DM841

Discrete Optimization

Part 2 – Lecture 5
Local Search Theory

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Outline

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LS Algorithm Components
Neighborhood function

Neighborhood function $\mathcal{N}_\pi : S_\pi \to 2^{S_\pi}$

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, π) is a directed graph: $G_{\mathcal{N}_\pi} := (V, A)$ with $V = S_\pi$ and $(uv) \in A \Leftrightarrow v \in N(u)$
  (if symmetric neighborhood $\rightsquigarrow$ undirected graph)

Notation: N when set, $\mathcal{N}$ when collection of sets or function

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

An operator Δ is a collection of operator functions $\delta : S \rightarrow S$ such that

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

Definition

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

Examples:

- 1-exchange (flip) neighborhood for SAT
  (solution components = single variable assignments)
- 2-exchange neighborhood for TSP
  (solution components = edges in given graph)

LS Algorithm Components

Definition:

- Local minimum: search position without improving neighbors wrt given evaluation function f and neighborhood $\mathcal{N}$, *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.

LS Algorithm Components

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.

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.*, $\mathcal{N}(s, s')$ 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

Outline

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 $\mathcal{N} : S \rightarrow 2^S$ is also defined through an operator. An operator Δ is a collection of operator functions $\delta : S \rightarrow S$ such that

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

Permutations

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

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

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

- π_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 π 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

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

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

Interchange operator

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

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

($\equiv$ set of all transpositions)

Insert operator

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

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

Circular Permutations

Reversal (2-edge-exchange)

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

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

Block moves (3-edge-exchange)

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

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

Short block move (Or-edge-exchange)

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

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

Assignments

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

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

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 $s : \{X\} \rightarrow \{C, \overline{C}\}$
(it can also be represented by a bit string)

One-addition operator

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

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

One-deletion operator

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

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

Swap operator

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

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

Outline

Distances

Set of paths in $\mathcal{N}$ with $s, s' \in S$:

$$\Phi(s, s') = \{(s_1, \ldots, s_h) \mid s_1 = s, s_h = s' \; \forall i : 1 \leq i \leq h-1, \langle s_i, s_{i+1} \rangle \in E_\mathcal{N}\}$$

If $\phi = (s_1, \ldots, s_h) \in \Phi(s, s')$ let $|\phi| = h$ be the length of the path; then the distance between any two solutions s, s' is the length of shortest path between s and s' in $\mathcal{N}$:

$$d_\mathcal{N}(s, s') = \min_{\phi \in \Phi(s, s')} |\Phi|$$

$\mathtt{diam}(\mathcal{N}) = \max\{d_\mathcal{N}(s, s') \mid s, s' \in S\}$ (= maximal distance between any two candidate solutions)
(= worst-case lower bound for number of search steps required for reaching (optimal) solutions)

Note: with permutations it is easy to see that:

$$d_\mathcal{N}(\pi, \pi') = d_\mathcal{N}(\pi^{-1} \cdot \pi', \iota)$$

Distances for Linear Permutation Representations

- Swap neighborhood operator
  computable in $O(n^2)$ by the precedence based distance metric:
  $d_S(\pi, \pi') = \#\{\langle i, j\rangle | 1 \leq i < j \leq n, pos_{\pi'}(\pi_j) < pos_{\pi'}(\pi_i)\}$.
  $\mathtt{diam}(G_{\mathcal{N}}) = n(n-1)/2$

- Interchange neighborhood operator
  Computable in $O(n) + O(n)$ since
  $d_X(\pi, \pi') = d_X(\pi^{-1} \cdot \pi', \iota) = n - c(\pi^{-1} \cdot \pi')$
  $c(\pi)$ is the number of disjoint cycles that decompose a permutation.
  $\mathtt{diam}(G_{\mathcal{N}_X}) = n - 1$

- Insert neighborhood operator
  Computable in $O(n) + O(n\, log(n))$ since
  $d_I(\pi, \pi') = d_I(\pi^{-1} \cdot \pi', \iota) = n - |lis(\pi^{-1} \cdot \pi')|$ where $lis(\pi)$ denotes the length of the longest increasing subsequence.
  $\mathtt{diam}(G_{\mathcal{N}_I}) = n - 1$

Distances for Circular Permutation Representations

- Reversal neighborhood operator
  sorting by reversal is known to be NP-hard
  surrogate in TSP: bond distance
- Block moves neighborhood operator
  unknown whether it is NP-hard but there does not exist a proved polynomial-time algorithm

Distances for Assignment Representations

- Hamming Distance

- An assignment can be seen as a partition of n in k mutually exclusive non-empty subsets

  One-exchange neighborhood operator
  The *partition-distance* $d_{1E}(\mathcal{P}, \mathcal{P}')$ between two partitions $\mathcal{P}$ and $\mathcal{P}'$ is the minimum number of elements that must be moved between subsets in $\mathcal{P}$ so that the resulting partition equals $\mathcal{P}'$.

  The partition-distance can be computed in polynomial time by solving an assignment problem. Given the assignment matrix M where in each cell (i, j) it is $|S_i \cap S'_j|$ with $S_i \in \mathcal{P}$ and $S'_j \in \mathcal{P}'$ and defined $A(\mathcal{P}, \mathcal{P}')$ the assignment of maximal sum then it is $d_{1E}(\mathcal{P}, \mathcal{P}') = n - A(\mathcal{P}, \mathcal{P}')$

Example: Search space size and diameter for SAT

SAT instance with n variables, 1-flip neighborhood:
$G_{\mathcal{N}} = n$-dimensional hypercube; diameter of $G_{\mathcal{N}} = n$.

Example: Search space size and diameter for the TSP

- Search space size = $(n-1)!/2$
- Insert neighborhood
  size = $(n-3)n$
  diameter = $n-2$
- 2-exchange neighborhood
  size = $\binom{n}{2} = n \cdot (n-1)/2$
  diameter in $[n/2, n-2]$
- 3-exchange neighborhood
  size = $\binom{n}{3} = n \cdot (n-1) \cdot (n-2)/6$
  diameter in $[n/3, n-1]$

Let $\mathcal{N}_1$ and $\mathcal{N}_2$ be two different neighborhood functions for the same instance (S, f, π) of a combinatorial optimization problem.

If for all solutions $s \in S$ we have $N_1(s) \subseteq N_2(s)$ then we say that $\mathcal{N}_2$ dominates $\mathcal{N}_1$

Example:

In TSP, 1-insert is dominated by 3-exchange.
(1-insert corresponds to 3-exchange and there are 3-exchanges that are not 1-insert)

Search Landscape

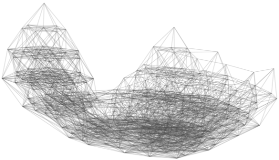
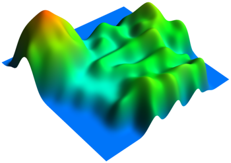
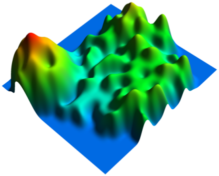
Given:

- Problem instance π
- Search space S_π
- Neighborhood function $\mathcal{N} : S \subseteq 2^S$
- Evaluation function $f_\pi : S \rightarrow \mathbf{R}$

Definition:

The **search landscape** L is the vertex-labeled neighborhood graph given by the triplet $\mathcal{L} = \langle S_\pi, N_\pi, f_\pi \rangle$.

Search Landscape

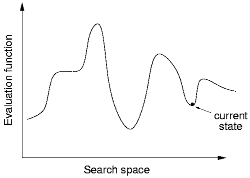
Transition Graph of Iterative Improvement

Given $\mathcal{L} = \langle S_\pi, N_\pi, f_\pi \rangle$, the transition graph of iterative improvement is a directed acyclic subgraph obtained from $\mathcal{L}$ by deleting all arcs (i, j) for which it holds that the cost of solution j is worse than or equal to the cost of solution i.

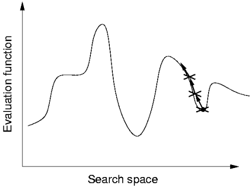
It can be defined for other algorithms as well and it plays a central role in the theoretical analysis of proofs of convergence.

Ideal visualization of landscapes principles

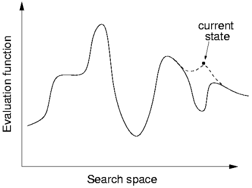
- Simplified landscape representation



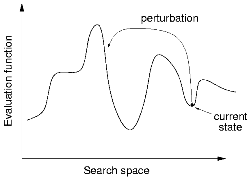
- Tabu Search



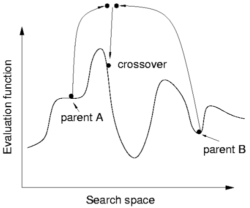
- Guided Local Search



- Iterated Local Search



- Evolutionary Alg.



Fundamental Properties

The behavior and performance of an LS algorithm on a given problem instance crucially depends on properties of the respective search landscape.

Simple properties:

- search space size $|S|$
- reachability: solution j is reachable from solution i if neighborhood graph has a path from i to j.
  - strongly connected neighborhood graph
  - weakly optimally connected neighborhood graph
- distance between solutions
- neighborhood size (ie, degree of vertices in neigh. graph)
- cost of fully examining the neighborhood
- relation between different neighborhood functions (if $N_1(s) \subseteq N_2(s)$ forall $s \in S$ then $\mathcal{N}_2$ dominates $\mathcal{N}_1$)

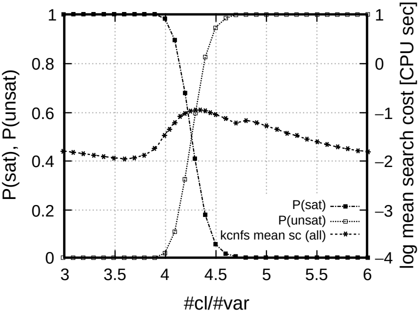
Outline

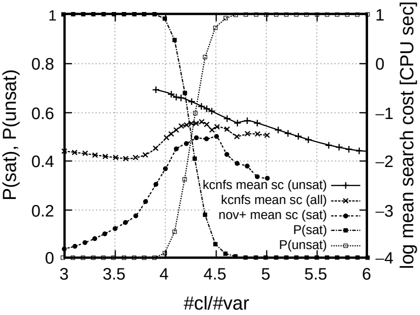
Other Search Space Properties

- number of (optimal) solutions $|S'|$, solution density $|S'|/|S|$
- distribution of solutions within the neighborhood graph

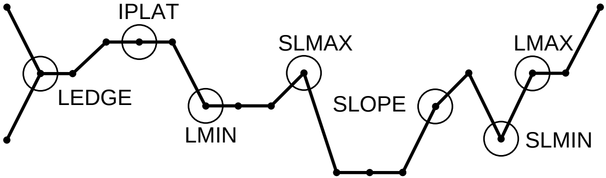
Phase Transition for 3-SAT

Random instances ⇝ m clauses of n uniformly chosen variables





Classification of search positions

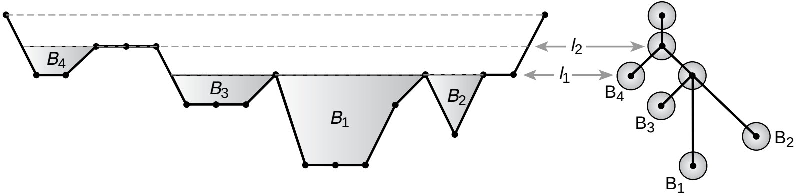


position type	>	=	<
SLMIN (strict local min)	+	–	–
LMIN (local min)	+	+	–
IPLAT (interior plateau)	–	+	–
SLOPE	+	–	+
LEDGE	+	+	+
LMAX (local max)	–	+	+
SLMAX (strict local max)	–	–	+

"+" = present, "–" absent; table entries refer to neighbors with larger (">") , equal ("="), and smaller ("<") evaluation function values

Other Search Space Properties

- plateux
- barrier and basins



Outline

Escaping Local Optima

Possibilities:

- Restart: re-initialize search whenever a local optimum is encountered.
  (Often rather ineffective due to cost of initialization.)
- 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.)
- Diversify the neighborhood: multiple, variable-size, rich (while still preserving incremental algorithmics insights)

Note: None of these mechanisms is guaranteed to always escape effectively from local optima.

Diversification *vs* Intensification

- Intensification: aims at greedily increasing solution quality, *e.g.*, by exploiting the evaluation function.
- Diversification: aims at preventing search stagnation, that is, the search process getting trapped in confined regions.
- Goal-directed and randomized components of LS strategy need to be balanced carefully.

Examples:

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

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

'Simple' Metaheuristics

Goal:

Effectively escape from local minima of given evaluation function.

General approach:

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

Specific methods:

- Stochastic Local Search
- Simulated Annealing
- (Guided Local Search)
- Tabu Search
- Iterated Local Search
- Variable Neighborhood Search
- Evolutionary Algorithms