DM841

Discrete Optimization

Lecture 12
Efficiency Issues
Neighborhoods and Landscapes

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Outline

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Summary: Local Search Algorithms
(as in [Hoos, Stützle, 2005])

For given problem instance π:

1. search space S_π
2. evaluation function $f_\pi : S \to \mathbf{R}$
3. neighborhood relation $\mathcal{N}_\pi \subseteq S_\pi \times S_\pi$
4. set of memory states M_π
5. initialization function $\texttt{init} : \emptyset \to S_\pi \times M_\pi)$
6. step function $\texttt{step} : S_\pi \times M_\pi \to S_\pi \times M_\pi$
7. termination predicate $\texttt{terminate} : S_\pi \times M_\pi \to \{\top, \bot\}$

Efficiency and Effectiveness

After implementation and test of the above components, improvements in efficiency (ie, computation time) can be achieved by:

A. fast incremental evaluation (ie, delta evaluation)

B. neighborhood pruning

C. clever use of data structures

Improvements in effectiveness, ie, quality, can be achieved by:

D. application of a metaheuristic

E. definition of a larger neighborhood

Outline

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Single Machine Total Weighted Tardiness Problem

- Interchange: size $\binom{n}{2}$ and $O(|i-j|)$ evaluation each
  - first-improvement: π_j, π_k
    - $p_{\pi_j} \leq p_{\pi_k}$ for improvements, $w_j T_j + w_k T_k$ must decrease because jobs in $\pi_j, \ldots, \pi_k$ can only increase their tardiness.
    - $p_{\pi_j} \geq p_{\pi_k}$ possible use of auxiliary data structure to speed up the computation
  - best-improvement: π_j, π_k
    - $p_{\pi_j} \leq p_{\pi_k}$ for improvements, $w_j T_j + w_k T_k$ must decrease at least as the best interchange found so far because jobs in $\pi_j, \ldots, \pi_k$ can only increase their tardiness.
    - $p_{\pi_j} \geq p_{\pi_k}$ possible use of auxiliary data structure to speed up the computation
- Swap: size $n-1$ and $O(1)$ evaluation each
- Insert: size $(n-1)^2$ and $O(|i-j|)$ evaluation each
  But possible to speed up with systematic examination by means of swaps: an interchange is equivalent to $|i-j|$ swaps hence overall examination takes $O(n^2)$

Outline

TSP

Efficient implementations of 2-opt, 2H-opt and 3-opt local search.

A. Delta evaluation already in $O(1)$

B. Fixed radius search + DLB

C. Data structures

Details at black board and references [Bentley, 1992; Johnson and McGeoch, 2002; Applegate et al., 2006]

Local Search for the Traveling Salesman Problem

- *k*-exchange heuristics
  - 2-opt
  - 2.5-opt
  - Or-opt
  - 3-opt
- complex neighborhoods
  - Lin-Kernighan
  - Helsgaun's Lin-Kernighan
  - Dynasearch
  - ejection chains approach

Implementations exploit speed-up techniques

1. neighborhood pruning: fixed radius nearest neighborhood search
2. neighborhood lists: restrict exchanges to most interesting candidates
3. don't look bits: focus perturbative search to "interesting" part
4. sophisticated data structures

Implementation examples by Stützle:
http://www.sls-book.net/implementations.html

TSP data structures

Tour representation:

- determine pos of v in π
- determine succ and prec
- check whether u_k is visited between u_i and u_j
- execute a k-exchange (reversal)

Possible choices:

- $|V| < 1.000$ array for π and π^{-1}
- $|V| < 1.000.000$ two level tree
- $|V| > 1.000.000$ splay tree

Moreover static data structure:

- priority lists
- k-d trees

Look at implementation of local search for TSP by T. Stützle:

File: http://www.imada.sdu.dk/~marco/DM811/Resources/ls.c

```
two_opt_b(tour); % best improvement, no speedup
two_opt_f(tour); % first improvement, no speedup
two_opt_best(tour); % first improvement including speed−ups (dlbs, fixed radius near
      neighbour searches, neughbourhood lists)
two_opt_first(tour); % best improvement including speed−ups (dlbs, fixed radius near
      neighbour searches, neughbourhood lists)
three_opt_first(tour); % first improvement
```

Table 17.1 Cases for k-opt moves.

k	No. of Cases
2	1
3	4
4	20
5	148
6	1,358
7	15,104
8	198,144
9	2,998,656
10	51,290,496

[Appelgate Bixby, Chvátal, Cook, 2006]

Table 17.2 Computer-generated source code for k-opt moves.

k	No. of Lines
6	120,228
7	1,259,863
8	17,919,296

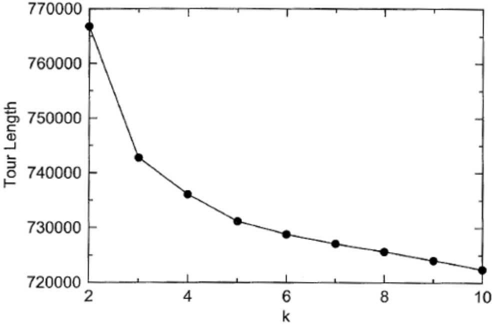

Figure 17.1 k-opt on a 10,000-city Euclidean TSP.

References

Applegate D.L., Bixby R.E., Chvátal V., and Cook W.J. (2006). **The Traveling Salesman Problem: A Computational Study**. Princeton University Press.

Bentley J. (1992). **Fast algorithms for geometric traveling salesman problems**. *ORSA Journal on Computing*, 4(4), pp. 387–411.

Johnson D.S. and McGeoch L.A. (2002). **Experimental analysis of heuristics for the STSP**. In *The Traveling Salesman Problem and Its Variations*, edited by G. Gutin and A. Punnen, pp. 369–443. Kluwer Academic Publishers, Boston, MA, USA.

Outline

Computational Complexity of LS

For a local search algorithm to be effective, search initialization and individual search steps should be efficiently computable.

Complexity class $\mathcal{PLS}$: class of problems for which a local search algorithm exists with polynomial time complexity for:

- search initialization
- any single search step, including computation of evaluation function value

For any problem in $\mathcal{PLS}$ ...

- local optimality can be verified in polynomial time
- improving search steps can be computed in polynomial time
- **but:** finding local optima may require super-polynomial time

Computational Complexity of LS

$\mathcal{PLS}$-complete: Among the most difficult problems in $\mathcal{PLS}$; if for any of these problems local optima can be found in polynomial time, the same would hold for all problems in $\mathcal{PLS}$.

Some complexity results:

- TSP with k-exchange neighborhood with $k > 3$ is $\mathcal{PLS}$-complete.
- TSP with 2- or 3-exchange neighborhood is in $\mathcal{PLS}$, but $\mathcal{PLS}$-completeness is unknown.

Outline

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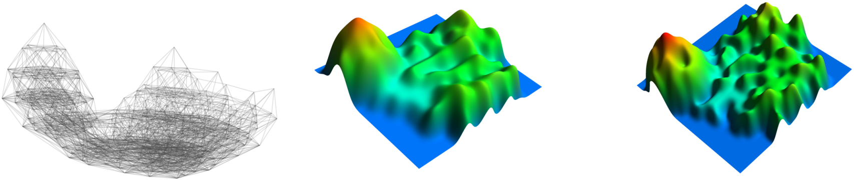
Definitions

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

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



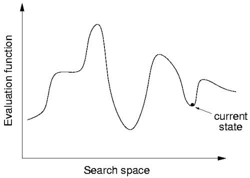
Transition Graph of Iterative Improvement

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.

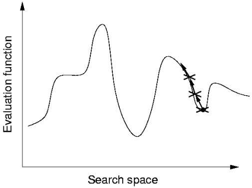
It can be defined for other algorithms as well and it plays a central role in the theoretical analysis of proofs of convergence.

Ideal visualization of landscapes principles

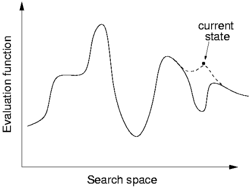
- Simplified landscape representation



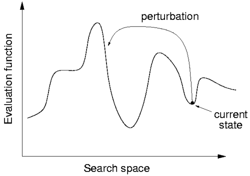
- Tabu Search



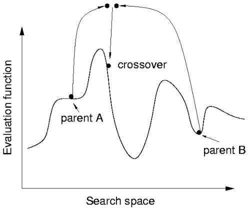
- Guided Local Search



- 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:
    for each pair i, j of solutions, j is reachable from i.
  - weakly optimally connected neighborhood graph:
    for each solution i, it contains a path from i to an optimal solution.
- 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

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

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

Permutations

$\Pi(n)$ 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 $\pi^{-1} \cdot \pi = \iota$
$\pi^{-1}(i) = pos_\pi(i)$

$$\Delta_N \subset \Pi$$

Linear Permutations

Swap operator

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

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

Interchange operator

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

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

($\equiv$ set of all transpositions)

Insert operator

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

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

Circular Permutations

Reversal (2-edge-exchange)

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

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

Block moves (3-edge-exchange)

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

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

Short block move (Or-edge-exchange)

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

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

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

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

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

Two-exchange operator

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

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

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

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

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

One-deletion operator

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

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

Swap operator

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

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

Outline

Distances

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

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

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 $\mathcal{L}$:

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

$\mathtt{diam}(\mathcal{L}) = \max\{d_{\mathcal{N}}(s, s') \mid s, s' \in S\}$ (= 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 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 $[n/3, n-1]$

Example: Search space size and diameter for SAT

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

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)

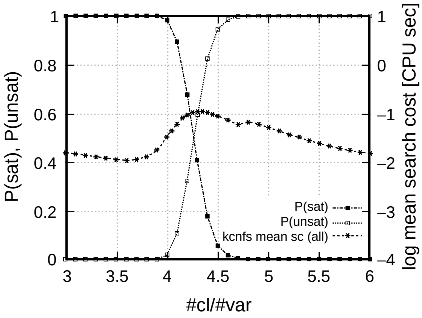
Outline

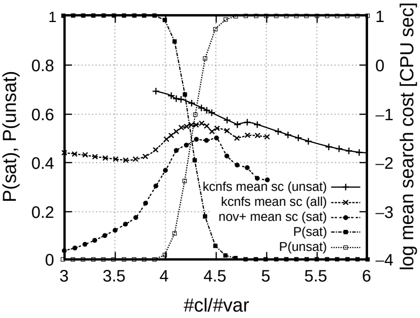
Other Search Space Properties

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

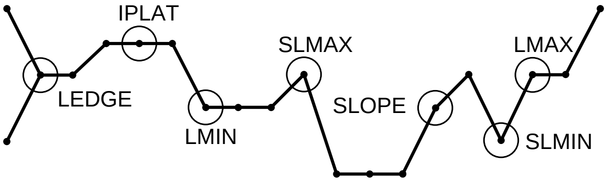
Phase Transition for 3-SAT

Random instances $\rightsquigarrow$ 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