combinatorial Problems

Combinatorial problems arise in many areas of computer science and application domains:

- finding shortest/cheapest round trips (TSP)
- finding models of propositional formulae (SAT)
- planning, scheduling, time-tabling
- internet data packet routing
- protein structure prediction
- combinatorial auctions winner determination

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Combinatorial problems involve finding a:

- *grouping*,
- *ordering*, or
- *assignment*

of a discrete, finite set of objects that satisfies given conditions.

Candidate solutions are combinations of *solution components* that may be encountered during a solutions attempt but need not satisfy all given conditions.

Solutions are *candidate solutions* that satisfy all given conditions.

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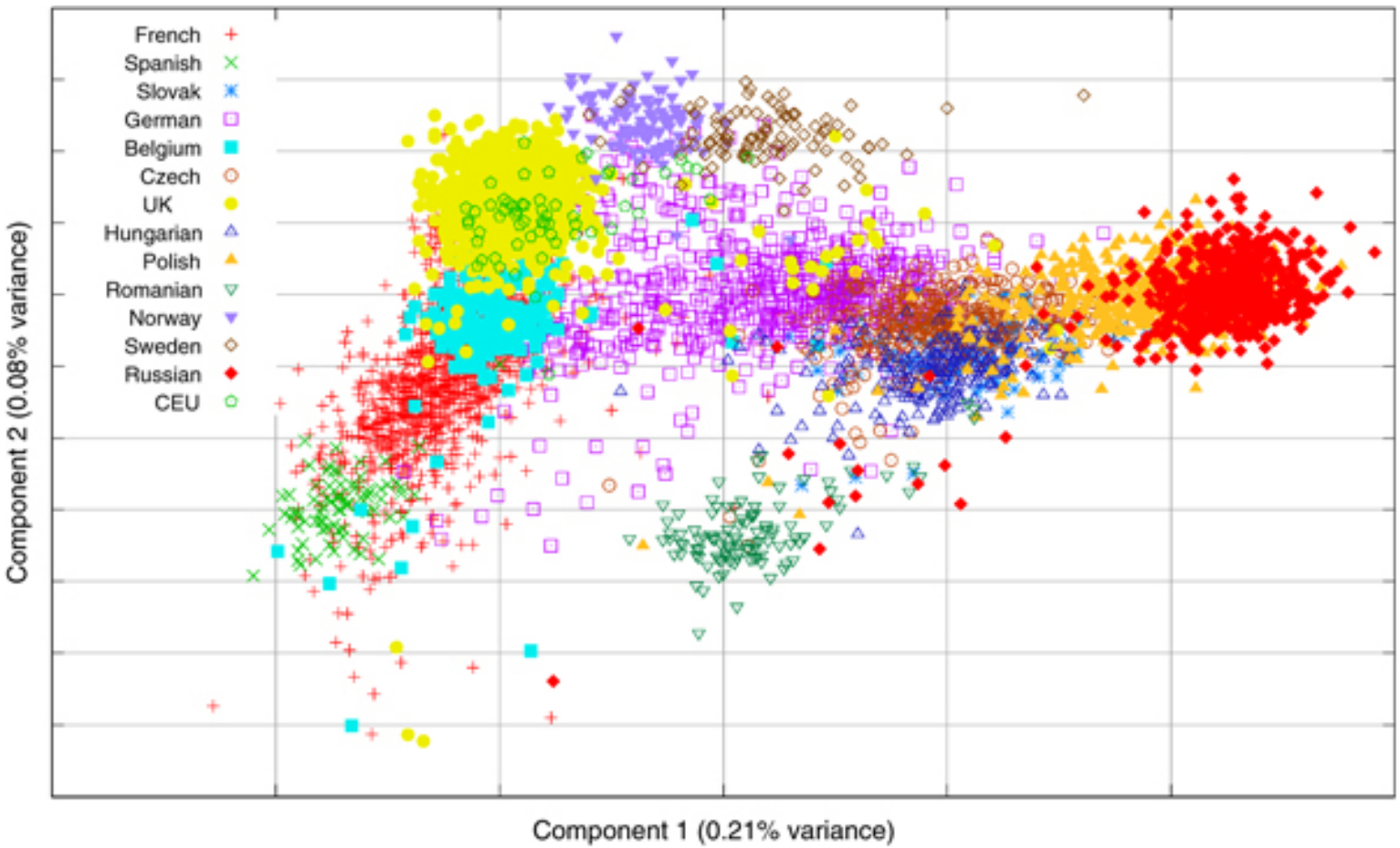
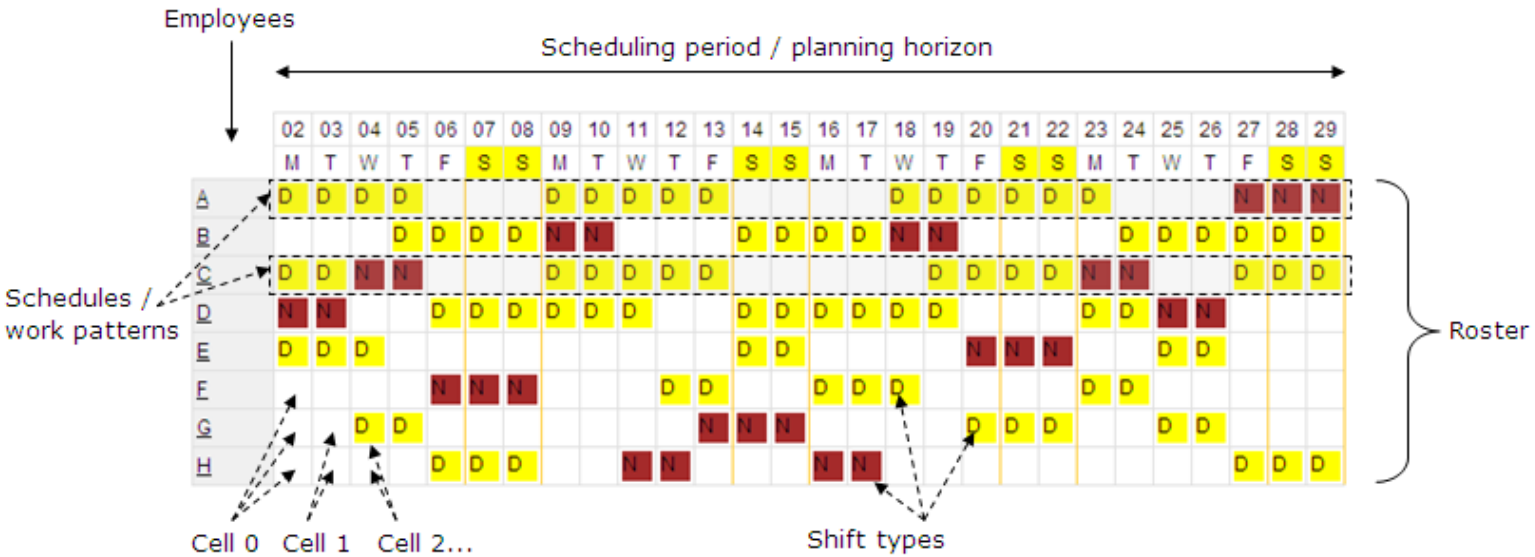
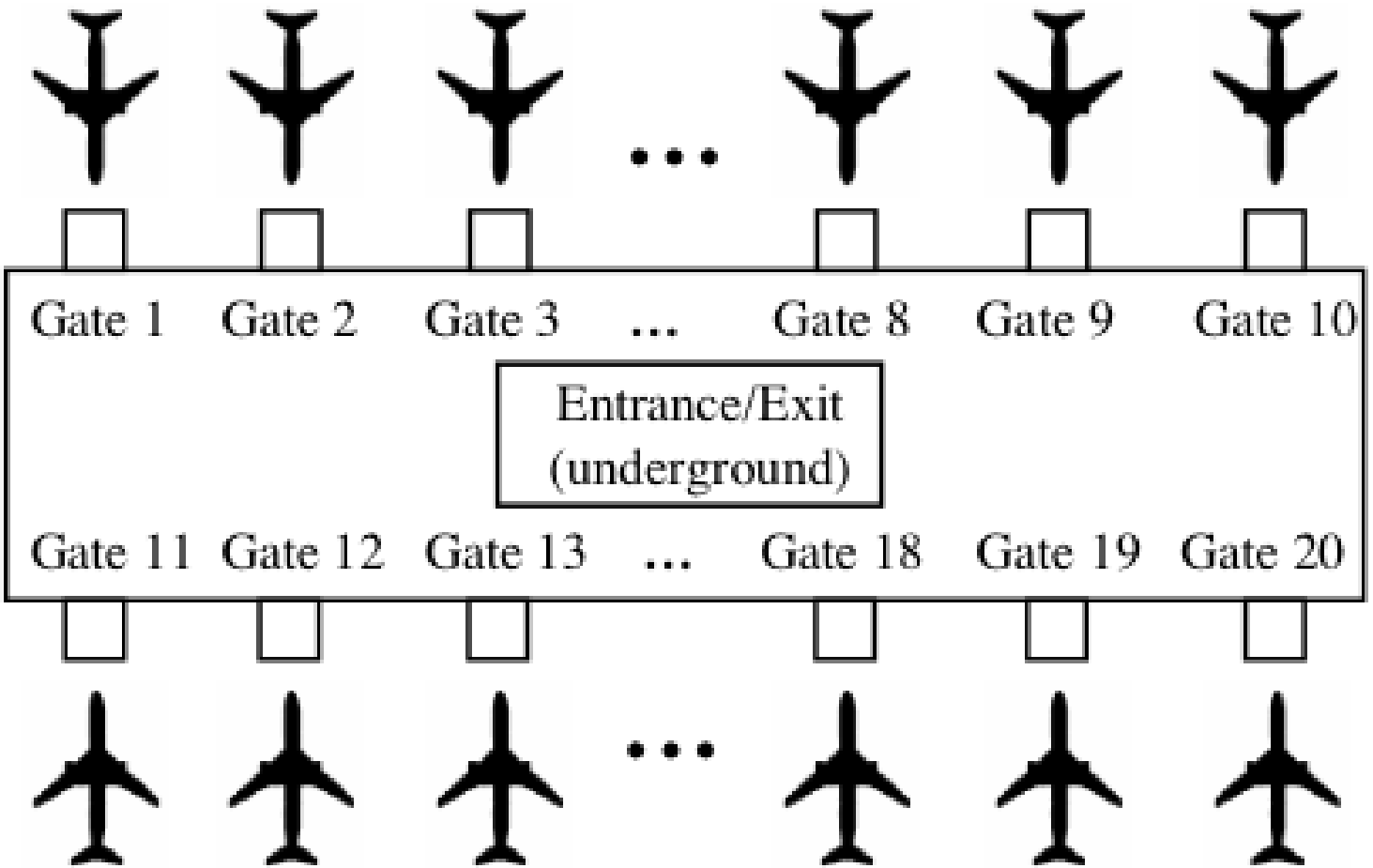
Grouping


French
Spanish
Slovak
German
Belgium
Czech
UK
Hungarian
Polish
Romanian
Norway
Sweden
Russian
CEU
Component 2 (0.08% variance)
Component 1 (0.21% variance)

Ordering


Employees
Scheduling period / planning horizon
02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
M T W T F S S M T W T F S S M T W T F S S M T W T F S S
A
B
C
D
E
F
G
H
Schedules / work patterns
Roster
Cell 0
Cell 1
Cell 2...
Shift types

Assignment


Gate 1
Gate 2
Gate 3
...
Gate 8
Gate 9
Gate 10
Entrance/Exit
(underground)
Gate 11
Gate 12
Gate 13
...
Gate 18
Gate 19
Gate 20

Example:

- *Given:* Set of points in the Euclidean plane
- *Objective:* Find the shortest round trip

- a round trip corresponds to a sequence of points (assignment of points to sequence positions)
- *solution component:* trip segment consisting of two points that are visited one directly after the other
- *candidate solution:* round trip
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Problem *vs* problem instance

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- *Problem instance:* Given *a specific* set of points P, find a shortest round trip
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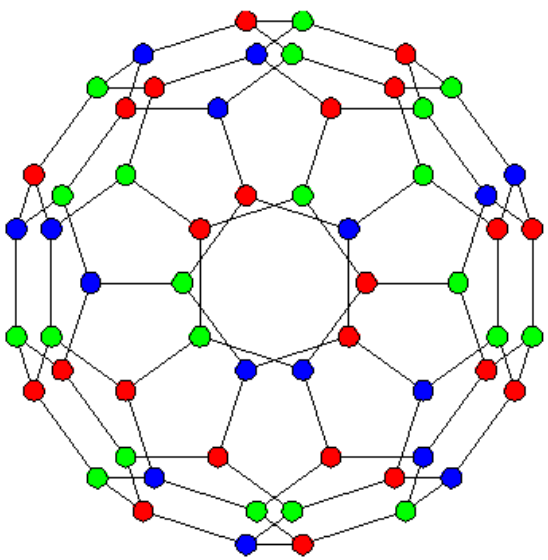
Decision problems

solutions = candidate solutions that satisfy given *logical conditions*

Example: The Graph Colouring Problem

- *Given:* Graph G and set of colours C
- *Objective:* Assign to all vertices of G a colour from C such that two vertices connected by an edge are never assigned the same colour



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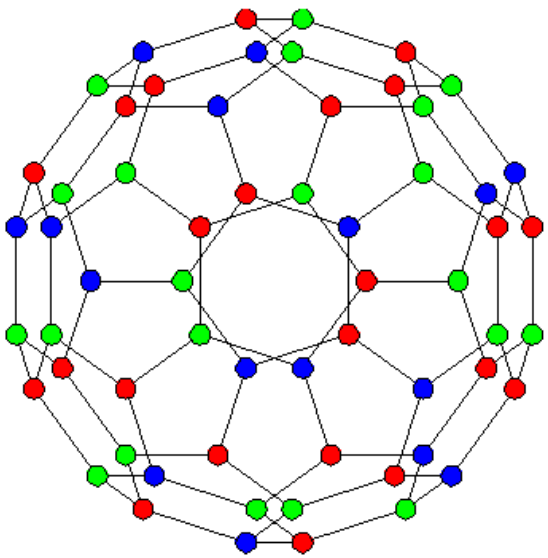

Search vs. decision variant

Every decision problem has two variants:

- *Search variant:* Find a solution for given problem instance (or determine that no solution exists)
- *Decision variant:* Determine whether solution for given problem instance exists

Search and decision variants are closely related; algorithms for one can be used for solving the other.

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Optimisation problems

- can be seen as generalisations of decision problems
- *objective function f* measures *solution quality* (often defined on all candidate solutions)
- typical goal: find solution with optimal quality
  minimisation problem: *minimal* value of f
  maximisation problem: *maximal* value of f

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Variants of optimisation problems

- *Search variant:* Find a solution with optimal objective function value for given problem instance
- *Evaluation variant:* Determine optimal objective function value for given problem instance

Every optimisation problem has associated decision problems:

Given a problem instance and a fixed solution quality bound b, find a solution with objective function value $\leq b$ (for minimisation problems) or determine that no such solution exists.

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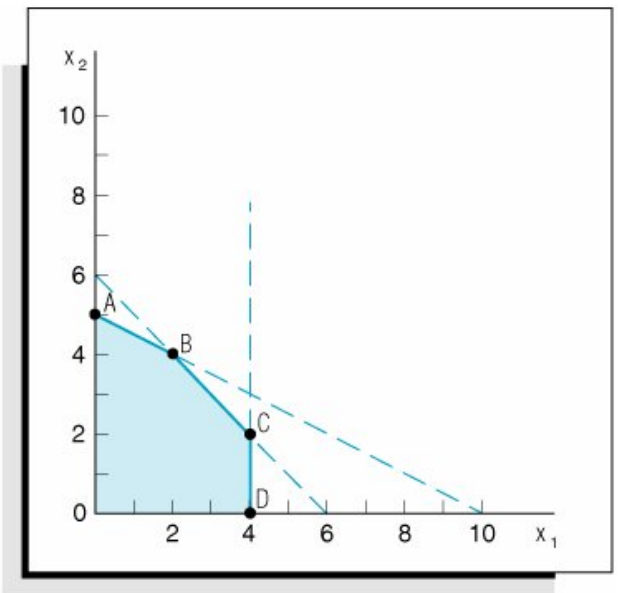
Many optimisation problems have an objective function as well as logical conditions that solutions must satisfy.

A candidate solution is called *feasible* (or *valid*) iff it satisfies the given logical conditions.

Note: Logical conditions can always be captured by an objective function such that feasible candidate solutions correspond to solutions of an associated decision problem with a specific bound.



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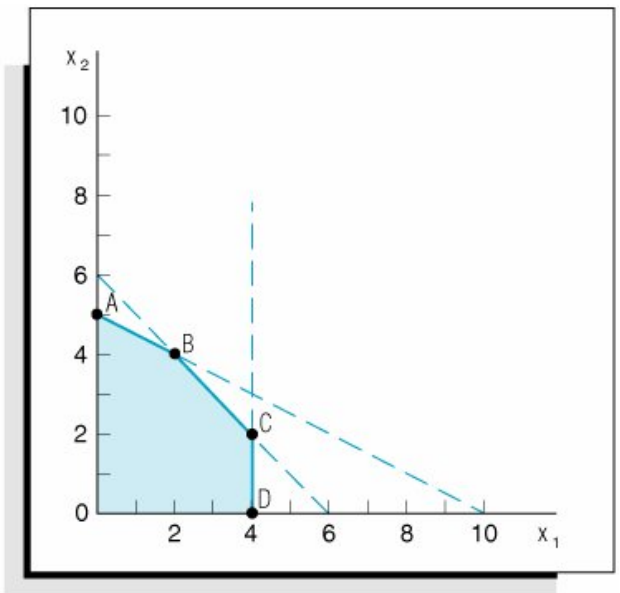

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Two Prototypical Combinatorial Problems

Studying conceptually simple problems facilitates development, analysis and presentation of algorithms

Two prominent, conceptually simple problems:

- Finding satisfying variable assignments of propositional formulae (SAT)
  – prototypical decision problem
- Finding shortest round trips in graphs (TSP)
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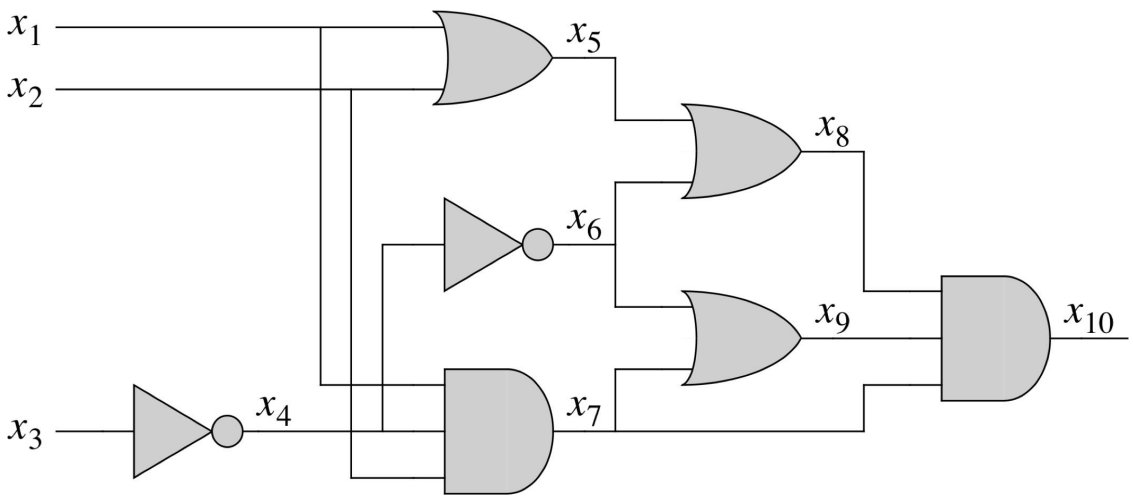
SAT: A simple example

General SAT Problem (search variant):

- *Given:* Formula F in propositional logic (e.g. $F := (x_1 \vee x_2) \wedge (\neg x_1 \vee \neg x_2)$)
- *Objective:* Find an assignment of truth values to variables in F that renders F true, or decide that no such assignment exists.



Definitions

- *Formula in propositional logic*: well-formed string that may contain
  - propositional variables $x_1, x_2, \ldots, x_n$;
  - truth values $\top$ ('true'), $\bot$ ('false');
  - operators $\neg$ ('not'), $\wedge$ ('and'), $\vee$ ('or');
  - parentheses (for operator nesting).

- *Model* (or *satisfying assignment*) of a formula F: Assignment of truth values to the variables in F under which F becomes true (under the usual interpretation of the logical operators)

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- A formula is in *conjunctive normal form (CNF)* iff it is of the form

$$\bigwedge_{i=1}^{m} \bigvee_{j=1}^{k(i)} l_{ij} = (l_{11} \vee \ldots \vee l_{1k(1)}) \ldots \wedge (l_{m1} \vee \ldots \vee l_{mk(m)})$$

  where each *literal* l_{ij} is a propositional variable or its negation. The disjunctions $(l_{i1} \vee \ldots \vee l_{ik(i)})$ are called *clauses*.

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Concise definition of SAT

- *Given:* Formula F in propositional logic.
- *Objective:* Decide whether F is satisfiable.

- In many cases, the restriction of SAT to CNF formulae is considered.
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Example:

$$
\begin{aligned}
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- F is in CNF.
- Is F satisfiable?

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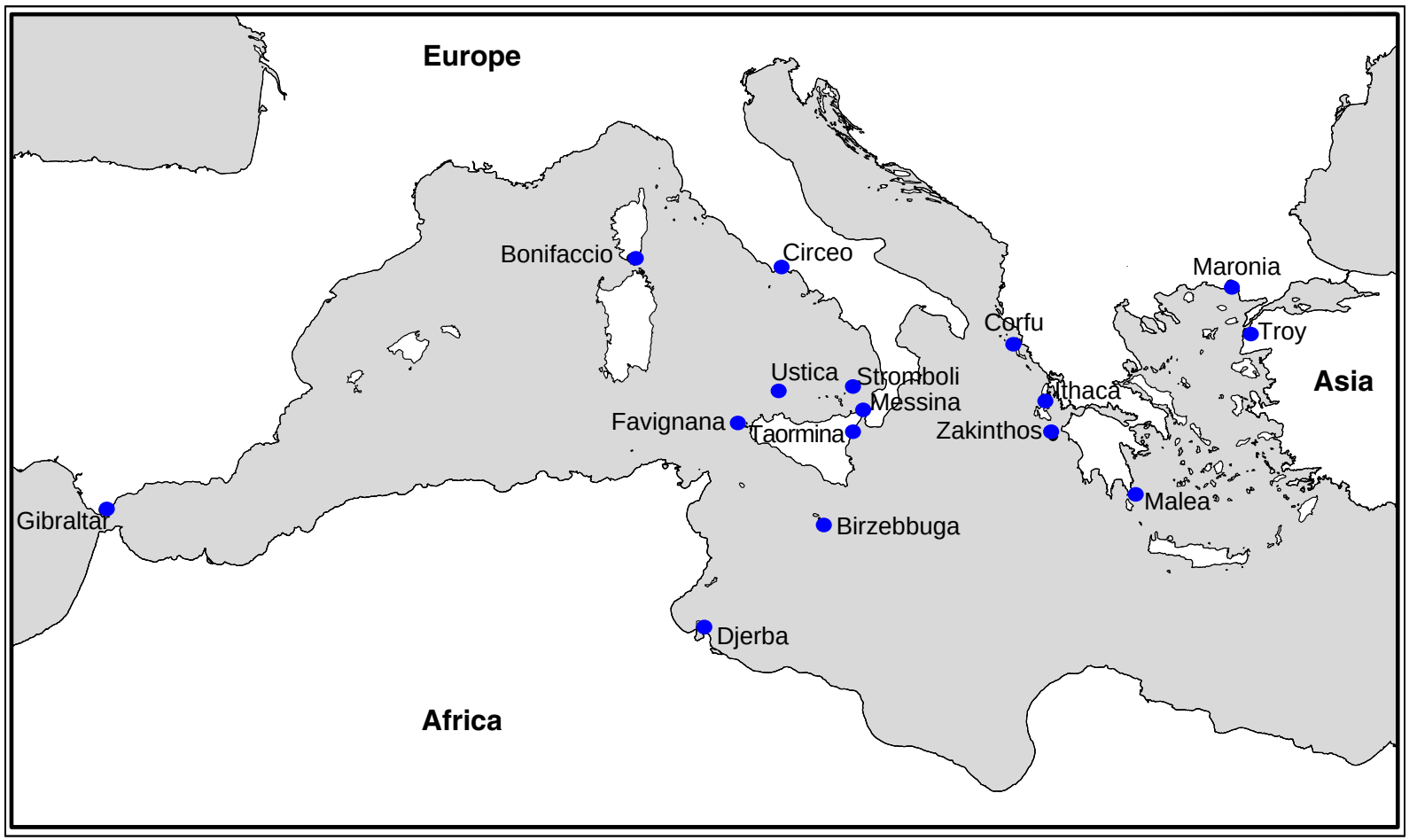
  Yes, *e.g.*, $x_1 := x_2 := \top$, $x_3 := x_4 := x_5 := \bot$ is a model of F.

TSP: A simple example



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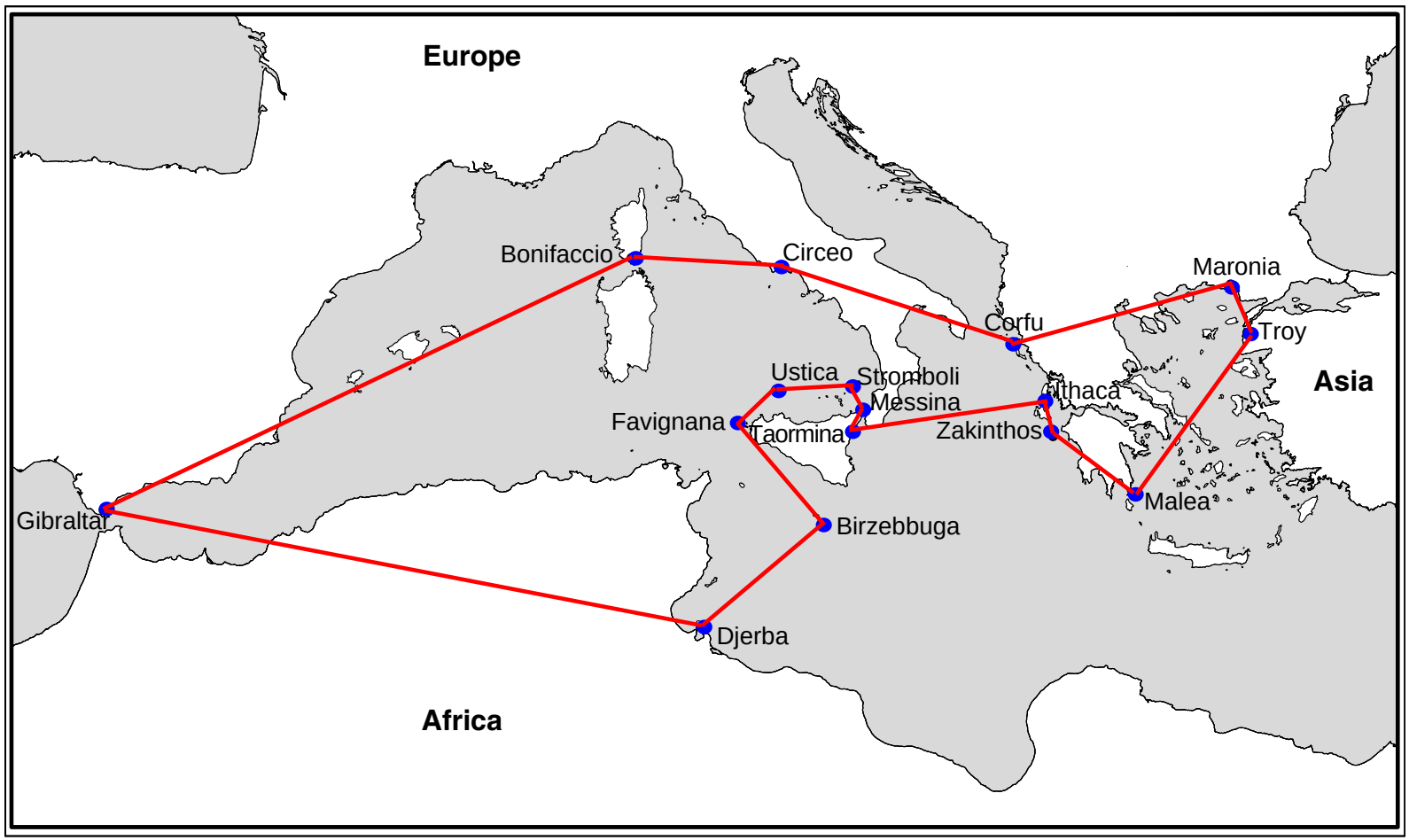

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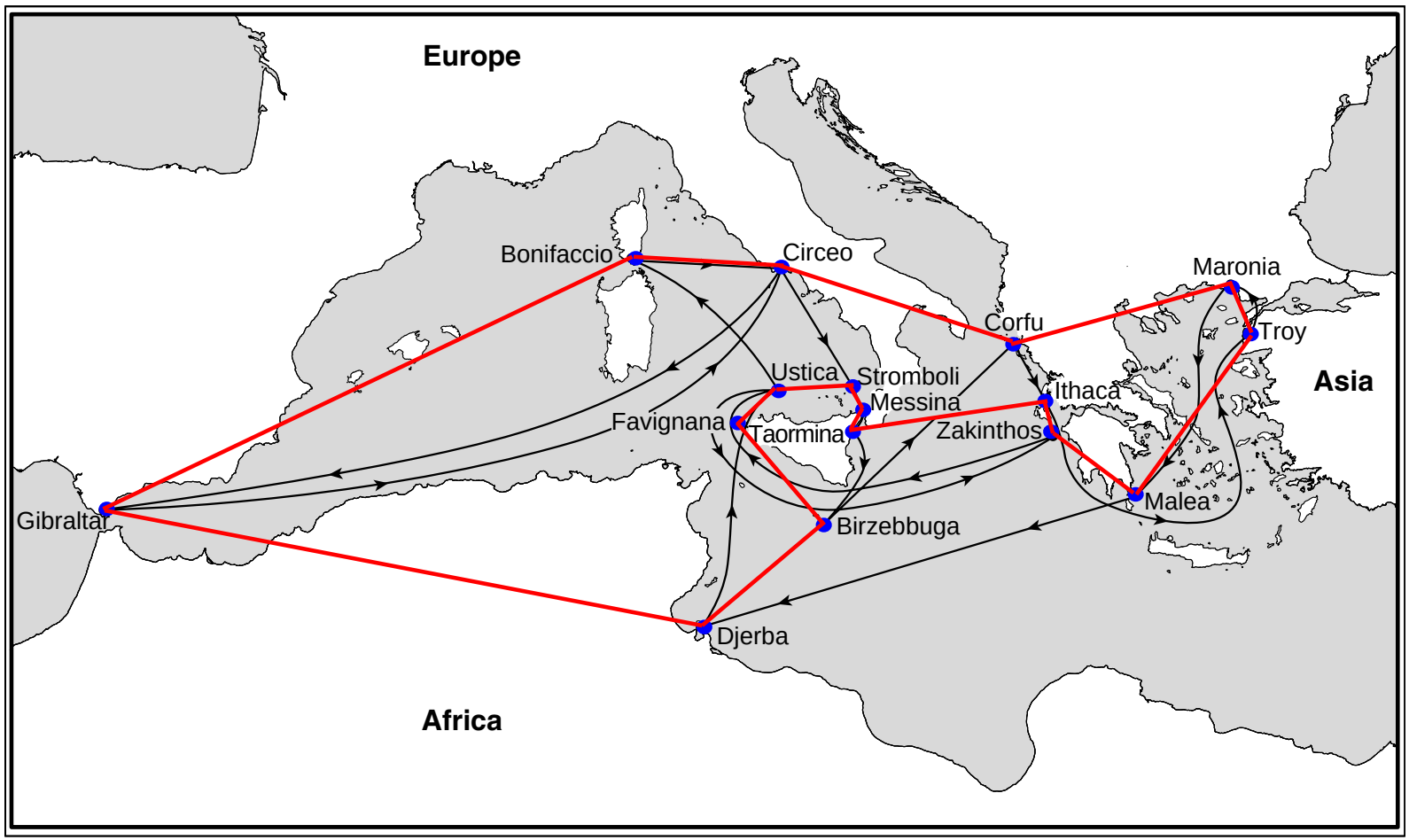

Definition

- *Hamiltonian cycle* in graph $G := (V, E)$: cyclic path that visits every vertex of G exactly once (except start/end point).

- *Weight* of path $p := (u_1, \ldots, u_k)$ in edge-weighted graph $G := (V, E, w)$: total weight of all edges on p, *i.e.*:

$$w(p) := \sum_{i=1}^{k-1} w((u_i, u_{i+1}))$$

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The Travelling Salesman Problem (TSP)

- *Given:* Directed, edge-weighted graph G.
- *Objective:* Find a minimal-weight Hamiltonian cycle in G.

Types of TSP instances:

- *Symmetric*: For all edges (v, v') of the given graph G, (v', v) is also in G, and $w((v, v')) = w((v', v))$. Otherwise: *asymmetric*.
- *Euclidean*: Vertices = points in a Euclidean space, weight function = Euclidean distance metric.
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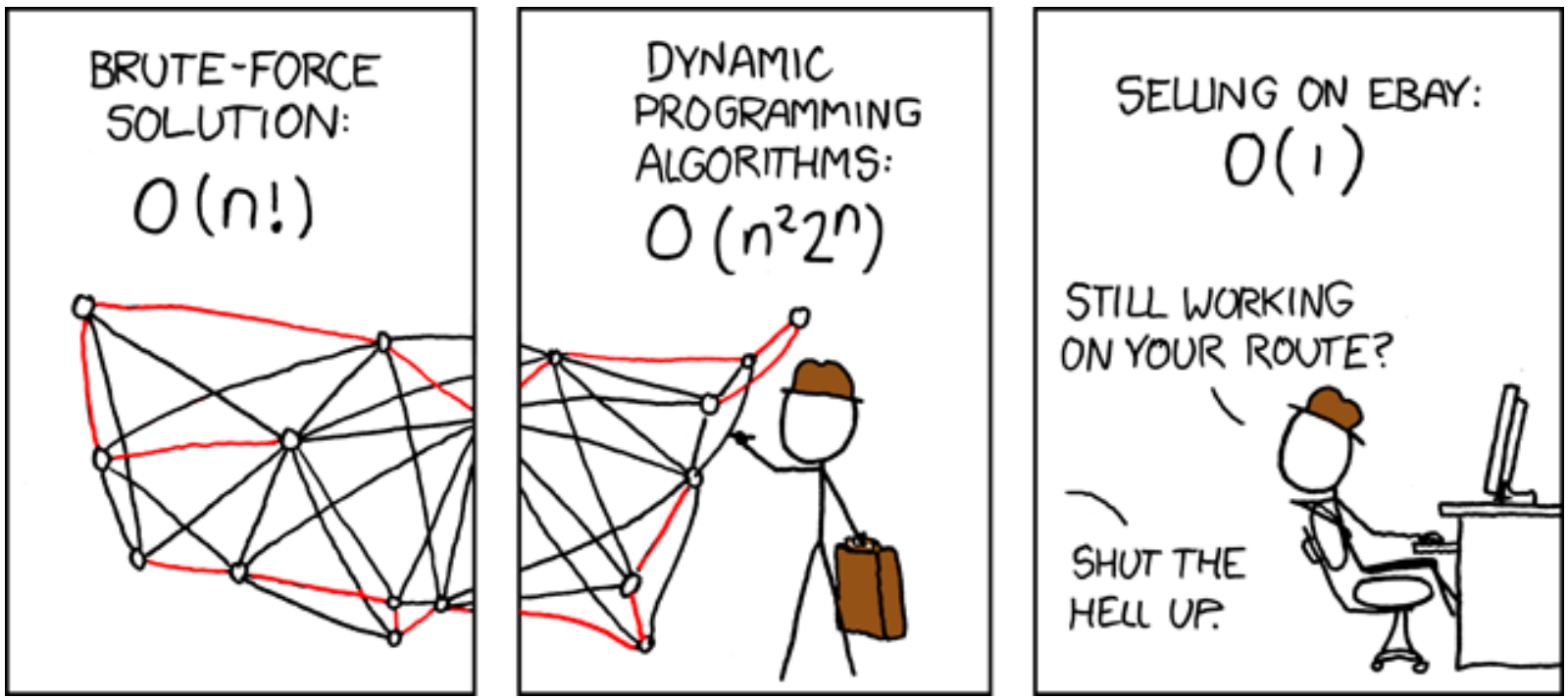
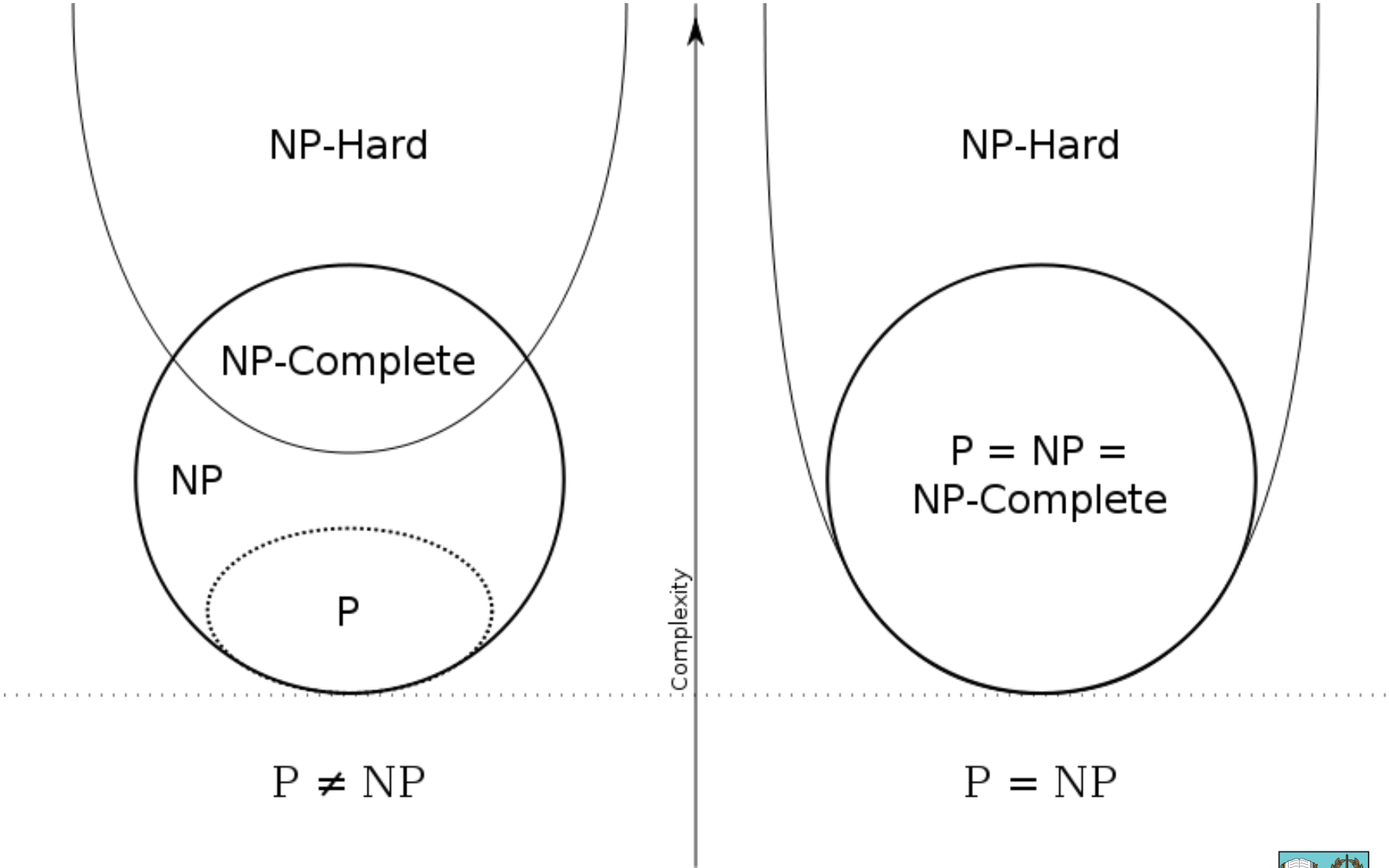


Complexity classes



Computational Complexity

Fundamental question: How hard is a given computational problem to solve?

Important concepts:

- *Time complexity of a problem Π:* Computation time required for solving a given instance π of Π using the most efficient algorithm for Π.
- *Worst-case time complexity:* Time complexity in the worst case over all problem instances of a given size, typically measured as a function of instance size, neglecting constants and lower-order terms ('$O(\ldots)$' and '$\Theta(\ldots)$' notations).

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  Note: nondeterministic $\neq$ randomised; non-deterministic machines are idealised models of computation that have the ability to make perfect guesses.

- $\mathcal{NP}$-complete: Among the most difficult problems in $\mathcal{NP}$; believed to have at least exponential time-complexity for any realistic machine or programming model.

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- SAT for 3-CNF is $\mathcal{NP}$-complete.
- TSP is $\mathcal{NP}$-hard, the associated decision problem (for any solution quality) is $\mathcal{NP}$-complete.
- The same holds for Euclidean TSP instances.
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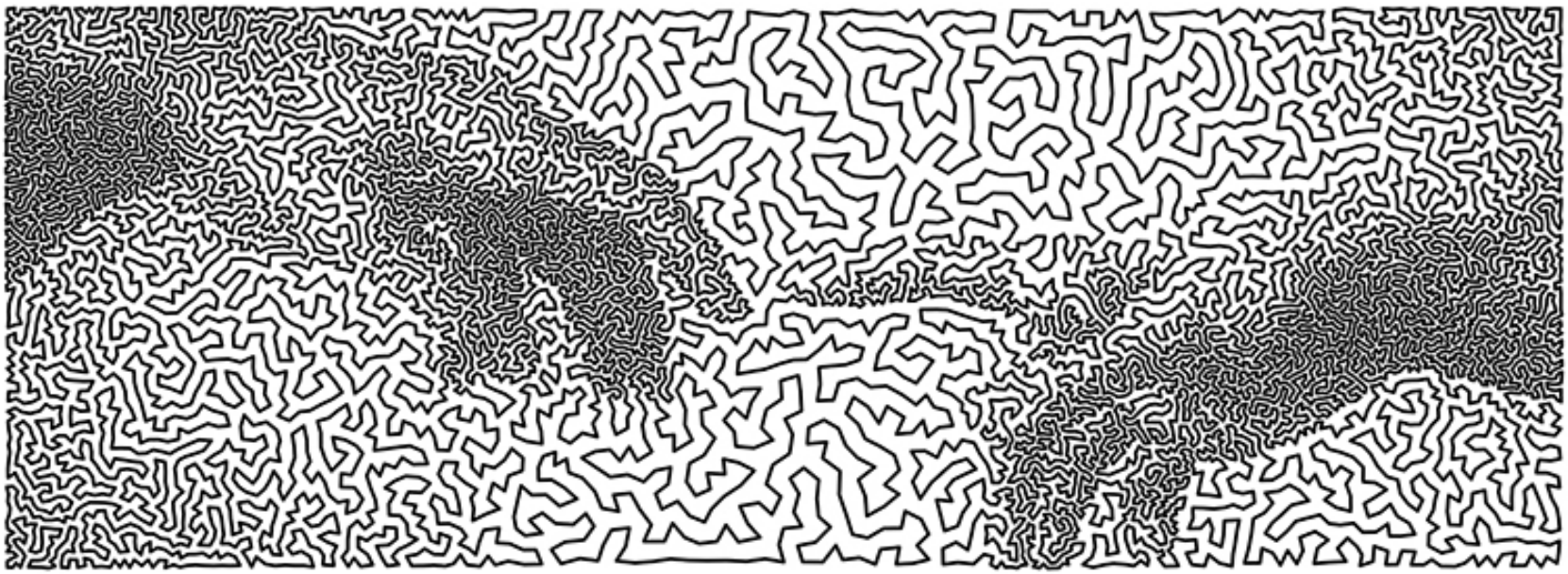
Search



Search Paradigms

Solving combinatorial problems through search:

- iteratively generate and evaluate candidate solutions
- decision problems: evaluation = test if solution
- optimisation problems: evaluation = check objective function value
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- search space = complete candidate solutions
- search step = modification of one or more solution components

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Example: Nearest Neighbour Heuristic (NNH) for TSP

- start with single vertex (chosen uniformly at random)
- in each step, follow minimal-weight edge to yet unvisited, next vertex
- complete Hamiltonian cycle by adding initial vertex to end of path

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procedure *URW-for-SAT*(F, *maxSteps*)
  input: *propositional formula* F, *integer maxSteps*
  output: *model of* F **or** $\emptyset$

  choose assignment a of truth values to all variables in F
    uniformly at random;
  steps := 0;
  while not((a satisfies F) **and** (*steps* $<$ *maxSteps*)) **do**
    randomly select variable x in F;
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Local search $\neq$ perturbative search:

- Construction heuristics can be seen as local search methods *e.g.*, the Nearest Neighbour Heuristic for TSP.

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Tree search

- Combination of constructive search and *backtracking*, *i.e.*, revisiting of choice points after construction of complete candidate solutions.
- Performs *systematic search* over constructions.
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Example: NNH + Backtracking

- Construct complete candidate round trip using NNH.
- Backtrack to most recent choice point with unexplored alternatives.
- Complete tour using NNH (possibly creating new choice points).
- Recursively iterate backtracking and completion.

Efficiency of tree search can be substantially improved by pruning choices that cannot lead to (optimal) solutions.

Example: Branch & bound / A* search for TSP

- Compute lower bound on length of completion of given partial round trip.
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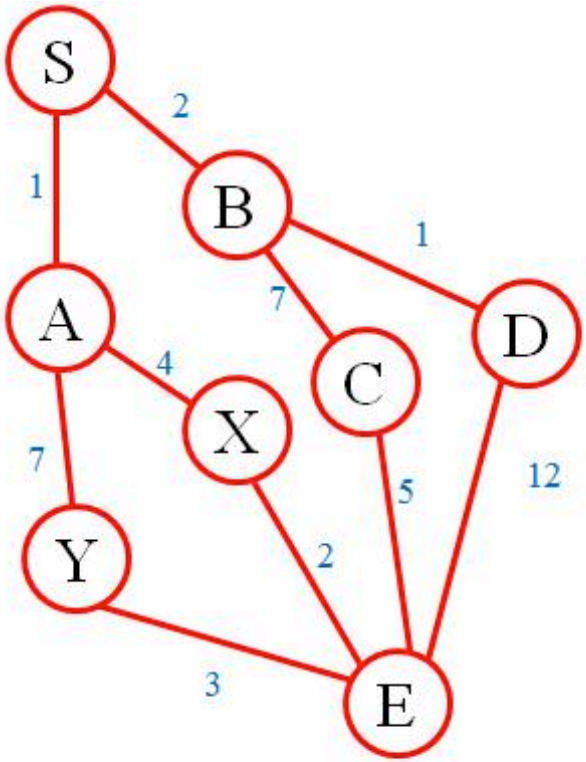

- Values for h:

  A:5, B:6, C:4, D:15, X:5, Y:8

Expand S

{S,A} f=1+5=6

{S,B} f=2+6=8

Expand A

{S,B} f=2+6=8

{S,A,X} f=(1+4)+5=10

{S,A,Y} f=(1+7)+8=16

Expand B

{S,A,X} f=(1+4)+5=10

{S,B,C} f= (2+7)+4=13

{S,A,Y} f=(1+7)+8=16

{S,B,D} f= (2+1)+15=18

Expand X

{S,A,X,E} is the best path... (costing 7)

Systematic *vs* Local Search

- **Completeness:** Advantage of systematic search, but not always relevant, *e.g.*, when existence of solutions is guaranteed by construction or in real-time situations.
- **Any-time property:** Positive correlation between run-time and solution quality or probability; typically more readily achieved by local search.
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- proofs of insolubility or optimality are required;
- time constraints are not critical;
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Stochastic Local Search

Many prominent local search algorithms use *randomised choices* in generating and modifying candidate solutions.

These *stochastic local search (SLS) algorithms* are one of the most successful and widely used approaches for solving hard combinatorial problems.

Some well-known SLS methods and algorithms:

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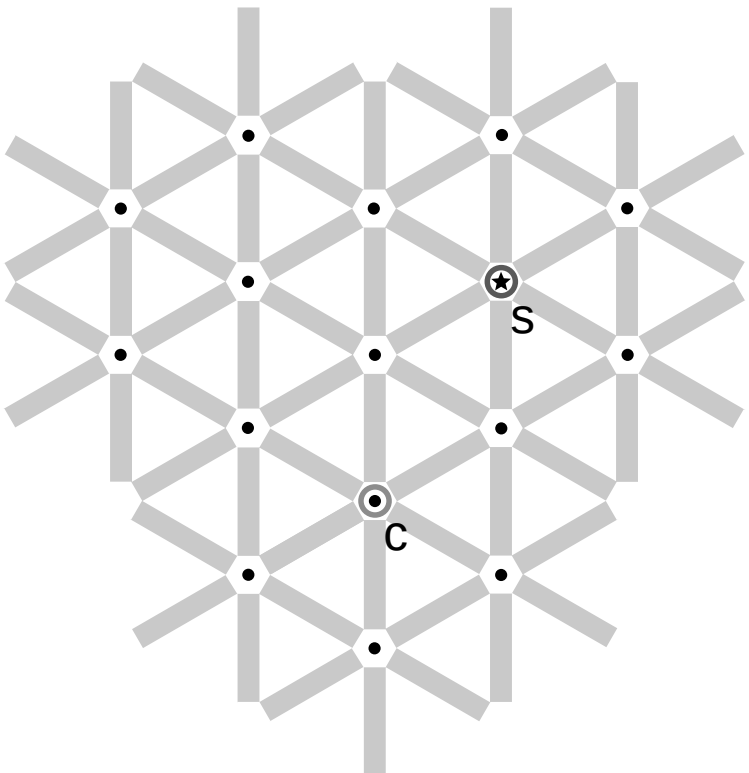
Stochastic local search — global view



- vertices: candidate solutions (search positions)
- edges: connect neighbouring positions
- s: (optimal) solution
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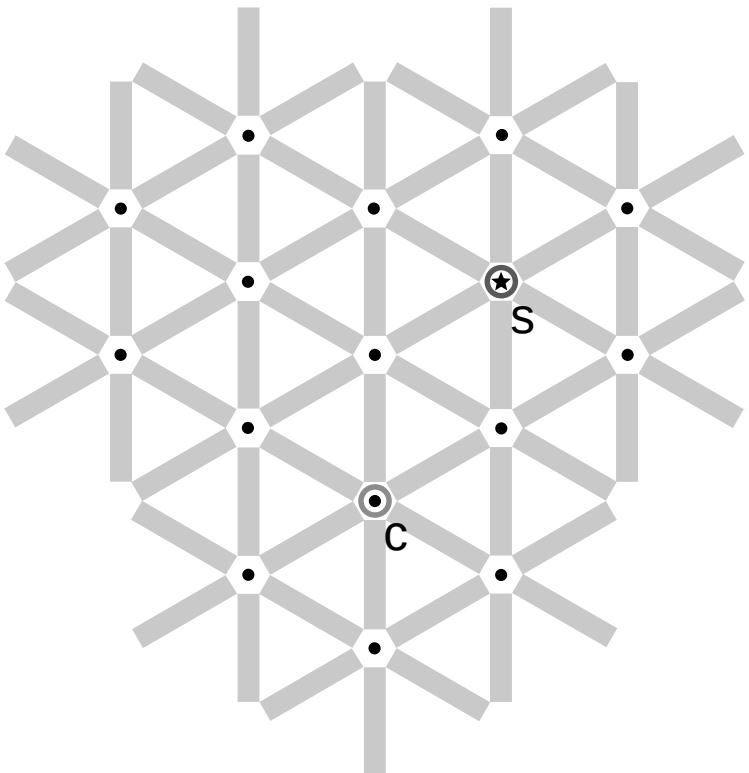

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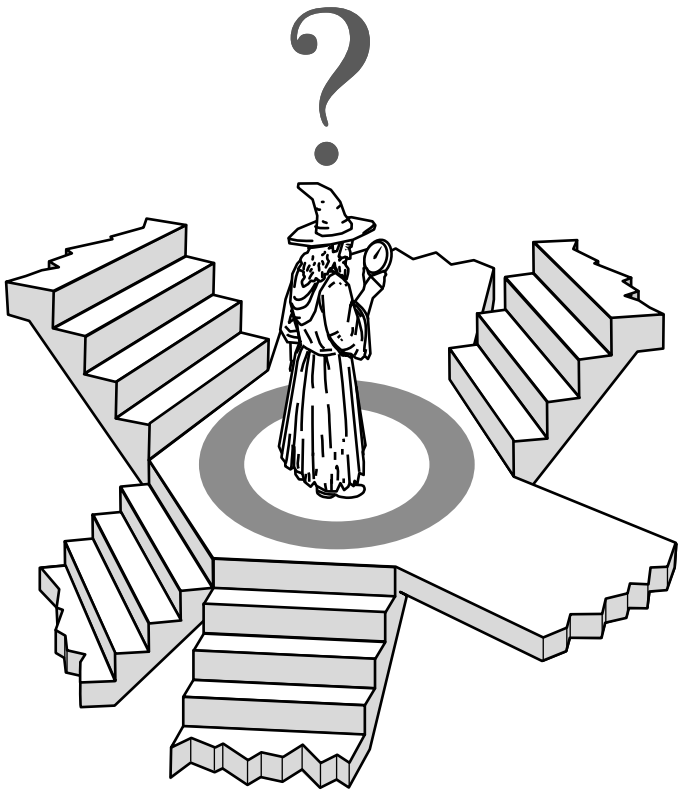

Next search position is selected

from local neighbourhood based on local information, *e.g.*, heuristic values.

Definition: **Stochastic Local Search Algorithm** (1)

For given problem instance π:

- *search space* $S(\pi)$ (*e.g.*, for SAT: set of all complete truth assignments to propositional variables)
- *solution set* $S'(\pi) \subseteq S(\pi)$ (*e.g.*, for SAT: models of given formula)
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  $\hat{s} := s$;
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- Procedural versions of *init*, *step* and *terminate* implement sampling from respective probability distributions.

- Memory state m can consist of multiple independent attributes, *i.e.*, $M(\pi) := M_1 \times M_2 \times \ldots \times M_{l(\pi)}$.

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- **initialisation:** uniform random choice from S, *i.e.*, $\mathit{init}()(a', m) := 1/\#S$ for all assignments a' and memory states m
- **step function:** uniform random choice from current neighbourhood, *i.e.*, $\mathit{step}(a, m)(a', m) := 1/\#N(a)$ for all assignments a and memory states m, where $N(a) := \{a' \in S \mid N(a, a')\}$ is the set of all neighbours of a.
- **termination:** when model is found, *i.e.*, $\mathit{terminate}(a, m)(\top) := 1$ if a is a model of F, and 0 otherwise.

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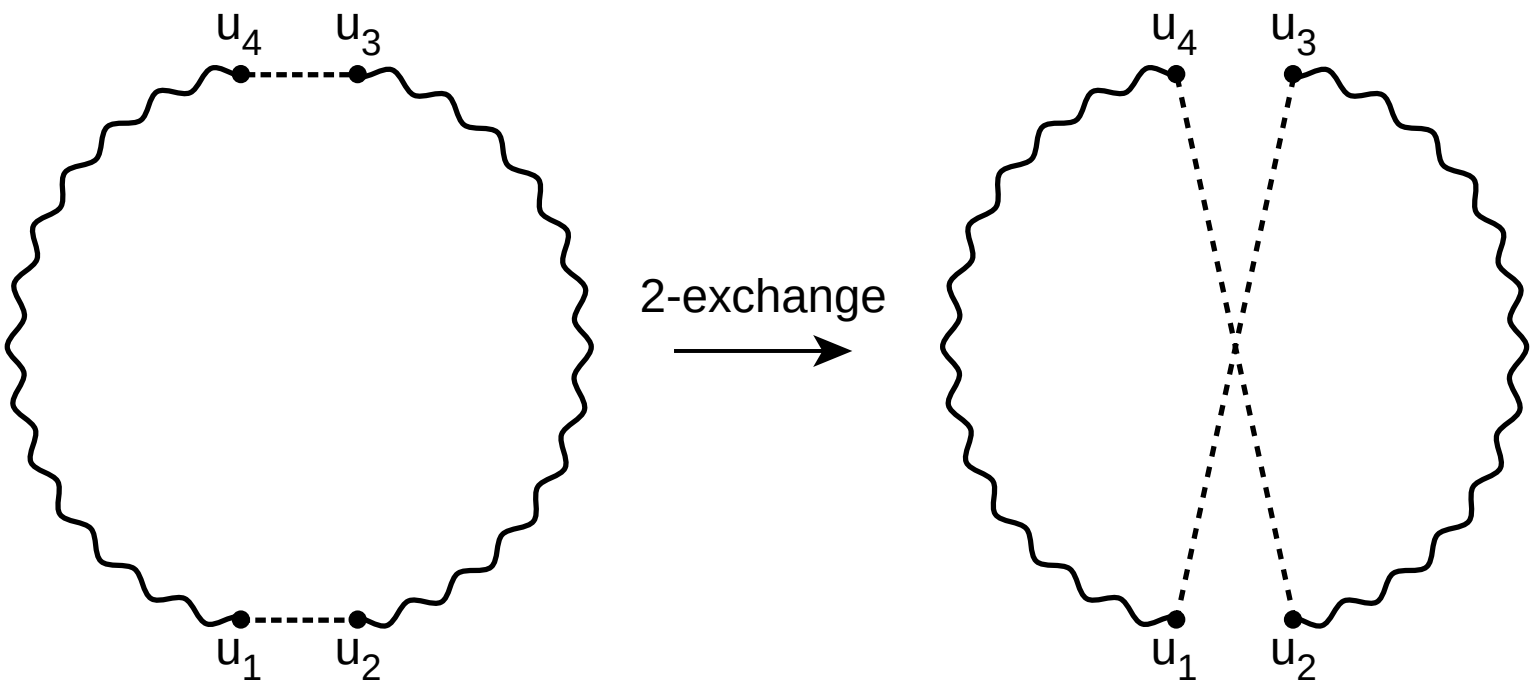
Search steps in the 2-exchange neighbourhood for the TSP



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- **Key idea:** calculate *effects of differences* between current search position s and neighbours s' on evaluation function value.
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Complexity class $\mathcal{PLS}$ (Polynomial Local Search): class of problems for which a local search algorithm exists with polynomial time complexity for:

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$\mathcal{PLS}$-complete: Among the most difficult problems in $\mathcal{PLS}$; if for any of these problems local optima can be found in polynomial time, the same would hold for all problems in $\mathcal{PLS}$.

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- TSP with k-exchange neighbourhood with $k > 3$ is $\mathcal{PLS}$-complete.
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