DM811
HEURISTICS AND LOCAL SEARCH ALGORITHMS FOR COMBINATORIAL OPTIMZATION

Lecture 11

Very Large Scale Neighborhoods

Marco Chiarandini

Outline

Outline

1. Very Large Scale Neighborhoods
   - Variable Depth Search
   - Ejection Chains
   - Dynasearch
   - Weighted Matching Neighborhoods
   - Cyclic Exchange Neighborhoods

2. Variable Neighborhood Search

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

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

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):

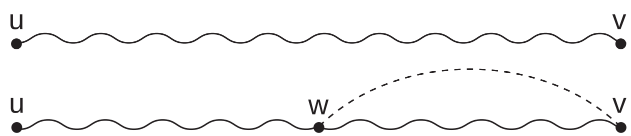
determine initial candidate solution s
$\hat{t} := s$
while s is not locally optimal **do**
  repeat
    select best feasible neighbor t
    if $g(t) < g(\hat{t})$ **then** $\hat{t} := t$
    $s := \hat{t}$
  until construction of complex step has been completed ;

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

- fast delta evaluations
- neighborhood pruning: fixed radius nearest neighborhood search
- neighborhood lists: restrict exchanges to most interesting candidates
- don't look bits: focus perturbative search to "interesting" part
- 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

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.

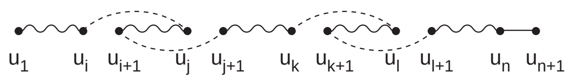
Example (on TSP):
successive 2-exchanges where each exchange involves one edge of the previous exchange

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.

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 w.r.t. 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*.

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

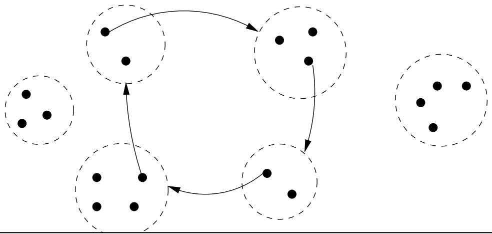
Example (TSP)
Neighborhood: Eject k nodes and reinsert them optimally

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

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

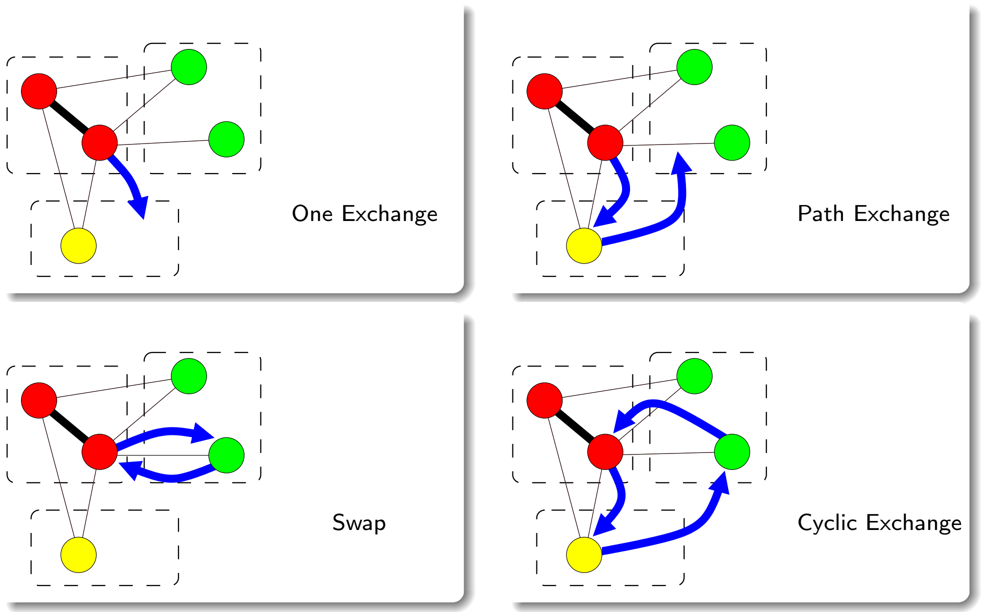
- Cyclic exchange:



Neighborhood search

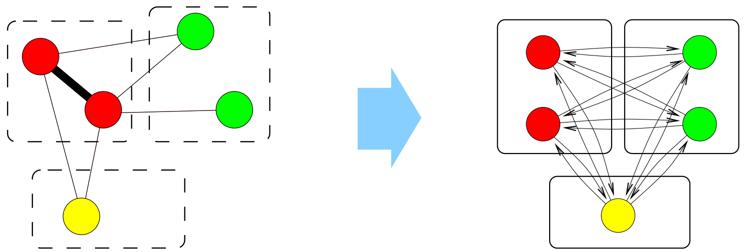
- Define an improvement graph
- Solve the relative
  - Subset Disjoint *Negative* Cost Cycle Problem
  - Subset Disjoint *Minimum* Cost Cycle Problem

Example (GCP)



Example (GCP)

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, 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 $(s(p), \dots, e(p), j)$ 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 $(s(p), \dots, e(p), j)$
        $c^* = c(q^*)$
  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)

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.

Iterative Improvement

Very Large Scale Neighborhood, effectiveness

Num. vertices	Num. distinct colorings	One exchange	Path and cyclic exchanges exhaustive	Path and cyclic exchanges 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

Outline

Variable Neighborhood Search (VNS)

Variable Neighborhood Search is an SLS method that is based on the systematic change of the neighborhood during the search.

Central observations

- a local minimum w.r.t. one neighborhood function is not necessarily locally minimal w.r.t. another neighborhood function
- a global optimum is locally optimal w.r.t. all neighborhood functions

- Principle: change the neighborhood during the search
- Several adaptations of this central principle
  - (Basic) Variable Neighborhood Descent (VND)
  - Variable Neighborhood Search (VNS)
  - Reduced Variable Neighborhood Search (RVNS)
  - Variable Neighborhood Decomposition Search (VNDS)
  - Skewed Variable Neighborhood Search (SVNS)
- Notation
  - $\mathcal{N}_k$, $k = 1, 2, \ldots, k_m$ is a set of neighborhood functions
  - $N_k(s)$ is the set of solutions in the k-th neighborhood of s

How to generate the various neighborhood functions?

- for many problems different neighborhood functions (local searches) exist / are in use
- change parameters of existing local search algorithms
- use k-exchange neighborhoods; these can be naturally extended
- many neighborhood functions are associated with distance measures; in this case increase the distance

Basic Variable Neighborhood Descent (BVND)

Procedure VND
input : $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{max}$, and an initial solution s
output: a local optimum s for $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{max}$
$k \leftarrow 1$
repeat
    $s' \leftarrow$ FindBestNeighbor(s,$\mathcal{N}_k$)
    if $g(s') < g(s)$ **then**
        $s \leftarrow s'$
        $(k \leftarrow 1)$
    else
        $k \leftarrow k + 1$
until $k = k_{max}$;

Variable Neighborhood Descent (VND)

Procedure VND
input : $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{max}$, and an initial solution s
output: a local optimum s for $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{max}$
$k \leftarrow 1$
repeat
    $s' \leftarrow$ IterativeImprovement(s,$\mathcal{N}_k$)
    if $g(s') < g(s)$ **then**
        $s \leftarrow s'$
        $(k \leftarrow 1)$
    else
        $k \leftarrow k + 1$
until $k = k_{max}$;

- Final solution is locally optimal w.r.t. all neighborhoods
- First improvement may be applied instead of best improvement
- Typically, order neighborhoods from smallest to largest
- If iterative improvement algorithms II_k, $k = 1, \ldots, k_{max}$ are available as black-box procedures:
  - order black-boxes
  - apply them in the given order
  - possibly iterate starting from the first one
  - order chosen by: *solution quality* and *speed*

Example

VND for single-machine total weighted tardiness problem

- Candidate solutions are permutations of job indexes
- Two neighborhoods: swap and insert
- Influence of different starting heuristics also considered

initial	swap		insert		swap+insert		insert+swap	
solution	Δavg	tavg	Δavg	tavg	Δavg	tavg	Δavg	tavg
EDD	0.62	0.140	1.19	0.64	0.24	0.20	0.47	0.67
MDD	0.65	0.078	1.31	0.77	0.40	0.14	0.44	0.79

Δavg deviation from best-known solutions, averaged over 100 instances

Basic Variable Neighborhood Search (VNS)

Procedure BVNS
input : $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{max}$, and an initial solution s
output: a local optimum s for $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{max}$
repeat
    $k \leftarrow 1$
    repeat
        $s' \leftarrow$ RandomPicking(s,$\mathcal{N}_k$)
        $s'' \leftarrow$ IterativeImprovement(s',$\mathcal{N}_k$)
        if $g(s'') < g(s)$ **then**
            $s \leftarrow s''$
            $k \leftarrow 1$
        else
            $k \leftarrow k + 1$
    until $k = k_{max}$;
until Termination Condition ;

To decide:

- which neighborhoods
- how many
- which order
- which change strategy

- Extended version: parameters k_{min} and k_{step}; set $k \leftarrow k_{min}$ and increase by k_{step} if no better solution is found (achieves diversification)

Extensions (1)

Reduced Variable Neighborhood Search (RVNS)

- same as VNS except that no IterativeImprovement procedure is applied
- only explores different neighborhoods randomly
- can be faster than standard local search algorithms for reaching good quality solutions

Extensions (2)

Variable Neighborhood Decomposition Search (VNDS)

- same as in VNS but in IterativeImprovement all solution components are kept fixed except k randomly chosen
- IterativeImprovement is applied on the k unfixed components

- IterativeImprovement can be substituted by exhaustive search up to a maximum size b (parameter) of the problem

Extensions (3)

Skewed Variable Neighborhood Search (SVNS)

- Derived from VNS
- Accept $s \leftarrow s''$ when s'' is worse
  - according to some probability
  - skewed VNS: accept if

$$g(s'') - \alpha \cdot d(s, s'') < g(s)$$

$d(s, s'')$ measure the distance between solutions

(underlying idea: avoiding degeneration to multi-start)