STOCHASTIC LOCAL SEARCH
FOUNDATIONS AND APPLICATIONS

Introduction: Combinatorial Problems and Search

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Outline

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

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

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

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 problems and vice versa.

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.

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.

Note:

- Algorithms for *optimisation problems* can be used to solve *associated decision problems*
- Algorithms for *decision problems* can often be extended to related *optimisation problems*.
- *Caution:* This does not always solve the given problem most efficiently.

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

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):

- *Given:* Formula F in propositional logic
- *Objective:* Find an assignment of truth values to variables in F that renders F true, or decide that no such assignment exists.

Definition:

- *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)

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

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, $k(i) = k$).

Note: For every propositional formula, there is an equivalent formula in 3-CNF.

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*.

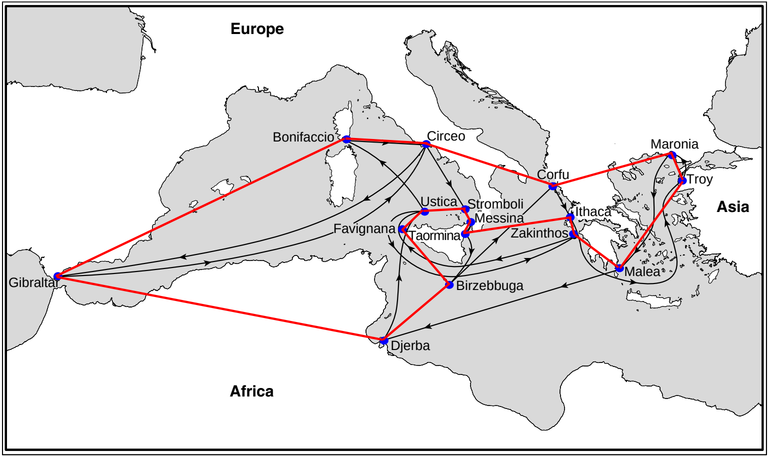
Example:

$$
\begin{aligned}
F := \; & (\neg x_2 \vee x_1) \\
& \wedge (\neg x_1 \vee \neg x_2 \vee \neg x_3) \\
& \wedge (x_1 \vee x_2) \\
& \wedge (\neg x_4 \vee x_3) \\
& \wedge (\neg x_5 \vee x_3)
\end{aligned}
$$

- 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



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.

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 ('$O(...)$' and '$\Theta(...)$' notations).

Important concepts (continued):

- *$\mathcal{NP}$:* Class of problems that can be solved in polynomial time by a nondeterministic machine.

  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.

- *$\mathcal{NP}$-hard:* At least as difficult as the most difficult problems in $\mathcal{NP}$, but possibly not in $\mathcal{NP}$ (*i.e.*, may have even worse complexity than $\mathcal{NP}$-complete problems).

Many combinatorial problems are hard:

- SAT for general propositional formulae is $\mathcal{NP}$-complete.
- 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.

- The Graph Colouring Problem is $\mathcal{NP}$-complete.
- Many scheduling and timetabling problems are $\mathcal{NP}$-hard.

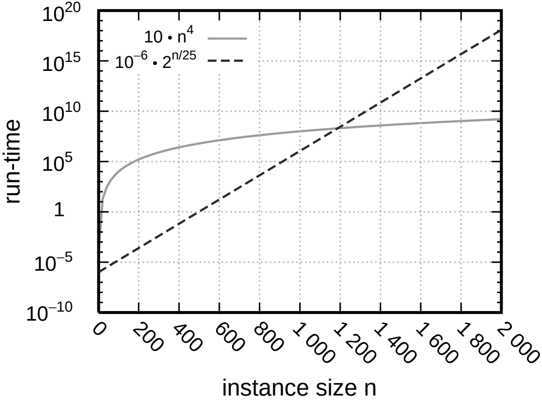
But: Some combinatorial problems can be solved efficiently:

- Shortest Path Problem (Dijkstra's algorithm);
- 2-SAT (linear time algorithm);
- many special cases of TSP, *e.g.*, Euclidean instances where all vertices lie on a circle;
- sequence alignment problems (dynamic programming).

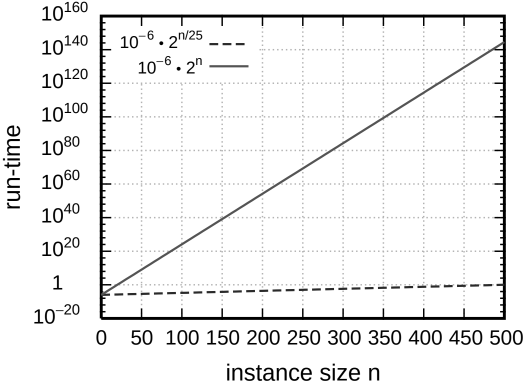
Practically solving hard combinatorial problems:

- Subclasses can often be solved efficiently
  (*e.g.*, 2-SAT);
- Average-case *vs* worst-case complexity
  (*e.g.* Simplex Algorithm for linear optimisation);
- Approximation of optimal solutions:
  sometimes possible in polynomial time (*e.g.*, Euclidean TSP),
  but in many cases also intractable (*e.g.*, general TSP);
- Randomised computation is often practically
  (and possibly theoretically) more efficient;
- Asymptotic bounds *vs* true complexity:
  constants matter!

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

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*

Local search $\neq$ perturbative search:

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

  Note: Many high-performance local search algorithms combine constructive and perturbative search.

- Perturbative search can provide the basis for systematic search methods.

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.
- **Complementarity:** Local and systematic search can be fruitfully combined, *e.g.*, by using local search for finding solutions whose optimality is proven using systematic search.

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

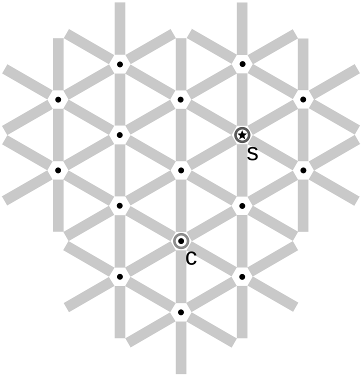
Many prominent local search algorithms use *randomised choices* in generating and modifying candidate solutions.

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:

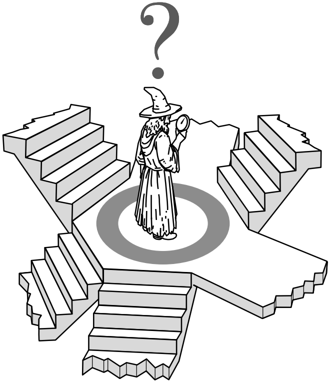
- Evolutionary Algorithms
- Simulated Annealing
- Lin-Kernighan Algorithm for TSP

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* $\mathit{init} : \emptyset \mapsto \mathcal{D}(S(\pi) \times M(\pi))$
  (specifies probability distribution over initial search positions and memory states)

- *step function* $\mathit{step} : S(\pi) \times M(\pi) \mapsto \mathcal{D}(S(\pi) \times M(\pi))$
  (maps each search position and memory state onto probability distribution over subsequent, neighbouring search positions and memory states)

- *termination predicate* $\mathit{terminate} : S(\pi) \times M(\pi) \mapsto \mathcal{D}(\{\top, \bot\})$
  (determines the termination probability for each search position and memory state)

```
procedure SLS-Decision(π)
    input: problem instance π ∈ Π
    output: solution s ∈ S'(π) or ∅
    (s, m) := init(π);

    while not terminate(π, s, m) do
        (s, m) := step(π, s, m);
    end



    if s ∈ S'(π) then
        return s
    else
        return ∅
    end
end SLS-Decision
```

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

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.*, $M(\pi) := M_1 \times M_2 \times \ldots \times M_{l(\pi)}$.
- SLS algorithms realise *Markov processes*: behaviour in any *search state* (s, m) depends only on current position s and (limited) memory m.

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.*, $M := \{0\}$

Example: Uninformed random walk for SAT (continued)

- **initialisation:** uniform random choice from S, *i.e.*, $init()(a', m) := 1/\#S$ for all assignments a' and memory states m
- **step function:** uniform random choice from current neighbourhood, *i.e.*, $step(a, m)(a', m) := 1/\#N(a)$ 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.*, $terminate(a, m)(\top) := 1$ if a is a model of F, and 0 otherwise.

Definition:

- *neighbourhood (set)* of candidate solution s:
  $N(s) := \{s' \in S \mid N(s, s')\}$

- *neighbourhood graph* of problem instance π:
  $G_N(\pi) := (S(\pi), N(\pi))$

Note: Diameter of G_N = worst-case lower bound for number of search steps required for reaching (optimal) solutions

Example:

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

Definition:

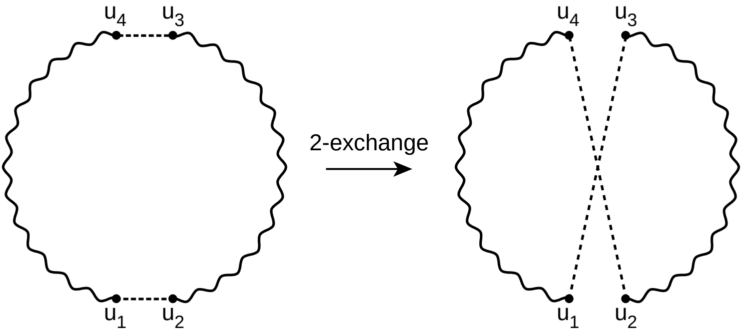
k-exchange neighbourhood: candidate solutions s, s' are neighbours iff s differs from s' in at most k solution components

Examples:

- 1-flip neighbourhood for SAT
  (solution components = single variable assignments)

- 2-exchange neighbourhood for TSP
  (solution components = edges in given graph)

Search steps in the 2-exchange neighbourhood for the TSP



Definition:

- *Search step* (or *move*): pair of search positions 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 $m, m' \in M$.
- *Search trajectory*: finite sequence of search positions $(s_0, s_1, \dots, s_k)$ such that (s_{i-1}, s_i) is a *search step* for any $i \in \{1, \dots, k\}$ and the probability of initialising the search at s_0 is greater zero, *i.e.*, $init(s_0, m) > 0$ for some memory state $m \in M$.
- *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,
  i.e., for all $s, s' \in S$, $init(s) := step(s)(s') := 1/\#S$

Uninformed Random Walk

- does not use memory
- *init*: uniform random choice from S
- *step*: uniform random choice from current neighbourhood,
  i.e., for all $s, s' \in S$, $step(s)(s') := 1/\#N(s)$ if $N(s, s')$,
  and 0 otherwise

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 (*e.g.*, dynamic local search).

Iterative Improvement (II)

- does not use memory
- *init*: uniform random choice from S
- *step*: uniform random choice from improving neighbours, *i.e.*, $step(s)(s') := 1/\#I(s)$ if $s' \in I(s)$, and 0 otherwise, where $I(s) := \{s' \in S \mid N(s,s') \wedge g(s') < g(s)\}$
- terminates when no improving neighbour available (to be revisited later)
- different variants through modifications of step function (to be revisited later)

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.*, $init()(a') := 1/\#S$ 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.

Incremental updates (aka delta evaluations)

- **Key idea:** calculate *effects of differences* between current search position s and neighbours s' on evaluation function value.
- Evaluation function values often consist of *independent contributions of solution components*; hence, $g(s)$ can be efficiently calculated from $g(s')$ by differences between s and s' in terms of solution components.
- Typically crucial for the efficient implementation of II algorithms (and other SLS techniques).

Example: Incremental updates for TSP

- solution components = edges of given graph G
- standard 2-exchange neighbhourhood, *i.e.*, neighbouring round trips p, p' differ in two edges
- $w(p') := w(p)$ − edges in p but not in p'
  + edges in p' but not in p

Note: Constant time (4 arithmetic operations), compared to linear time (n arithmetic operations for graph with n vertices) for computing $w(p')$ from scratch.

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.