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Heuristics and Approximation Algorithms

# (Stochastic) Local Search Algorithms

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# Outline

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1. Definitions

2. Local Search Algorithms

3. Local Search Revisited
   Components

# Definitions
## Neighborhood function

Neighborhood function $N : S_\pi \to 2^S$

Also defined as: $\mathcal{N} : S \times S \to \{T, F\}$ or $\mathcal{N} \subseteq S \times S$

- neighborhood (set) of candidate solution $s$: $N(s) := \{s' \in S \mid \mathcal{N}(s, s')\}$
- neighborhood size is $|N(s)|$
- neighborhood is symmetric if: $s' \in N(s) \Rightarrow s \in N(s')$
- neighborhood graph of $(S, N, \pi)$ is a directed graph: $G_N := (V, A)$ with $V = S$ and $(uv) \in A \Leftrightarrow v \in N(u)$
  (if symmetric neighborhood $\rightsquigarrow$ undirected graph)

A neighborhood function is also defined by means of an operator (aka move).

An operator $\Delta$ is a collection of operator functions $\delta : S \to S$ such that

$$s' \in N(s) \quad \Longrightarrow \quad \exists\, \delta \in \Delta, \delta(s) = s'$$

### Definition

*k*-exchange neighborhood: candidate solutions $s, s'$ are neighbors iff $s$ differs from $s'$ in at most $k$ solution components

### Examples:

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

# Neighborhood Operator

Goal: providing a formal description of neighborhood functions for the three main solution representations:

- Permutation
  - linear permutation: Single Machine Total Weighted Tardiness Problem
  - circular permutation: Traveling Salesman Problem
- Assignment: SAT, CSP
- Set, Partition: Max Independent Set

A neighborhood function $N : S \to 2^S$ is also defined through an operator.
An operator $\Delta$ is a collection of operator functions $\delta : S \to S$ such that

$$s' \in N(s) \iff \exists \delta \in \Delta \mid \delta(s) = s'$$

# Permutations

$S_n$ indicates the set all permutations of the numbers $\{1, 2, \ldots, n\}$

$(1, 2 \ldots, n)$ is the identity permutation $\iota$.

If $\pi \in \Pi(n)$ and $1 \leq i \leq n$ then:

- $\pi_i$ is the element at position $i$
- $pos_\pi(i)$ is the position of element $i$

Alternatively, a permutation is a bijective function $\pi(i) = \pi_i$

The permutation product $\pi \cdot \pi'$ is the composition $(\pi \cdot \pi')_i = \pi'(\pi(i))$

For each $\pi$ there exists a permutation such that $\pi^{-1} \cdot \pi = \iota$
$\pi^{-1}(i) = pos_\pi(i)$

$$\Delta_N \subset S_n$$

# Linear Permutations

Swap operator

$$\Delta_S = \{\delta_S^i \mid 1 \leq i \leq n\}$$

$$\delta_S^i(\pi_1 \ldots \pi_i \pi_{i+1} \ldots \pi_n) = (\pi_1 \ldots \pi_{i+1} \pi_i \ldots \pi_n)$$

Interchange operator

$$\Delta_X = \{\delta_X^{ij} \mid 1 \leq i < j \leq n\}$$

$$\delta_X^{ij}(\pi) = (\pi_1 \ldots \pi_{i-1} \pi_j \pi_{i+1} \ldots \pi_{j-1} \pi_i \pi_{j+1} \ldots \pi_n)$$

($\equiv$ set of all transpositions)
Insert operator

$$\Delta_I = \{\delta_I^{ij} \mid 1 \leq i \leq n, 1 \leq j \leq n, j \neq i\}$$

$$\delta_I^{ij}(\pi) = \begin{cases} (\pi_1 \ldots \pi_{i-1} \pi_{i+1} \ldots \pi_j \pi_i \pi_{j+1} \ldots \pi_n) & i < j \\ (\pi_1 \ldots \pi_j \pi_i \pi_{j+1} \ldots \pi_{i-1} \pi_{i+1} \ldots \pi_n) & i > j \end{cases}$$

# Circular Permutations

Reversal (2-edge-exchange)

$$\Delta_R = \{\delta_R^{ij} \mid 1 \le i < j \le n\}$$

$$\delta_R^{ij}(\pi) = (\pi_1 \dots \pi_{i-1}\pi_j \dots \pi_i\pi_{j+1} \dots \pi_n)$$

Block moves (3-edge-exchange)

$$\Delta_B = \{\delta_B^{ijk} \mid 1 \le i < j < k \le n\}$$

$$\delta_B^{ij}(\pi) = (\pi_1 \dots \pi_{i-1}\pi_j \dots \pi_k\pi_i \dots \pi_{j-1}\pi_{k+1} \dots \pi_n)$$

Short block move (Or-edge-exchange)

$$\Delta_{SB} = \{\delta_{SB}^{ij} \mid 1 \le i < j \le n\}$$

$$\delta_{SB}^{ij}(\pi) = (\pi_1 \dots \pi_{i-1}\pi_j\pi_{j+1}\pi_{j+2}\pi_i \dots \pi_{j-1}\pi_{j+3} \dots \pi_n)$$

# Assignments

An assignment can be represented as a mapping $\sigma : \{X_1 \dots X_n\} \to \{v : v \in D, |D| = k\}$:

$$\sigma = \{X_i = v_i, X_j = v_j, \dots\}$$

One-exchange operator

$$\Delta_{1E} = \{\delta_{1E}^{il} \mid 1 \leq i \leq n, 1 \leq l \leq k\}$$

$$\delta_{1E}^{il}(\sigma) = \left\{\sigma' : \sigma'(X_i) = v_l \text{ and } \sigma'(X_j) = \sigma(X_j)\ \forall j \neq i\right\}$$

Two-exchange operator

$$\Delta_{2E} = \{\delta_{2E}^{ij} \mid 1 \leq i < j \leq n\}$$

$$\delta_{2E}^{ij}(\sigma) = \left\{\sigma' : \sigma'(X_i) = \sigma(X_j),\ \sigma'(X_j) = \sigma(X_i) \ \text{ and } \ \sigma'(X_l) = \sigma(X_l)\ \forall l \neq i, j\right\}$$

# Partitioning

An assignment can be represented as a partition of objects selected and not selected
$s : \{X\} \to \{C, \overline{C}\}$ (it can also be represented by a bit string)

One-addition operator

$$\Delta_{1E} = \{\delta_{1E}^{v} \mid v \in \bar{C}\}$$

$$\delta_{1E}^{v}(s) = \left\{s : C' = C \cup v \text{ and } \bar{C}' = \bar{C} \setminus v\right\}$$

One-deletion operator

$$\Delta_{1E} = \{\delta_{1E}^{v} \mid v \in C\}$$

$$\delta_{1E}^{v}(s) = \left\{s : C' = C \setminus v \text{ and } \bar{C}' = \bar{C} \cup v\right\}$$

Swap operator

$$\Delta_{1E} = \{\delta_{1E}^{v} \mid v \in C, u \in \bar{C}\}$$

$$\delta_{1E}^{v}(s) = \left\{s : C' = C \cup u \setminus v \text{ and } \bar{C}' = \bar{C} \cup v \setminus u\right\}$$

# Definitions

Definition:

- Local minimum: search position without improving neighbors wrt given evaluation function $f$ and neighborhood function $N$,
  *i.e.*, position $s \in S$ such that $f(s) \leq f(s')$ for all $s' \in N(s)$.
- Strict local minimum: search position $s \in S$ such that $f(s) < f(s')$ for all $s' \in N(s)$.
- *Local maxima* and *strict local maxima*: defined analogously.

# Outline

# Local Search

- Model
  - Variables $\rightsquigarrow$ solution representation, search space
  - Constraints:
    – implicit
    – one-way defining invariants
    – soft
  - evaluation function
- Search (solve an optimization problem)
  - Construction heuristics
  - Neighborhoods, Iterative Improvement, (Stochastic) local search
  - Metaheuristics: Tabu Search, Simulated Annealing, Iterated Local Search
  - Population based metaheuristics

# Local Search Algorithms

Given a (combinatorial) optimization problem $\Pi$ and one of its instances $\pi$:

1. search space $S(\pi)$

   - specified by the definition of (finite domain, integer) variables and their values handling implicit constraints
   - all together they determine the representation of candidate solutions
   - common solution representations are discrete structures such as: sequences, permutations, partitions, graphs

   Note: solution set $S'(\pi) \subseteq S(\pi)$

# Local Search Algorithms (cntd)

2. evaluation function $f_\pi : S(\pi) \to \mathbf{R}$
   - it handles the soft constraints and the objective function
3. neighborhood function, $N_\pi : S \to 2^{S(\pi)}$
   - defines for each solution $s \in S(\pi)$ a set of solutions $N(s) \subseteq S(\pi)$ that are in some sense close to $s$.

# Local Search Algorithms (cntd)

## Further components [according to [HS]]

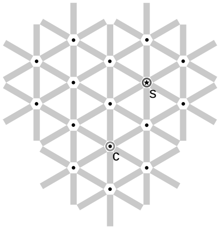
4. set of memory states $M(\pi)$
   (may consist of a single state, for LS algorithms that do not use memory)

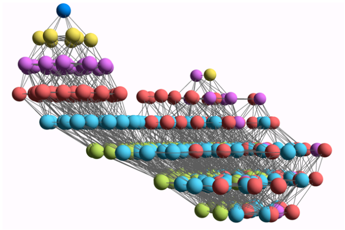
5. initialization function $\texttt{init} : \emptyset \to S(\pi)$
   (can be seen as a probability distribution $\Pr(S(\pi) \times M(\pi))$ over initial search positions and memory states)

6. step function $\texttt{step} : S(\pi) \times M(\pi) \to S(\pi) \times M(\pi)$
   (can be seen as a probability distribution $\Pr(S(\pi) \times M(\pi))$ over subsequent, neighboring search positions and memory states)

7. termination predicate $\texttt{terminate} : S(\pi) \times M(\pi) \to \{\top, \bot\}$
   (determines the termination state for each search position and memory state)

# Local search — global view



Neighborhood graph

- vertices: candidate solutions (search positions)
- vertex labels: evaluation function
- edges: connect "neighboring" positions
- s: (optimal) solution
- c: current search position

# Local Search Algorithms

Note:

- Local search implements a walk through the neighborhood graph
- Procedural versions of `init`, `step` and `terminate` implement sampling from respective probability distributions.
- Local search algorithms can be described as Markov processes:
  behavior in any search state $\{s, m\}$ depends only
  on current position $s$
  higher order MP if (limited) memory $m$.

# Local Search (LS) Algorithm Components
## Step function

Search step (or move):
pair of search positions $s, s'$ for which
$s'$ can be reached from $s$ in one step, *i.e.*, $s' \in N(s)$ and
$\texttt{step}(\{s, m\}, \{s', m'\}) > 0$ for some memory states $m, m' \in M$.

- Search trajectory: finite sequence of search positions $\langle s_0, s_1, \ldots, s_k \rangle$ such that $(s_{i-1}, s_i)$ is a *search step* for any $i \in \{1, \ldots, k\}$
  and the probability of initializing the search at $s_0$
  is greater than zero, *i.e.*, $\texttt{init}(\{s_0, m\}) > 0$
  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 LS algorithm.
  - random
  - based on evaluation function
  - based on memory

# Iterative Improvement

**Iterative Improvement (II):**
determine initial candidate solution $s$
**while** $s$ has better neighbors **do**
  choose a neighbor $s'$ of $s$ such that $f(s') < f(s)$
  $s := s'$

- If more than one neighbor has better cost then need to choose one (heuristic pivot rule)
- The procedure ends in a local optimum $\hat{s}$:
  Def.: Local optimum $\hat{s}$ w.r.t. $N$ if $f(\hat{s}) \leq f(s)\ \forall s \in N(\hat{s})$
- Issue: how to avoid getting trapped in bad local optima?
  - use more complex neighborhood functions
  - restart
  - allow non-improving moves

# Metaheuristics

- “Restart” + parallel search
  Avoid local optima
  Improve search space coverage

- Variable Neighborhood Search and Large Scale Neighborhood Search
  diversified neighborhoods + incremental algorithmics
  ("diversified" $\equiv$ multiple, variable-size, and rich).

- Tabu Search: Online learning of moves
  Discard undoing moves,
  Discard inefficient moves
  Improve efficient moves selection

- Simulated annealing
  Allow degrading solutions

# Summary: Local Search Algorithms

For given problem instance $\pi$:

1. search space $S_\pi$, solution representation: variables + implicit constraints
2. evaluation function $f_\pi : S \to \mathbf{R}$, soft constraints + objective
3. neighborhood relation $\mathcal{N}_\pi \subseteq S_\pi \times S_\pi$
4. set of memory states $M_\pi$
5. initialization function $\mathtt{init} : \emptyset \to S_\pi \times M_\pi$
6. step function $\mathtt{step} : S_\pi \times M_\pi \to S_\pi \times M_\pi$
7. termination predicate $\mathtt{terminate} : S_\pi \times M_\pi \to \{\top, \bot\}$

# Decision vs Minimization

**LS-Decision**$(\pi)$
**input:** problem instance $\pi \in \Pi$
**output:** solution $s \in S'(\pi)$ **or** $\emptyset$

$(s, m) := \texttt{init}(\pi)$

**while** not $\texttt{terminate}(\pi, \texttt{s}, \texttt{m})$ **do**
    $(s, m) := \texttt{step}(\pi, \texttt{s}, \texttt{m})$

**if** $s \in S'(\pi)$ **then**
    **return** $s$
**else**
    **return** $\emptyset$

**LS-Minimization**$(\pi')$
**input:** problem instance $\pi' \in \Pi'$
**output:** solution $s \in S'(\pi')$ **or** $\emptyset$

$(s, m) := \texttt{init}(\pi')$;
$s_b := s$;
**while** not $\texttt{terminate}(\pi', \texttt{s}, \texttt{m})$ **do**
    $(s, m) := \texttt{step}(\pi', \texttt{s}, \texttt{m})$;
    **if** $f(\pi', s) < f(\pi', s_b)$ **then**
        $s_b := s$;

**if** $s_b \in S'(\pi')$ **then**
    **return** $s_b$
**else**
    **return** $\emptyset$

However, the algorithm on the left has little guidance, hence most often decision problems are transformed in optimization problems by, eg, couting number of violations.

# Outline

# LS Algorithm Components

## Search space

### Search Space

Solution representations defined by the variables and the implicit constraints:

- permutations (implicit: alldiffrerent)
  - linear (scheduling problems)
  - circular (traveling salesman problem)
- arrays (implicit: assign exactly one, assignment problems: GCP)
- sets (implicit: disjoint sets, partition problems: graph partitioning, max indep. set)

$\rightsquigarrow$ Multiple viewpoints are useful in local search!

# LS Algorithm Components
## Evaluation function

### Evaluation (or cost) function:

- function $f_\pi : S_\pi \to \mathbf{Q}$ that maps candidate solutions of a given problem instance $\pi$ onto rational numbers (most often integer), such that global optima correspond to solutions of $\pi$;
- used for assessing or ranking neighbors of current search position to provide guidance to search process.

### Evaluation *vs* objective functions:

- *Evaluation function*: part of LS algorithm.
- *Objective function*: integral part of optimization problem.
- Some LS methods use evaluation functions different from given objective function (*e.g.*, guided local search).

# Constrained Optimization Problems

Constrained Optimization Problems exhibit two issues:

- feasibility
  eg, treveling salesman problem with time windows: customers must be visited within their time window.
- optimization
  minimize the total tour.

How to combine them in local search?

- sequence of feasibility problems
- staying in the space of feasible candidate solutions
- considering feasible and infeasible configurations

# Constraint-based local search

## From Van Hentenryck and Michel

If infeasible solutions are allowed, we count violations of constraints.

What is a violation?
Constraint specific:

- decomposition-based violations
  number of violated constraints, eg: alldiff
- variable-based violations
  min number of variables that must be changed to satisfy $c$.
- value-based violations
  for constraints on number of occurences of values
- arithmetic violations
- combinations of these

# Constraint-based local search

## From Van Hentenryck and Michel

Combinatorial constraints

- $\texttt{alldiff}(x_1, \ldots, x_n)$:
  Let $a$ be an assignment with values $V = \{a(x_1), \ldots, a(x_n)\}$ and $c_v = \#_a(v, x)$ be the number of occurrences of $v$ in $a$.
  Possible definitions for violations are:
  - $\text{viol} = \sum_{v \in V} I(\max\{c_v - 1, 0\} > 0)$ value-based
  - $\text{viol} = \max_{v \in V} \max\{c_v - 1, 0\}$ value-based
  - $\text{viol} = \sum_{v \in V} \max\{c_v - 1, 0\}$ value-based
  - $\#$ variables with same value, variable-based, here leads to same definitions as previous three

Arithmetic constraints

- $l \leq r \leadsto \text{viol} = \max\{l - r, 0\}$
- $l = r \leadsto \text{viol} = |l - r|$
- $l \neq r \leadsto \text{viol} = 1$ if $l = r$, $0$ otherwise