DM811 – Fall 2009
Heuristics for Combinatorial Optimization

Lecture 13

Very Large Scale Neighborhoods

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Outline

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
- allows 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

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

➤ Idea: turn a special case into a neighborhood
VLSN allows to use the literature on polynomial time algorithms

Outline

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
$\hat{t} := s$
while s is not locally optimal **do**
  repeat
    select best feasible neighbor t
    if $g(t) < g(\hat{t})$ **then** $\hat{t} := t$
    $s := \hat{t}$
  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:

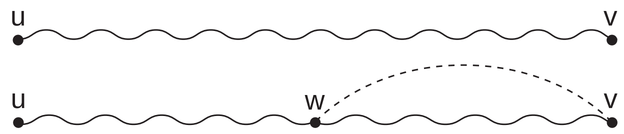
- it is admissible, ie, $|V_i| \leq p$ for all i and
- it has minimum cost, ie, the sum of c_{ij}, i, j that belong to different subsets is mimimal

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 $(u, \dots, v)$:

- 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.

Additional 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)]

Elements for an efficient neighborhood search

1. fast delta evaluations
2. neighborhood pruning: fixed radius nearest neighborhood search
   - problem insights
   - neighborhood lists: restrict exchanges to most interesting candidates
   - don't look bits: focus perturbative search to "interesting" part
3. sophisticated data structures for fast updates

TSP data structures

Static data structures:

- priority lists
- k-d trees

Tour representation. Operations needed:

- `reverse`(a, b)
- `succ`(a)
- `prec`(a)
- `sequence(a,b,c)` – check whether `b` is within `a` and `b`

Possible choices (dynamic data structure):

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

Outline

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.

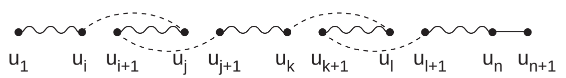
Outline

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

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*.

Outline

1. Variable Depth Search
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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 (non-)bipartite improvement graph

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

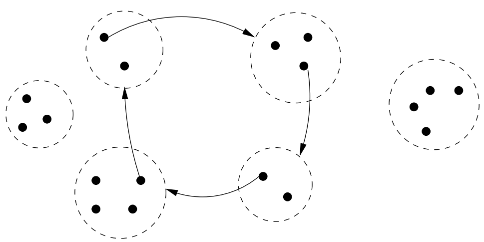
Outline

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:

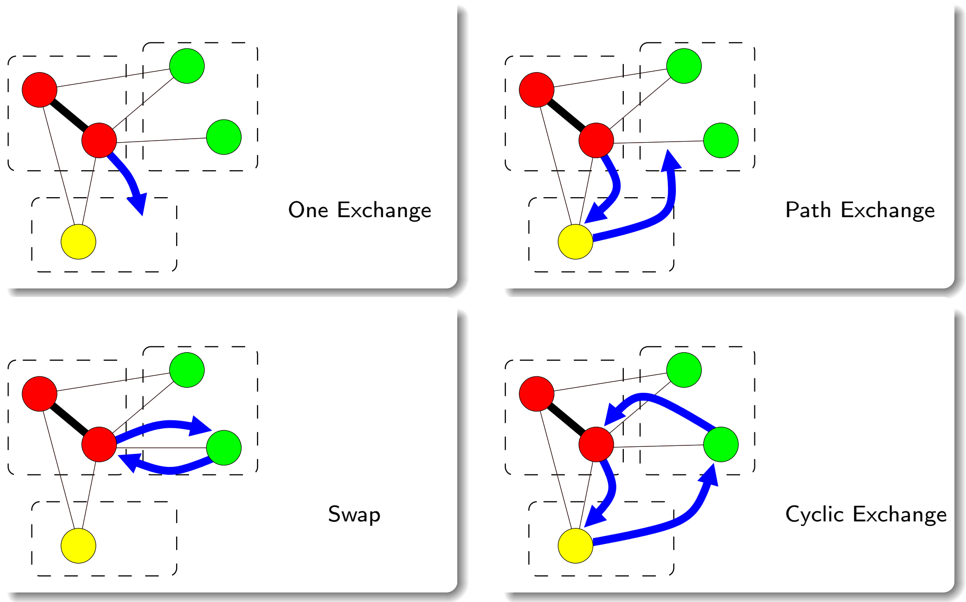


Neighborhood search

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

Example (GCP)

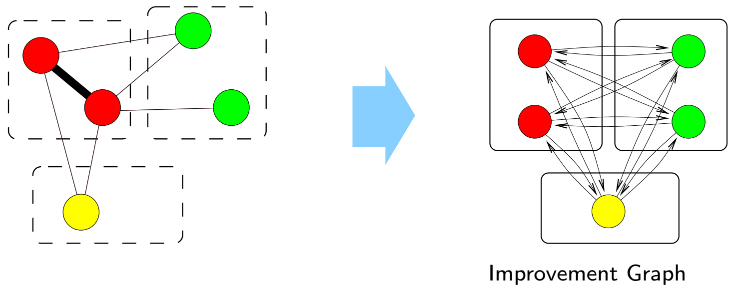
Neighborhood Structures: Very Large Scale Neighborhood



Example (GCP)

Examination of the Very Large Scale Neighborhood

Exponential size but can be searched efficiently



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, heuristics 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^*

Example (GCP)

Very Large Scale Neighborhood, dynamic programming for SDNCCP

Cyclic exchanges

- negative cost cycles can be detected rather *easily* thanks to Lin-Kernighan Lemma
  If a sequence of edge costs has negative sum, then there is a cyclic permutation of these edges such that every partial sum is negative.

Path exchanges

- dynamic programming algorithm requires modification to also check for path exchanges (easy)
- require a correction term due to the definition of the improvement graph
- unfortunately, the above lemma is not anymore applicable if we require to find all path exchanges.

Very Large Scale Neighborhood, effectiveness

Num. vertices	Num. distinct colorings	One exchange	Path and cyclic exchanges	
			exhaustive	truncated
3	7 (2)	0	0	0
4	63 (6)	1	0	1
5	756 (21)	10	0	9
6	14113 (112)	83	4	52
7	421555 (853)	532	15	260
8	22965511 (11117)	348	11	134
9	2461096985 (261080)	134	1	54