STOCHASTIC LOCAL SEARCH
FOUNDATIONS AND APPLICATIONS

Introduction: Combinatorial Problems and Search

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Outline

1. Combinatorial Problems
2. Two Prototypical Combinatorial Problems
3. Search Paradigms
4. 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

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.

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
- *candidate solution:* round trip
- *solution*: round trip with minimal length

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

Technically, problems can be formalised as sets of problem instances.

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

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
  maximisation problem: optimal quality = *maximal* value of f

Example:

Variant of the Graph Colouring Problem where the objective is to find a valid colour assignment that uses a minimal number of colours.

Note: Every minimisation problem can be formulated as a maximisation problem and vice versa.

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.

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)
  – prototypical optimisation problem

Concise definition of SAT:

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

Note:

- In many cases, the restriction of SAT to CNF formulae is considered.
- The restriction of SAT to k-CNF formulae is called *k-SAT*.

Definition:

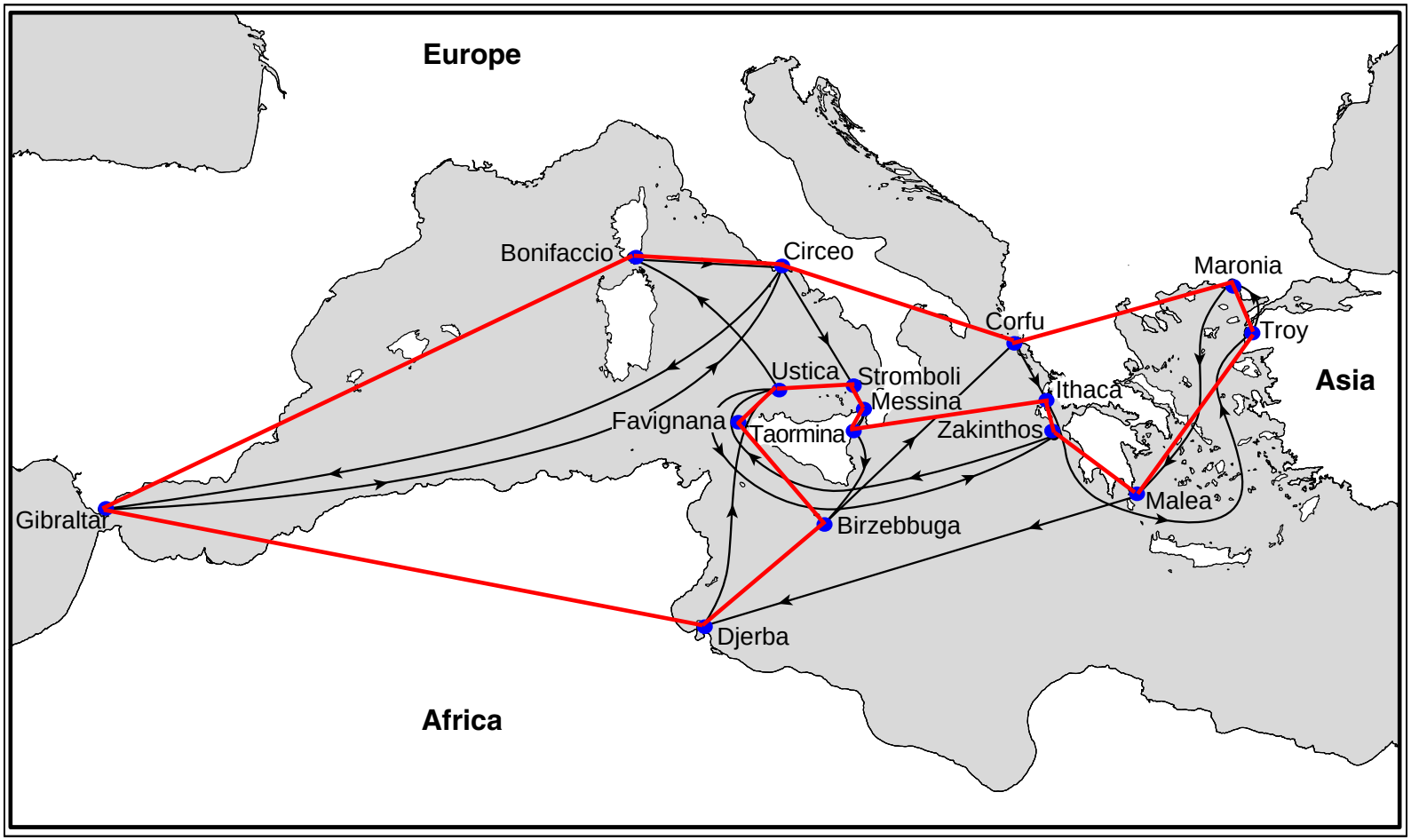
- A formula is in *conjunctive normal form (CNF)* iff it is of the form

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

  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*.

- A formula is in *k-CNF* iff it is in CNF and all clauses contain exactly k literals (*i.e.*, for all i, $k(i) = k$).

TSP: A simple example



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.*:

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

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.

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

Perturbative search

- search space = complete candidate solutions
- search step = modification of one or more solution components

Example: SAT

- search space = complete variable assignments
- search step = modification of truth values for one or more variables

Constructive search (aka construction heuristics)

- search space = partial candidate solutions
- search step = extension with one or more solution components

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

Note: NNH typically does not find very high quality solutions, but it is often and successfully used in combination with perturbative search methods.

Systematic search:

- traverse search space for given problem instance in a systematic manner
- *complete*: guaranteed to eventually find (optimal) solution, or to determine that no solution exists

Local Search:

- start at some position in search space
- iteratively move from position to neighbouring position
- typically *incomplete*: not guaranteed to eventually find (optimal) solutions, cannot determine insolubility with certainty

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;
  end
  if a satisfies F **then**
    return a
  else
    return $\emptyset$
  end
end *URW-for-SAT*

Systematic search is often better suited when ...

- proofs of insolubility or optimality are required;
- time constraints are not critical;
- problem-specific knowledge can be expoited.

Local search is often better suited when ...

- reasonably good solutions are required within a short time;
- parallel processing is used;
- problem-specific knowledge is rather limited.

Stochastic Local Search

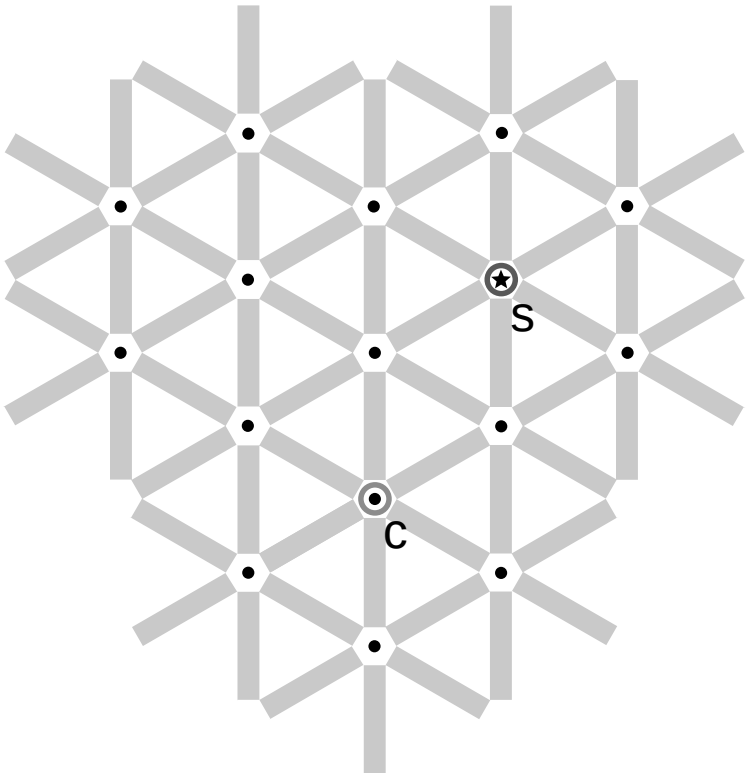
Many prominent local search algorithms use *randomised choices* in generating and modifying candidate solutions.

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:

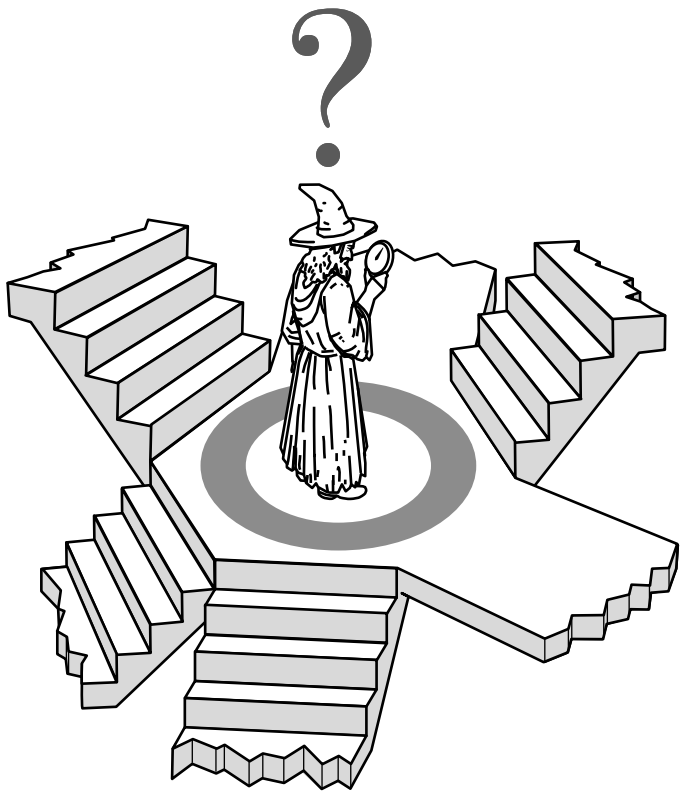
- Evolutionary Algorithms
- Simulated Annealing
- Lin-Kernighan Algorithm for TSP

Stochastic local search — global view



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

Stochastic local search — local view



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)
- *neighbourhood relation* $N(\pi) \subseteq S(\pi) \times S(\pi)$
  (*e.g.*, for SAT: neighbouring variable assignments differ in the truth value of exactly one variable)

Definition: **Stochastic Local Search Algorithm** (2)

- *set of memory states* $M(\pi)$
  (may consist of a single state, for SLS algorithms that do not use memory)
- *initialisation function* $init : \emptyset \mapsto \mathcal{D}(S(\pi) \times M(\pi))$
  (specifies probability distribution over initial search positions and memory states)
- *step function* $step : S(\pi) \times M(\pi) \mapsto \mathcal{D}(S(\pi) \times M(\pi))$
  (maps each search position and memory state onto probability distribution over subsequent, neighbouring search positions and memory states)
- *termination predicate* $terminate : S(\pi) \times M(\pi) \mapsto \mathcal{D}(\{\top, \bot\})$
  (determines the termination probability for each search position and memory state)

procedure *SLS-Minimisation*(π')
  input: *problem instance* $\pi' \in \Pi'$
  output: *solution* $s \in S'(\pi')$ **or** $\emptyset$
  $(s, m) := \mathit{init}(\pi')$;
  $\hat{s} := s$;
  while not $\mathit{terminate}(\pi', s, m)$ **do**
    $(s, m) := \mathit{step}(\pi', s, m)$;
    if $f(\pi', s) < f(\pi', \hat{s})$ **then**
      $\hat{s} := s$;
    end
  end
  if $\hat{s} \in S'(\pi')$ **then**
    return $\hat{s}$
  else
    return $\emptyset$
  end
end *SLS-Minimisation*

Example: Uninformed random walk for SAT

- **search space S:** set of all truth assignments to variables in given formula F
- **solution set S':** set of all models of F
- **neighbourhood relation N:** *1-flip neighbourhood*, *i.e.*, assignments are neighbours under N iff they differ in the truth value of exactly one variable
- **memory:** not used, *i.e.*, $M := \{0\}$
- **initialisation:** uniform random choice from S
- **step function:** uniform random choice from current neighbourhood
- **termination:** when model is found

Definition:

- *Search step* (or *move*): pair of search positions s, s' for which s' can be reached from s in one step,
- *Search trajectory*: finite sequence of search positions $(s_0, s_1, \ldots, s_k)$ such that (s_{i-1}, s_i) is a *search step* for any $i \in \{1, \ldots, k\}$ and the probability of initialising the search at s_0 is greater than zero,
- *Search strategy*: specified by *init* and *step* function; to some extent independent of problem instance and other components of SLS algorithm.

Uninformed Random Picking

- $N := S \times S$
- does not use memory
- *init*, *step*: uniform random choice from S,

Uninformed Random Walk

- does not use memory
- *init*: uniform random choice from S
- *step*: uniform random choice from current neighbourhood,

Note: These uninformed SLS strategies are quite ineffective,
but play a role in combination with more directed search strategies.

Evaluation function:

- function $g(\pi) : S(\pi) \mapsto \mathbb{R}$ that maps candidate solutions of a given problem instance π onto real numbers, such that global optima correspond to solutions of π;
- used for ranking or assessing neighbhours of current search position to provide guidance to search process.

Evaluation *vs* objective functions:

- *Evaluation function*: part of SLS algorithm.
- *Objective function*: integral part of optimisation problem.
- Some SLS methods use evaluation functions different from given objective function

Iterative Improvement (II)

- does not use memory
- *init*: uniform random choice from S
- *step*: uniform random choice from improving neighbours,
- terminates when no improving neighbour available
  (to be revisited later)
- different variants through modifications of step function

Note: II is also known as *iterative descent* or *hill-climbing*.

Example: Iterative Improvement for SAT

- **search space S:** set of all truth assignments to variables in given formula F
- **solution set S':** set of all models of F
- **neighbourhood relation N:** 1-flip neighbourhood (as in Uninformed Random Walk for SAT)
- **memory:** not used, *i.e.*, $M := \{0\}$
- **initialisation:** uniform random choice from S, *i.e.*, $\mathit{init}()(a') := 1/\#S$ for all assignments a'

Example: Iterative Improvement for SAT (continued)

- **evaluation function:** $g(a) :=$ number of clauses in F that are *unsatisfied* under assignment a
  (*Note:* $g(a) = 0$ iff a is a model of F.)
- **step function**: uniform random choice from improving neighbours, *i.e.*, $step(a)(a') := 1/\#I(a)$ if $s' \in I(a)$, and 0 otherwise, where $I(a) := \{a' \mid N(a, a') \wedge g(a') < g(a)\}$
- **termination**: when no improving neighbour is available
  i.e., $terminate(a)(\top) := 1$ if $I(a) = \emptyset$, and 0 otherwise.

Definition:

- *Local minimum:* search position without improving neighbours w.r.t. given evaluation function g and neighbourhood N, *i.e.*, position $s \in S$ such that $g(s) \leq g(s')$ for all $s' \in N(s)$.
- *Strict local minimum:* search position $s \in S$ such that $g(s) < g(s')$ for all $s' \in N(s)$.
- *Local maxima* and *strict local maxima*: defined analogously.

Simple mechanisms for escaping from local optima:

- *Restart:* re-initialise search whenever a local optimum is encountered.
  (Often rather ineffective due to cost of initialisation.)
- *Non-improving steps*: in local optima, allow selection of candidate solutions with equal or worse evaluation function value, *e.g.*, using minimally worsening steps.
  (Can lead to long walks in *plateaus*, *i.e.*, regions of search positions with identical evaluation function.)

Note: Neither of these mechanisms is guaranteed to always escape effectively from local optima.

Diversification *vs* Intensification

- Goal-directed and randomised components of SLS strategy need to be balanced carefully.
- *Intensification*: aims to greedily increase solution quality or probability, *e.g.*, by exploiting the evaluation function.
- *Diversification*: aim to prevent search stagnation by preventing search process from getting trapped in confined regions.

Examples:

- Iterative Improvement (II): *intensification* strategy.
- Uninformed Random Walk (URW): *diversification* strategy.

Balanced combination of intensification and diversification mechanisms forms the basis for advanced SLS methods.