STOCHASTIC LOCAL SEARCH
FOUNDATIONS AND APPLICATIONS

Introduction: Combinatorial Problems and Search

Holger H. Hoos & Thomas Stützle

Outline

1. Combinatorial Problems
2. Two Prototypical Combinatorial Problems
3. Computational Complexity
4. Search Paradigms
5. 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
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Example:

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

Note:

- 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
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Problem *vs* problem instance:

- *Problem:* Given *any* set of points X, find a shortest round trip
- *Solution:* Algorithm that finds shortest round trips for any X

- *Problem instance:* Given *a specific* set of points P, find a shortest round trip
- *Solution:* Shortest round trip for P

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Decision problems:

solutions = candidate solutions that satisfy given *logical conditions*

Example: The Graph Colouring Problem

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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

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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: optimal quality = *minimal* value of f
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Variant of the Graph Colouring Problem where the objective is to find a valid colour assignment that uses a minimal number of colours.

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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

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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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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 roundtrips in graphs (TSP)
  – prototypical optimisation problem

SAT: A simple example

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

General SAT Problem (search variant):

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Definition:

- *Formula in propositional logic*: well-formed string that may contain
  - propositional variables $x_1, x_2, \ldots, x_n$;
  - truth values $\top$ ('true'), $\perp$ ('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)

- Formula F is *satisfiable* iff there exists at least one model of F, *unsatisfiable* otherwise.

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

  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.
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Note:

- In many cases, the restriction of SAT to CNF formulae is considered.
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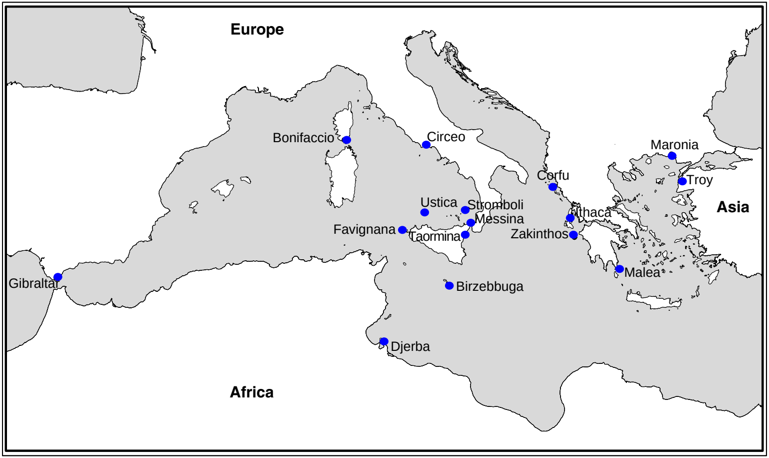
- F is in CNF.
- Is F satisfiable?
  Yes, *e.g.*, $x_1 := x_2 := \top$, $x_3 := x_4 := x_5 := \bot$ is a model of F.

TSP: A simple example



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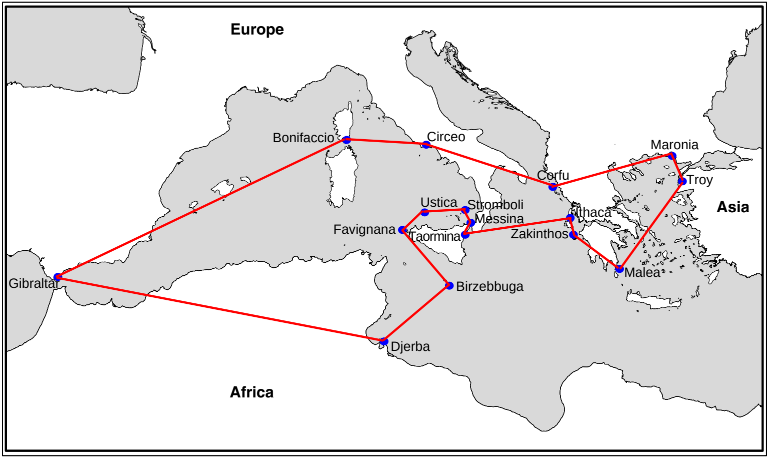

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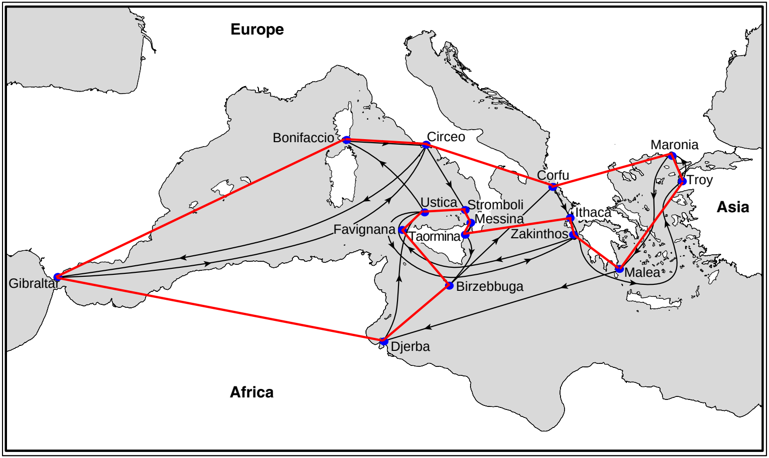

Definition:

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

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

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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.
- *Geographic*: Vertices = points on a sphere, weight function = geographic (great circle) distance.

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Computational Complexity

Fundamental question:

How hard is a given computational problems 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 ('$O(...)$' and '$\Theta(...)$' notations).

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Important concepts (continued):

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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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Many combinatorial problems are hard:

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- SAT for 3-CNF is $\mathcal{NP}$-complete.

- TSP is $\mathcal{NP}$-hard, the associated decision problem for optimal solution quality is $\mathcal{NP}$-complete.
- The same holds for Euclidean TSP instances.

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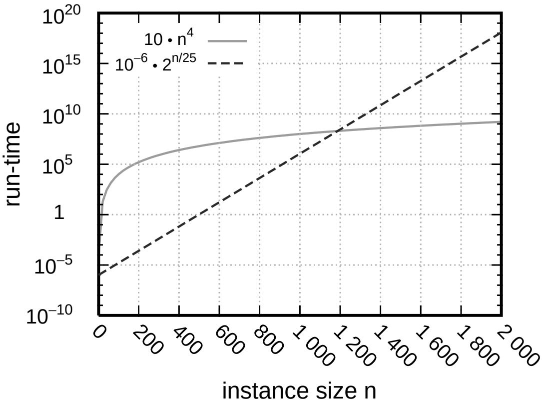
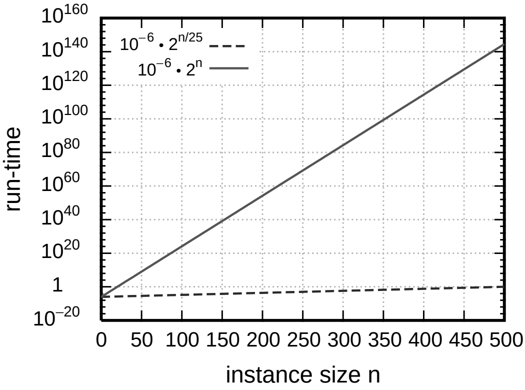
Example: Polynomial *vs* exponential growth



Example: Impact of constants



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
- evaluating candidate solutions is typically computationally much cheaper than finding (optimal) solutions

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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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- traverse search space for given problem instance in a systematic manner
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Example: Uninformed random walk for SAT

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;
    change value of x in a;
    steps $:=$ *steps*$+1$;
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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.
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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.
- Terminate search on branch if length of current partial round trip + lower bound on length of completion exceeds length of shortest complete round trip found so far.

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- Dynamical selection of solution components in construction or choice points in backtracking.
- Backtracking to other than most recent choice points (*back jumping*).
- Randomisation of construction method or selection of choice points in backtracking $\rightsquigarrow$ *randomised systematic search*.

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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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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.

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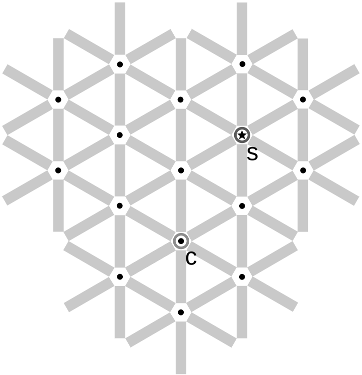
Stochastic local search — global view



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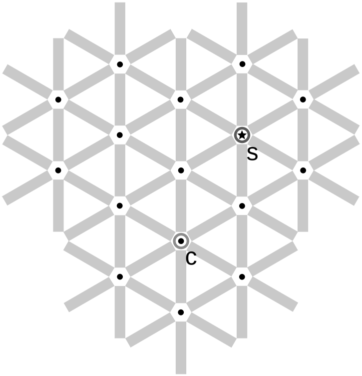

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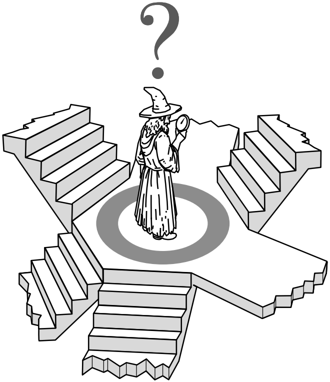

Next search position is selected from local neighbourhood based on local information, *e.g.*, heuristic values.

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* $S'(\pi) \subseteq S(\pi)$
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Note:

- 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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- **search space S:** set of all truth assignments to variables in given formula F
- **solution set S':** set of all models of F
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Note: Diameter of G_N = worst-case lower bound for number of search steps required for reaching (optimal) solutions

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SAT instance with n variables, 1-flip neighbourhood:
G_N = n-dimensional hypercube; diameter of $G_N = n$.

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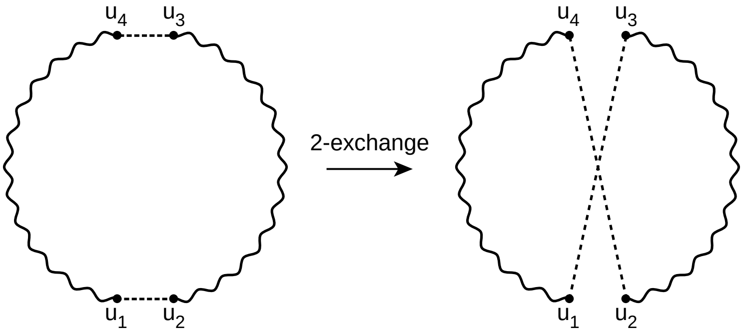
Search steps in the 2-exchange neighbourhood for the TSP



Definition:

- *Search step* (or *move*): pair of search states s, s' for which s can be reached from s in one step, *i.e.*, $N(s, s')$ and $step(s, m)(s', m') > 0$ for some memory states $m, m' \in M$.
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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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- solution components = edges of given graph G
- standard 2-exchange neighbhourhood, *i.e.*, neighbouring round trips p, p' differ in two edges
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For a local search algorithm to be effective, search initialisation and individual search steps should be efficiently computable.

Complexity class $\mathcal{PLS}$: class of problems for which a local search algorithm exists with polynomial time complexity for:

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