STOCHASTIC LOCAL SEARCH
FOUNDATIONS AND APPLICATIONS

SLS Methods: An Overview

Holger H. Hoos & Thomas Stützle

Outline

1. Iterative Improvement (Revisited)
2. 'Simple' SLS Methods
3. Hybrid SLS Methods
4. Population-based SLS Methods

Iterative Improvement (Revisited)

Iterative Improvement (II):

determine initial candidate solution s
While s is not a local optimum:
  choose a neighbour s' of s such that $g(s') < g(s)$
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Main Problem:
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- Larger neighbourhoods $N(s)$ induce
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Trade-off:

- Using larger neighbourhoods can improve performance of II (and other SLS methods).
- *But:* time required for determining improving search steps increases with neighbhourhood size.

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Neighbourhood Pruning:

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Example: Candidate lists for the TSP

- *Intuition:* High-quality solutions likely include short edges.
- *Candidate list* of vertex v: list of v's nearest neighbours (limited number), sorted according to increasing edge weights.
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In II, various mechanisms (*pivoting rules*) can be used for choosing improving neighbour in each step:

- *Best Improvement* (aka *gradient descent*, *greedy hill-climbing*): Choose maximally improving neighbour, *i.e.*, randomly select from $I^*(s) := \{s' \in N(s) \mid g(s') = g^*\}$, where $g^* := \min\{g(s') \mid s' \in N(s)\}$.

  Note: Requires evaluation of all neighbours in each step.

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- **Given:** TSP instance G with vertices $v_1, v_2, \ldots, v_n$.
- search space: Hamiltonian cycles in G;
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- **Initialisation:**

  search position := fixed canonical path $(v_1, v_2, \ldots, v_n, v_1)$
  P := random permutation of {1,2, . . . , n}
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Empirical performance evaluation:

- Perform 1000 runs of algorithm on benchmark instance `pcb3038`.
- Record *relative solution quality* (= percentage deviation from known optimum) of final tour obtained in each run.
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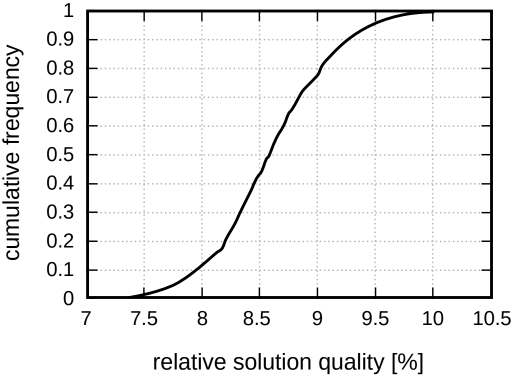
Result: Substantial variability in solution quality between runs.



Variable Neighbourhood Descent

- *Recall:* Local minima are relative to neighbourhood relation.
- **Key idea:** To escape from local minimum of given neighbourhood relation, switch to different neighbhourhood relation.
- Use k neighbourhood relations $N_1, \ldots, N_k$, (typically) ordered according to increasing neighbourhood size.
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determine initial candidate solution s
$i := 1$
Repeat:
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Until $i > k$

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- Many variants exist that switch between neighbhourhoods in different ways.
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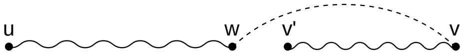

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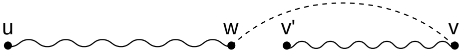

- *Note:* Hamiltonian path can be completed into Hamiltonian cycle by adding edge (v', u):

Construction of complex LK steps:

1. start with current candidate solution (Hamiltonian cycle) s; set $t^* := s$; set $p := s$
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4. if $w(t) < w(t^*)$ then set $t^* := t$; $p := p'$; go to step 2
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Additional mechanisms used by LK algorithm:

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Note:

Variable depth search algorithms have been very successful for other problems, including:

- the Graph Partitioning Problem [Kernigan and Lin, 1970];
- the Unconstrained Binary Quadratic Programming Problem [Merz and Freisleben, 2002];
- the Generalised Assignment Problem [Yagiura *et al.*, 1999].

Dynasearch (1)

- Iterative improvement method based on building complex search steps from combinations of simple search steps.
- Simple search steps constituting any given complex step are required to be *mutually independent*, *i.e.*, do not interfere with each other w.r.t. effect on evaluation function and feasibility of candidate solutions.

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Goal:

Effectively escape from local minima of given evaluation function.

General approach:

For fixed neighbourhood, use step function that permits *worsening search steps*.

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Randomised Iterative Improvement

Key idea: In each search step, with a fixed probability perform an uninformed random walk step instead of an iterative improvement step.

Randomised Iterative Improvement (RII):

determine initial candidate solution s
While termination condition is not satisfied:
  With probability wp:
    choose a neighbour s' of s uniformly at random
  Otherwise:
    choose a neighbour s' of s such that $g(s') < g(s)$ or,
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Note:

- No need to terminate search when local minimum is encountered

  Instead: Bound number of search steps or CPU time from beginning of search or after last improvement.

- Probabilistic mechanism permits arbitrary long sequences of random walk steps

  Therefore: When run sufficiently long, RII is guaranteed to find (optimal) solution to any problem instance with arbitrarily high probability.

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Example: Randomised Iterative Best Improvement for SAT

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procedure GUWSAT(F, wp, maxSteps)
   input: propositional formula F, probability wp, integer maxSteps
   output: model of F or ∅

   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
      with probability wp do
         select x uniformly at random from set of all variables in F;
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         select x uniformly at random from {x' | x' is a variable in F and
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Key idea: Accept worsening steps with probability that depends on respective deterioration in evaluation function value: bigger deterioration $\cong$ smaller probability

Realisation:

- Function $p(g, s)$: determines probability distribution over neighbours of s based on their values under evaluation function g.
- Let $step(s)(s') := p(g, s)(s')$.

Note:

- Behaviour of PII crucially depends on choice of p.
- II and RII are special cases of PII.

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Example: Metropolis PII for the TSP (1)

- **Search space:** set of all Hamiltonian cycles in given graph G.
- **Solution set:** same as search space (*i.e.*, all candidate solutions are considered feasible).
- **Neighbourhood relation:** reflexive variant of 2-exchange neighbourhood relation (includes s in $N(s)$, *i.e.*, allows for steps that do not change search position).

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Simulated Annealing

Key idea: Vary temperature parameter, *i.e.*, probability of accepting worsening moves, in Probabilistic Iterative Improvement according to *annealing schedule* (aka *cooling schedule*).

Inspired by physical annealing process:

- candidate solutions $\cong$ states of physical system
- evaluation function $\cong$ thermodynamic energy
- globally optimal solutions $\cong$ ground states
- parameter $T \cong$ physical temperature

Note: In physical process (*e.g.*, annealing of metals), perfect ground states are achieved by very slow lowering of temperature.

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determine initial candidate solution s
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While termination condition is not satisfied:
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Note:

- 2-stage step function based on
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Extension of previous PII algorithm for the TSP, with

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  instead of computing exponential function $\exp(\Delta/T)$ for each step with $\Delta := f(s) - f(s')$ (expensive!), use precomputed table for range of argument values Δ/T.

'Convergence' result for SA:

Under certain conditions (extremely slow cooling),
any sufficiently long trajectory of SA is guaranteed to end in
an optimal solution [Geman and Geman, 1984; Hajek, 1998].

Note:

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Key idea: Use aspects of search history (memory) to escape from local minima.

Simple Tabu Search:

- Associate *tabu attributes* with candidate solutions or solution components.
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- Non-tabu search positions in $N(s)$ are called *admissible neighbours of s*.
- After a search step, the current search position or the solution components just added/removed from it are declared *tabu* for a fixed number of subsequent search steps (*tabu tenure*).
- Often, an additional *aspiration criterion* is used: this specifies conditions under which tabu status may be overridden (*e.g.*, if considered step leads to improvement in incumbent solution).

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- **Search space:** set of all truth assignments for propositional variables in given CNF formula F.
- **Solution set:** models of F.
- Use 1-flip **neighbourhood relation**, *i.e.*, two truth assignments are neighbours iff they differ in the truth value assigned to one variable.
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- *GSAT/Tabu* used to be state of the art for SAT solving.
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- tt too low ⇒ search stagnates due to inability to escape from local minima;
- tt too high ⇒ search becomes ineffective due to overly restricted search path (admissible neighbourhoods too small)

Advanced TS methods:

- **Robust Tabu Search** [Taillard, 1991]:
  repeatedly choose tt from given interval;
  also: force specific steps that have not been made for a long time.
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- Occasionally backtrack to *elite candidate solutions*, *i.e.*, high-quality search positions encountered earlier in the search; when doing this, all associated tabu attributes are cleared.
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determine *initial candidate solution s*
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While *termination criterion* is not satisfied:
| compute *modified evaluation function g'* from *g*
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  $$g'(\pi, s) := g(\pi, s) + \sum_{i \in SC(\pi', s)} penalty(i),$$

  where $SC(\pi', s)$ = set of solution components of problem instance π' used in candidate solution s.

- **Penalty initialisation:** For all i: $penalty(i) := 0$.

- **Penalty update** in local minimum s: Typically involves *penalty increase* of some or all solution components of s; often also occasional *penalty decrease* or *penalty smoothing*.

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Solution components required for (optimal) solution may also be present in many local minima.

Possible solutions:

A: Occasional decreases/smoothing of penalties.

B: Only increase penalties of solution components that are least likely to occur in (optimal) solutions.

Implementation of **B**:

[Voudouris and Tsang, 1995]

Only increase penalties of solution components i with maximal utility:

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[Voudouris and Tsang 1995; 1999]

- **Given:** TSP instance G
- Search space: Hamiltonian cycles in G with n vertices; use standard 2-exchange neighbourhood;
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  $f(G, p) := w(p)$; $f_e(G, p) := w(e)$;
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- GENET [Davenport *et al.*, 1994]
- Clause weighting methods for SAT
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Simple examples:

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Iterated Local Search

Key Idea: Use two types of SLS steps:

- *subsidiary local search* steps for reaching local optima as efficiently as possible (intensification)
- *perturbation steps* for effectively escaping from local optima (diversification).

Also: Use *acceptance criterion* to control diversification *vs* intensification behaviour.

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Iterated Local Search (ILS):

determine initial candidate solution s
perform *subsidiary local search* on s
While termination criterion is not satisfied:
  $r := s$
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Note:

- *Subsidiary local search* results in a local minimum.
- ILS trajectories can be seen as walks in the space of local minima of the given evaluation function.
- *Perturbation phase* and *acceptance criterion* may use aspects of *search history* (*i.e.*, limited memory).
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- Always accept the *better* of the two candidate solutions

  ⇒ ILS performs Iterative Improvement in the space of local optima reached by subsidiary local search.

- Always accept the *more recent* of the two candidate solutions

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- Intermediate behaviour: select between the two candidate solutions based on the *Metropolis criterion* (*e.g.*, used in *Large Step Markov Chains* [Martin *et al.*, 1991].

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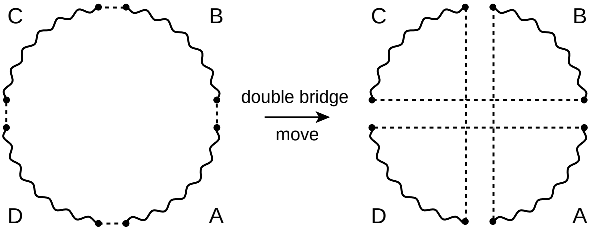

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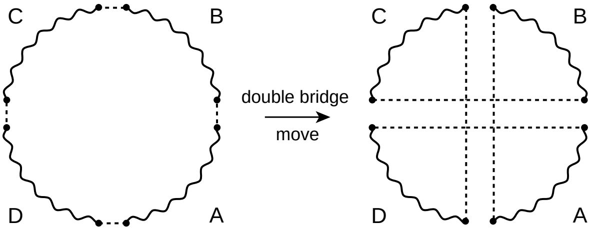

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Iterated local search algorithms . . .

- are typically rather easy to implement (given existing implementation of subsidiary simple SLS algorithms);
- achieve state-of-the-art performance on many combinatorial problems, including the TSP.

There are many SLS approaches that are closely related to ILS, including:

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- Chained Local Search [Martin and Otto, 1996]
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Key Idea: Combine randomised constructive search with subsequent perturbative local search.

Motivation:

- Candidate solutions obtained from construction heuristics can often be substantially improved by perturbative local search.
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While *termination criterion* is not satisfied:

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- Each step of *constructive search* adds a solution component selected uniformly at random from a *restricted candidate list (RCL)*.
- RCLs are constructed in each step usig a *heuristic function* h.
- RCLs based on *cardinality restriction* comprise the k best-ranked solution components. (k is a parameter of the algorithm.)
- RCLs based on *value restriction* comprise all solution components l for which $h(l) \leq h_{min} + \alpha \cdot (h_{max} - h_{min})$, where h_{min} = minimal value of h and h_{max} = maximal value of h for any l. (α is a parameter of the algorithm.)

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- **Given:** CNF formula F over variables $x_1, \ldots, x_n$
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  - in each step, add one atomic assignment (*i.e.*, assignment of a truth value to a currently unassigned variable)
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Key Idea: Alternate construction and perturbative local search phases as in GRASP, exploiting experience gained during the search process.

Realisation:

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- Initialise all weights to some small value τ_0 at beginning of search process.
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(Based on Ant System for the TSP [Dorigo *et al.*, 1991].)

- Search space and solution set as usual (all Hamiltonian cycles in given graph G).
- Associate weight τ_{ij} with each edge (i, j) in G.
- Use heuristic values $\eta_{ij} := 1/w((i, j))$.
- Initialise all weights to a small value τ_0 (parameter).
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  - stochastic tree search [Bresina, 1996],
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SLS methods discussed so far manipulate one candidate solution of given problem instance in each search step.

Straightforward extension: Use *population* (*i.e.*, set) of candidate solutions instead.

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- The use of populations provides a generic way to achieve search diversification.
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Key idea: Can be seen as population-based extension of AICS where population of agents – *(artificial) ants* – communicate via common memory – *(simulated) pheromone trails*.

Inspired by foraging behaviour of real ants:

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Application to combinatorial problems:
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- Ants iteratively construct candidate solutions.
- Solution construction is probabilistically biased by pheromone trail information, heuristic information and partial candidate solution of each ant.
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Note:

- In each cycle, each ant creates one candidate solution using a *constructive search procedure*.
- *Subsidiary local search* is applied to individual candidate solutions. (Some ACO algorithms do not use a subsidiary local search procedure.)
- All *pheromone trails* are initialised to the same value, τ_0.
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Example: A simple ACO algorithm for the TSP (1)

(Variant of Ant System for the TSP [Dorigo *et al.*, 1991; 1996].)

- Search space and solution set as usual (all Hamiltonian cycles in given graph G).
- Associate pheromone trails τ_{ij} with each edge (i,j) in G.
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Motivation: Edges belonging to highest-quality candidate solutions and/or that have been used by many ants should be preferably used in subsequent constructions.

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- *Termination:* After fixed number of cycles (= construction + local search phases).

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- Ants can be seen as walking along edges of given graph (using memory to ensure their tours correspond to Hamiltonian cycles) and depositing pheromone to reinforce edges of tours.
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Enhancements:

- use of look-ahead in construction phase;
- pheromone updates during construction phase;
- bounds on range and smoothing of pheromone levels.

Advanced ACO methods:

- Ant Colony System [Dorigo and Gambardella, 1997]
- $\mathcal{MAX}-\mathcal{MIN}$ Ant System [Stützle and Hoos, 1997; 2000]
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Ant Colony Optimisation ...

- has been applied very successfully to a wide range of combinatorial problems, including
  - the Open Shop Scheduling Problem,
  - the Sequential Ordering Problem, and
  - the Shortest Common Supersequence Problem;
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Note:

A general algorithmic framework for solving static and dynamic combinatorial problems using ACO techniques is provided by the *ACO metaheuristic* [Dorigo and Di Caro, 1999; Dorigo et al., 1999].

For further details on Ant Colony Optimisation, see the book by Dorigo and Stützle [2004].

Evolutionary Algorithms

Key idea: Iteratively apply *genetic operators* *mutation*, *recombination*, *selection* to a population of candidate solutions.

Inspired by simple model of biological evolution:

- *Mutation* introduces random variation in the genetic material of individuals.
- *Recombination* of genetic material during sexual reproduction produces *offspring* that combines features inherited from both *parents*.
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determine initial population *sp*

While *termination criterion* is not satisfied:

generate set *spr* of new candidate solutions
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Solution: Apply subsidiary local search after initialisation, mutation and recombination.

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Initialisation

- *Often:* independent, uninformed random picking from given search space.
- *But:* can also use multiple runs of construction heuristic.

Recombination

- Typically repeatedly selects a set of *parents* from current population and generates *offspring* candidate solutions from these by means of *recombination operator*.
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Example: One-point binary crossover operator

Given two parent candidate solutions $x_1 x_2 \ldots x_n$ and $y_1 y_2 \ldots y_n$:

1. choose index i from set $\{2, \ldots, n\}$ uniformly at random;
2. define offspring as $x_1 \ldots x_{i-1} y_i \ldots y_n$ and $y_1 \ldots y_{i-1} x_i \ldots x_n$.

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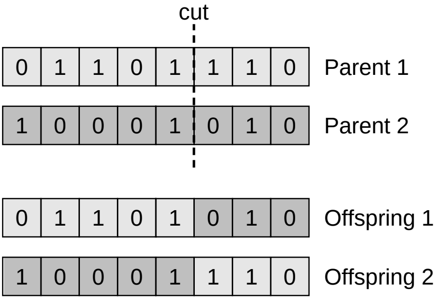

Mutation

- *Goal:* Introduce relatively small perturbations in candidate solutions in current population + offspring obtained from *recombination*.
- Typically, perturbations are applied stochastically and independently to each candidate solution; amount of perturbation is controlled by *mutation rate*.
- Can also use *subsidiary selection function* to determine subset of candidate solutions to which mutation is applied.
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Selection (1)

- Determines population for next cycle (*generation*) of the algorithm by selecting individual candidate solutions from current population + new candidate solutions obtained from *recombination*, *mutation* (+ *subsidiary local search*).
- *Goal:* Obtain population of high-quality solutions while maintaining *population diversity*.
- Selection is based on evaluation function (*fitness*) of candidate solutions such that better candidate solutions have a higher chance of 'surviving' the selection process.

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- Many selection schemes involve probabilistic choices, *e.g.*, *roulette wheel selection*, where the probability of selecting any candidate solution s is proportional to its fitness value, $g(s)$.
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- *Search space:* set of all truth assignments for propositional variables in given CNF formula F; *solution set:* models of F; use *1-flip neighbourhood relation*; *evaluation function:* number of unsatisfied clauses in F.
- *Note:* truth assignments can be naturally represented as bit strings.
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