DM841
Discrete Optimization

Part 2 – Heuristics
Very Large Scale Neighborhoods

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Course Overview

- ✔ Combinatorial Optimization
- ✔ Local Search: Components, Basic Algorithms
- ✔ Local Search: Neighborhoods and Search Landscape
- ✔ Stochastic Local Search & Metaheuristics
- ✔ Efficient Local Search: data structures, incremental updates and neighborhood pruning
- ✔ Working Environment and Solver Systems (EasyLocal)
- ✔ Methods for the Analysis of Experimental Results
- ✔ Algorithm Configuration: iRace tool
- ✖ Very Large Scale Neighborhoods

Examples: GCP, CSP, TSP, SAT, SMTWP, Steiner Tree, Unrelated Parallel Machines, p-median,

Very Large Scale Neighborhoods

Small neighborhoods:

- might be short-sighted
- need many steps to traverse the search space

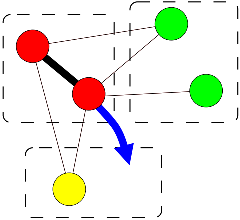
Large neighborhoods

- introduce large modifications to reach higher quality solutions
- allow to traverse the search space in few steps

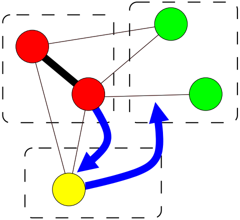
Key idea: use very large neighborhoods that can be searched efficiently (preferably in polynomial time) or are searched heuristically

Example (GCP)

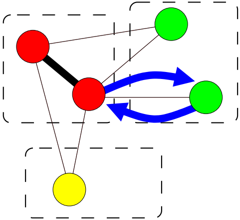
Neighborhood Structures: Very Large Scale Neighborhood



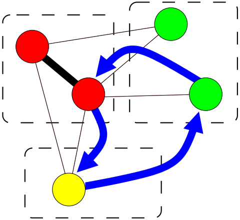
One Exchange



Path Exchange



Swap



Cyclic Exchange

Very large scale neighborhood search

1. define an exponentially large neighborhood
   (though, $O(n^3)$ might already be large)
2. define a polynomial time search algorithm to search the neighborhood
   (= solve the neighborhood search problem, NSP)
   - exactly (leads to a best improvement strategy)
   - heuristically (some improving moves might be missed)

Examples of VLSN Search

[Ahuja, Ergun, Orlin, Punnen, 2002]

- based on concatenation of simple moves
  - Variable Depth Search (TSP, GP)
  - Ejection Chains
- based on Dynamic Programming or Network Flows
  - Dynasearch (ex. SMTWTP)
  - Weighted Matching based neighborhoods (ex. TSP)
  - Cyclic exchange neighborhood (ex. VRP)
  - Shortest path
- based on polynomially solvable special cases of hard combinatorial optimization problems
  - Pyramidal tours
  - Halin Graphs

Outline

1. Variable Depth Search
2. Ejection Chains
3. Dynasearch
4. Weighted Matching Neighborhoods
5. Cyclic Exchange Neighborhoods

Variable Depth Search

- **Key idea:** *Complex steps* in large neighborhoods = variable-length sequences of *simple steps* in small neighborhood.
- Use various *feasibility restrictions* on selection of simple search steps to limit time complexity of constructing complex steps.
- Perform Iterative Improvement w.r.t. complex steps.

Variable Depth Search (VDS):

```
determine initial candidate solution s
while s is not locally optimal do
    t̂ := s
    repeat
        select best feasible neighbor t of t̂
        if f(t) < f(t̂) then
            t̂ := t
            s := t̂
    until construction of complex step has been completed;
```

Graph Partitioning

Graph Partitioning

Given: $G = (V, E)$, weighted function $\omega : V \to \mathbf{R}$, a positive number p: $0 < w_i \leq p,\ \forall i$ and a connectivity matrix $C = [c_{ij}] \in \mathbf{R}^{|V| \times |V|}$.

Task: A k-partition of G, $V_1, V_2, \ldots, V_k$: $\bigcup_{i=1}^{n} V_i = G$ such that:

- it is admissible, ie, $|V_i| \leq p$ for all i and
- it has minimum cost, ie, the sum of c_{ij}, i, j that belong to different subsets is mimimal

VLSN for the Traveling Salesman Problem

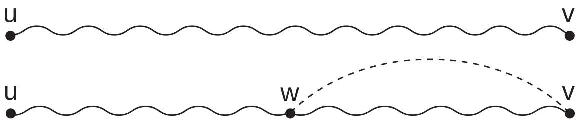
- k-exchange heuristics
  - 2-opt [Flood, 1956, Croes, 1958]
  - 2.5-opt or 2H-opt
  - Or-opt [Or, 1976]
  - 3-opt [Block, 1958]
  - k-opt [Lin 1965]

- complex neighborhoods
  - Lin-Kernighan [Lin and Kernighan, 1965]
  - Helsgaun's Lin-Kernighan
  - Dynasearch
  - Ejection chains approach

The Lin-Kernighan (LK) Algorithm for the TSP (1)

- Complex search steps correspond to sequences of 2-exchange steps and are constructed from sequences of *Hamiltonian paths*

- *δ-path:* Hamiltonian path p + 1 edge connecting one end of p to interior node of p

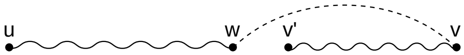


Basic LK exchange step:

- Start with Hamiltonian path $(u, \ldots, v)$:

- Obtain δ-path by adding an edge (v, w):

- Break cycle by removing edge (w, v'):



- *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 $p := s$
2. obtain δ-path p' by replacing one edge in p
3. consider Hamiltonian cycle t obtained from p by (uniquely) defined edge exchange
4. if $w(t) < w(t^*)$ then
   set $t^* := t$; $p := p'$; go to step 2
   else accept t^* as new current candidate solution s

Note: This can be interpreted as sequence of 1-exchange steps that alternate between δ-paths and Hamiltonian cycles.

Mechanisms used by LK algorithm:

- *Pruning exact rule:* If a sequence of numbers has a positive sum, there is a cyclic permutation of these numbers such that every partial sum is positive.
  ➨ need to consider only gains whose partial sum remains positive

- *Tabu restriction:* Any edge that has been added cannot be removed and any edge that has been removed cannot be added in the same LK step.
  Note: This limits the number of simple steps in a complex LK step.

- *Limited form of backtracking* ensures that local minimum found by the algorithm is optimal w.r.t. standard 3-exchange neighborhood

- (For further details, see original article)

[LKH Helsgaun's implementation
http://www.akira.ruc.dk/~keld/research/LKH/ (99 pages report)]

Outline

1. Variable Depth Search
2. Ejection Chains
3. Dynasearch
4. Weighted Matching Neighborhoods
5. Cyclic Exchange Neighborhoods

Ejection Chains

- Attempt to use large neighborhoods without examining them exhaustively
- Sequences of successive steps each influenced by the precedent and determined by myopic choices
- Limited in length
- Local optimality in the large neighborhood is not guaranteed.

Example (on TSP):
successive 2-exchanges where each exchange involves one edge of the previous exchange

Example (on GCP):
successive 1-exchanges: a vertex v_1 changes color from $\varphi(v_1) = c_1$ to c_2, in turn forcing some vertex v_2 with color $\varphi(v_2) = c_2$ to change to another color c_3 (which may be different or equal to c_1) and again forcing a vertex v_3 with color $\varphi(v_3) = c_3$ to change to color c_4.

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Dynasearch

- Iterative improvement method based on building complex search steps from combinations of mutually independent search steps
- Mutually independent search steps do not interfere with each other wrt effect on evaluation function and feasibility of candidate solutions.

Example: Independent 2-exchange steps for the TSP:

Therefore: Overall effect of complex search step = sum of effects of constituting simple steps;
complex search steps maintain feasibility of candidate solutions.

- **Key idea:** Efficiently find optimal combination of mutually independent simple search steps using *Dynamic Programming*.

Dynasearch for SMTWTP

- two interchanges δ_{jk} and δ_{lm} are independent if $\max\{j,k\} < \min\{l,m\}$ or $\min\{j,k\} > \max\{l,m\}$;
- the dynasearch neighborhood is obtained by a series of independent interchanges;
- it has size $2^{n-1} - 1$ (the number of subsets of $n-1$ pairwise jobs);
- but a best move can be found in $O(n^3)$ searched by dynamic programming;
- it yields in average better results than the interchange neighborhood alone.

Table 1 Data for the Problem Instance

Job j	1	2	3	4	5	6
Processing time p_j	3	1	1	5	1	5
Weight w_j	3	5	1	1	4	4
Due date d_j	1	5	3	1	3	1

Table 2 Swaps Made by Best-Improve Descent

Iteration	Current Sequence	Total Weighted Tardiness
	1 2 3 4 5 6	109
1	1 2 3 5 4 6	90
2	1 2 3 5 6 4	75
3	5 2 3 1 6 4	70

Table 3 Dynasearch Swaps

Iteration	Current Sequence	Total Weighted Tardiness
	1 2 3 4 5 6	109
1	1 3 2 5 4 6	89
2	1 5 2 3 6 4	68
3	5 1 2 3 6 4	67

- state (k, π)
- π_k is the partial sequence at state (k, π) that has min $\sum wT$
- π_k is obtained from state (i, π)

$$\begin{cases} \text{appending job } \pi(k) \text{ after } \pi(i) & i = k-1 \\ \text{appending job } \pi(k) \text{ and interchanging } \pi(i+1) \text{ and } \pi(k) & 0 \leq i < k-1 \end{cases}$$

- $F(\pi_0) = 0; \qquad F(\pi_1) = w_{\pi(1)} \left(p_{\pi(1)} - d_{\pi(1)}\right)^+;$

$$F(\pi_k) = \min \begin{cases} F(\pi_{k-1}) + w_{\pi(k)} \left(C_{\pi(k)} - d_{\pi(k)}\right)^+, \\ \min\limits_{1 \leq i < k-1} \{F(\pi_i) + w_{\pi(k)} \left(C_{\pi(i)} + p_{\pi(k)} - d_{\pi(k)}\right)^+ + \\ \quad + \sum_{j=i+2}^{k-1} w_{\pi(j)} \left(C_{\pi(j)} + p_{\pi(k)} - p_{\pi(i+1)} - d_{\pi(j)}\right)^+ + \\ \quad + w_{\pi(i+1)} \left(C_{\pi(k)} - d_{\pi(i+1)}\right)^+ \} \end{cases}$$

- The best choice is computed by recursion in $O(n^3)$ and the optimal series of interchanges for $F(\pi_n)$ is found by backtrack.

- Local search with dynasearch neighborhood starts from an initial sequence, generated by ATC, and at each iteration applies the best dynasearch move, until no improvement is possible (that is, $F(\pi_n^t) = F(\pi_n^{(t-1)})$, for iteration t).

- Speedups:
  - pruning with considerations on $p_{\pi(k)}$ and $p_{\pi(i+1)}$
  - maintainig a string of late, no late jobs
  - h_t largest index s.t. $\pi^{(t-1)}(k) = \pi^{(t-2)}(k)$ for $k = 1, \ldots, h_t$ then $F(\pi_k^{(t-1)}) = F(\pi_k^{(t-2)})$ for $k = 1, \ldots, h_t$ and at iter t no need to consider $i < h_t$.

Dynasearch, refinements:

- [Grosso et al. 2004] add insertion moves to interchanges.
- [Ergun and Orlin 2006] show that dynasearch neighborhood can be searched in $O(n^2)$.

Performance:

- exact solution via branch and bound feasible up to 40 jobs [Potts and Wassenhove, Oper. Res., 1985]
- exact solution via time-indexed integer programming formulation used to lower bound in branch and bound solves instances of 100 jobs in 4-9 hours [Pan and Shi, Math. Progm., 2007]
- dynasearch: results reported for 100 jobs within a 0.005% gap from optimum in less than 3 seconds [Grosso et al., Oper. Res. Lett., 2004]

Outline

Weighted Matching Neighborhoods

- **Key idea** use basic polynomial time algorithms, example: weighted matching in bipartied graphs, shortest path, minimum spanning tree.
- Neighborhood defined by finding a minimum cost matching on a (bipartite) improvement graph

Example (TSP)
Neighborhood: Eject k nodes and reinsert them optimally

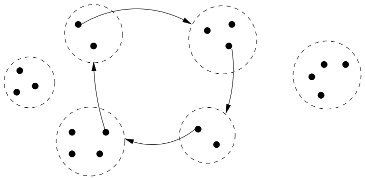
Outline

Cyclic Exchange Neighborhoods

- Possible for problems where solution can be represented as form of partitioning
- Definition of a partitioning problem:
  Given: a set W of n elements, a collection $\mathcal{T} = \{T_1, T_2, \ldots, T_k\}$ of subsets of W, such that $W = T_1 \cup \ldots \cup T_k$ and $T_i \cap T_j = \emptyset$, and a cost function $c : \mathcal{T} \to \mathbf{R}$:
  Task: Find another partition $\mathcal{T}'$ of W by means of single exchanges between the sets such that

$$\min \sum_{i=1}^{k} c(T_i)$$

- Cyclic exchange:

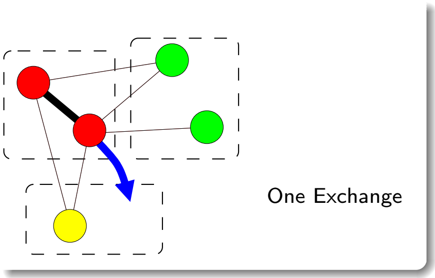


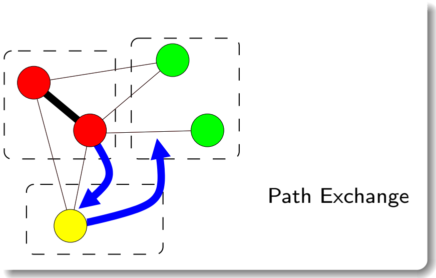
Neighborhood search

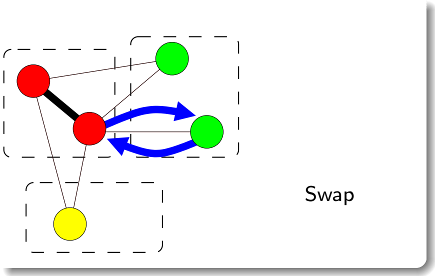
- Define an improvement graph
- Solve the relative
  - Subset Disjoint *Negative* Cost Cycle Problem
  - Subset Disjoint *Minimum* Cost Cycle Problem

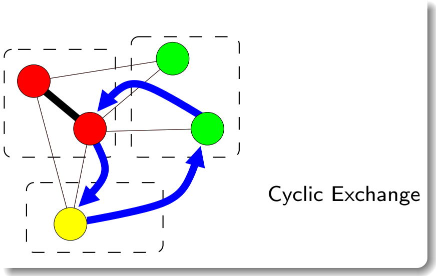
Example (GCP)

Neighborhood Structures: Very Large Scale Neighborhood



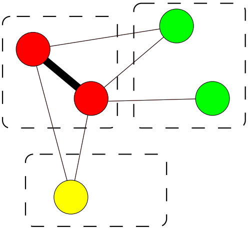


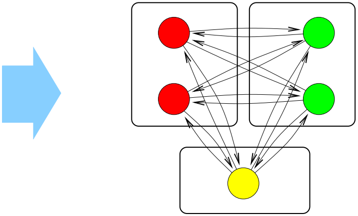




Example (GCP)
Examination of the Very Large Scale Neighborhood

Exponential size but can be searched efficiently





Improvement Graph

A Subset Disjoint Negative Cost Cycle Problem in the Improvement Graph can be solved by dynamic programming in $\mathcal{O}(|V|^2 2^k |D'|)$.
Yet, heuristic rules can be adopted to reduce the complexity to $\mathcal{O}(|V'|^2)$

Procedure SDNCC($G'(V', D')$)

Let $\mathcal{P}$ all negative cost paths of length 1, Mark all paths in $\mathcal{P}$ as untreated

Initialize the best cycle $q^* = ()$ and $c^* = 0$

for all $p \in \mathcal{P}$ **do**

  if $(e(p), s(p)) \in D'$ and $c(p) + c(e(p), s(p)) < c^*$ **then**

    q^* = the cycle obtained by closing p and $c^* = c(q^*)$

while $\mathcal{P} \neq \emptyset$ **do**

  Let $\widehat{\mathcal{P}} = \mathcal{P}$ be the set of untreated paths

  $\mathcal{P} = \emptyset$

  while $\exists\, p \in \widehat{\mathcal{P}}$ untreated **do**

    Select some untreated path $p \in \widehat{\mathcal{P}}$ and mark it as treated

    for all $(e(p), j) \in D'$ s.t. $w_{\varphi(v_j)}(p) = 0$ and $c(p) + c(e(p), j) < 0$ **do**

      Add the extended path $(s(p), \ldots, e(p), j)$ to $\mathcal{P}$ as untreated

      if $(j, s(p)) \in D'$ and $c(p) + c(e(p), j) + c(j, s(p)) < c^*$ **then**

        q^* = the cycle obtained closing the path $(s(p), \ldots, e(p), j)$

        $c^* = c(q^*)$

  for all $p' \in \mathcal{P}$ subject to $w(p') = w(p),\ s(p') = s(p),\ e(p') = e(p)$ **do**

    Remove from $\mathcal{P}$ the path of higher cost between p and p'

return a minimal negative cost cycle q^* of cost c^*