Heuristic Algorithms

Master's Degree in Computer Science/Mathematics

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Complexity

Algorithm SteepestDescent$\left(I, x^{(0)}\right)$

$x := x^{(0)}$;

Stop $:=$ *false*;

While Stop $=$ *false do* $\{\ t_{\max}$ iterations $\}$

$\quad \tilde{x} := \arg\min_{x' \in N(x)} f(x)$;

$\quad$ *If* $f(\tilde{x}) \geq f(x)$ *then* Stop $:=$ *true*; *else* $x := \tilde{x}$;

EndWhile;

Return $(x, f(x))$;

The complexity of the *steepest descent* heuristic depends on

1. the number of iterations $t_{\max}$ from $x^{(0)}$ to the local optimum found, which depends on the structure of the search graph (width of the attraction basins) and is hard to estimate *a priori*
2. the search for the best solution in the neighbourhood ($\tilde{x}$), which depends on how the search itself is performed, but whose complexity estimation is usually standard

The exploration of the neighbourhood

Two strategies to explore the neighbourhood are possible

1. exhaustive search: evaluate all the neighbour solutions; the complexity of a single step is the product of
   - the number of neighbour solutions ($|N(x)|$)
   - the evaluation of the cost of each solution ($\gamma_f(|B|, x)$)

   If it is not possible to generate only feasible solution:
   - visit a superset of the neighbourhood ($\tilde{N}(x) \supset N(x)$)
   - for each element x, evaluate the feasibility ($\gamma_X(|B|, x)$)
   - for the feasible ones, evaluate the cost ($\gamma_f(|B|, x)$)
2. efficient exploration of the neighbourhood without a complete visit: find the best neighbour solution solving an auxiliary problem

Only some special neighbourhoods allow that

Exhaustive visit of the neighbourhood

Algorithm SteepestDescent$\left(I, x^{(0)}\right)$

$x := x^{(0)}$;

Stop $:=$ *false*;

While Stop $=$ *false do*

  $\tilde{x} := x$; $\{\ \tilde{x} := \arg \min\limits_{x' \in N(x)} f(x')\ \}$

  For each $x' \in \tilde{N}(x)$ *do*

    If $x' \in N(x)$ *then*

      If $f(x') < f(\tilde{x})$ *then* $\tilde{x} := x'$;

    EndIf;

  EndFor;

  If $f(\tilde{x}) \geq f(x)$ *then* Stop $:=$ *true*; *else* $x := \tilde{x}$;

EndWhile;

Return $(x, f(x))$;

The complexity of the neighbourhood exploration combines three terms

1. $|\tilde{N}(x)|$: the number of subsets visited
2. γ_X: the time to evaluate their feasibility
3. γ_f: the time to evaluate the objective for a feasible solution

Evaluating or updating the objective: the additive case

The first way to accelerate an exchange algorithm is to minimize the time to evaluate the objective: in particular, it is faster to update $f(x)$ rather than to recompute it

The update of an additive objective $f(x) = \sum_{j \in x} \phi_j$ requires to

- sum ϕ_i for each element $i \in A$, added to x
- subtract ϕ_j for each element $j \in D$, deleted from x

$$\delta f(x, A, D) = f(x \cup A \setminus D) - f(x) = \sum_{i \in A} \phi_i - \sum_{j \in D} \phi_j$$

Examples: swap of objects (KP), columns (SCP), edges ($CMSTP$), ...

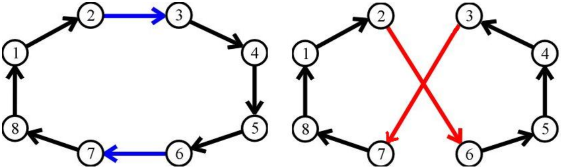
This update has two fundamental properties:

- it takes constant time for a constant number of elements $|A| + |D|$
- $\delta f(x, A, D)$ does not depend on x (*we will talk about it later*)

Example: the symmetric *TSP*

To generate neighbourhood $N_{\mathcal{R}_2}$ for the *TSP* we

- delete two nonconsecutive arcs (s_i, s_{i+1}) and (s_j, s_{j+1})
- add the two arcs (s_i, s_j) and (s_{i+1}, s_{j+1})
- revert the path $(s_{i+1}, \ldots, s_j)$ (modifying $O(n)$ arcs!)



If the graph and the cost function are symmetric, the variation of $f(x)$ is

$$\delta f(x, A, D) = c_{s_i,s_j} + c_{s_{i+1},s_{j+1}} - c_{s_i,s_{i+1}} - c_{s_j,s_{j+1}}$$

but this it not true for the asymmetric *TSP*

What if the objective function is not additive?

Evaluating or updating the objective: the quadratic case

The *MDP* has a quadratic objective function: computing it costs $\Theta\left(n^2\right)$

Moving from x to $x' = x \setminus \{i\} \cup \{j\}$ (neighbourhood $N_{\mathcal{S}_1}$), the update is

$$\delta f(x,i,j) = f(x \setminus \{i\} \cup \{j\}) - f(x) = \sum_{h,k \in x \setminus \{i\} \cup \{j\}} d_{hk} - \sum_{h,k \in x} d_{hk}$$

which depends on $O(n)$ distance terms, related to points i and j

There is a general trick for the simmetric quadratic functions with $d_{ii} = 0$

$$\begin{aligned} \delta f(x,i,j) &= \sum_{h \in x \setminus \{i\} \cup \{j\}} \sum_{k \in x \setminus \{i\} \cup \{j\}} d_{hk} - \sum_{h \in x} \sum_{k \in x} d_{hk} \Rightarrow \\ \Rightarrow \delta f(x,i,j) &= 2 \sum_{k \in x} d_{jk} - 2 \sum_{k \in x} d_{ik} - 2 d_{ij} = 2 \left(D_j(x) - D_i(x) - d_{ij}\right) \end{aligned}$$

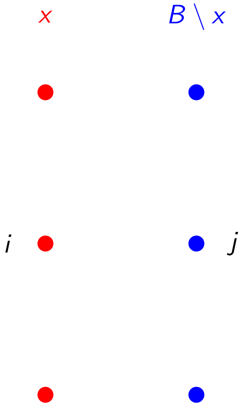
If $D_\ell(x) = \sum_{k \in x} d_{\ell k}$ is known for each $\ell \in B$, the computation takes $O(1)$

Example: the *MDP*

Let us consider $f(x)/2$
Evaluate the exchange

$$x \to x' = x \setminus \{i\} \cup \{j\}$$

with $i \in x$ and $j \in B \setminus x$



$$f(x') = f(x) - D_i + D_j - d_{ij}$$

- the pairs including i are lost
- the pairs including j are acquired
- but the pair (i,j) is in excess

The cost is computed in $O(1)$ time for each solution

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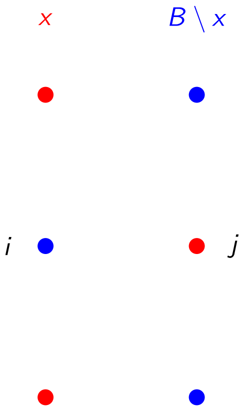

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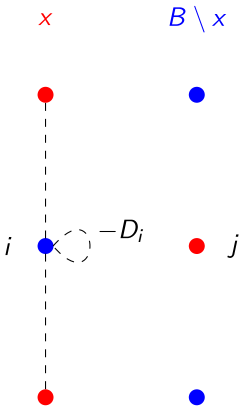

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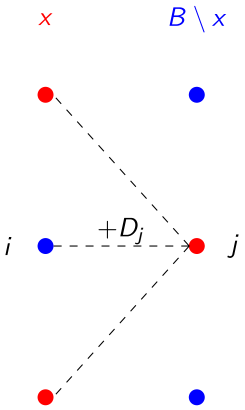

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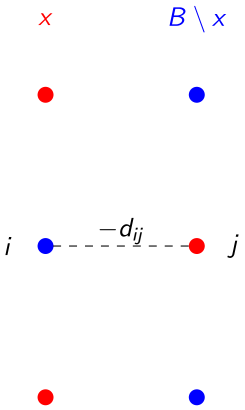

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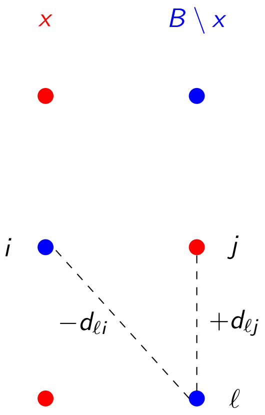
Example: the *MDP*



Update of the data structures:

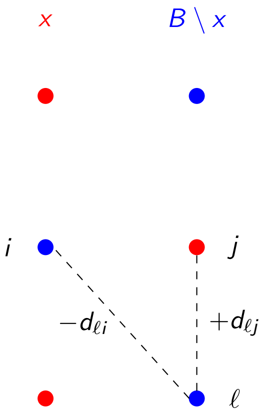
- $D_\ell = D_\ell - d_{\ell i} + d_{\ell j}\ ,\ \ell \in B$

For each element $\ell \in B$

- $d_{\ell i}$ disappears
- $d_{\ell j}$ appears

The auxiliary data structure is updated in $O(n)$ time for each iteration

Example: the *MDP*



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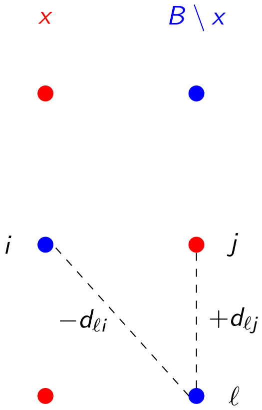

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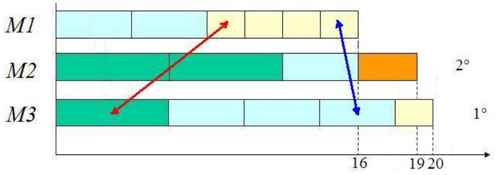
Updating the objective function: nonlinear examples

Many nonlinear functions can be updated with similar tricks

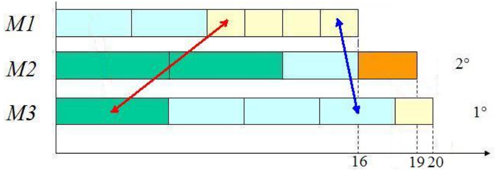
- save aggregated information on the current solution $x^{(t)}$
- use it to compute $f\left(x'\right)$ efficiently for each $x' \in N\left(x^{(t)}\right)$
- update it when moving to the following solution $x^{(t+1)}$

Using the transfer $\left(N_{\mathcal{T}_1}\right)$ and swap $\left(N_{\mathcal{S}_1}\right)$ neighbourhoods for the *PMSP*, the objective can be updated in constant time by managing

1. the completion time for each machine
2. the indices of the machines with the first and second maximum time



Example: the *PMSP*



Consider the swap $o = (i, j)$ of tasks i and j
(i on machine M_i, j on machine M_j)

- compute in constant time the new completion times:
  one increases, the other decreases (or both remain constant)
- test in constant time whether either exceeds the maximum
- if the maximum time decreases, test in constant time whether the other time or the second maximum time becomes the maximum

Once the neighbourhood is visited and the exchange selected, update

- the two modified completion times (each one in constant time)
- their positions in a max-heap (each one in time $O(\log |M|)$)

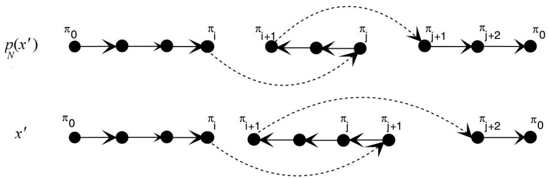
Use of local auxiliary information

The auxiliary information used to compute $f(x')$ can be

- global, that is referring to the current solution x
- local, that is referring to the solution $p_N(x')$ visited before x' in neighbourhood $N(x)$ according to a suitable order

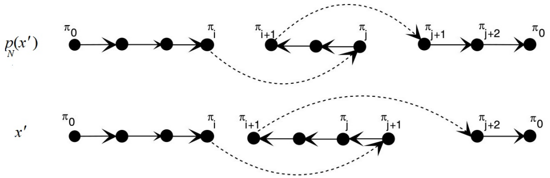
Consider the neighbourhood $N_{\mathcal{R}_2}$ for the asymmetric TSP:

- the neighbour solutions differ from x for $O(n)$ arcs
- general neighbour solutions differ from each other for $O(n)$ arcs
- if the pairs of arcs (s_i, s_{i+1}) and (s_j, s_{j+1}) follow the lexicographic order, the reverted path changes only by one arc



Example: the asymmetric *TSP*

Let $p_N(x') = o_{s_i,s_j}(x)$ and $x' = o_{s_i,s_{j+1}}(x)$ be subsequent neighbours of x



The variation of the objective from x to $o_{s_i,s_j}(x)$ is

$$\delta f(x,i,j) = c_{s_i,s_j} + c_{s_{i+1},s_{j+1}} - c_{s_i,s_{i+1}} - c_{s_j,s_{j+1}} + c_{s_j \ldots s_{i+1}} - c_{s_{i+1} \ldots s_j}$$

The variation of the objective from x to $o_{s_i,s_{j+1}}(x)$ is different, but

- the first four terms (single arcs) can be recomputed in constant time
- the last two terms (paths) can be updated in constant time

$$\begin{cases} c_{s_{j+1} \ldots s_{i+1}} = c_{s_j \ldots s_{i+1}} + c_{s_{j+1},s_j} \\ c_{s_{i+1} \ldots s_{j+1}} = c_{s_{i+1} \ldots s_j} + c_{s_j,s_{j+1}} \end{cases}$$

Is it acceptable to explore the neighbourhood in a predefined order ?

What about feasibility?

Defining neighbourhoods with the Hamming distance or with operations can generate also unfeasible subsets, that must be removed

$$\tilde{N}_{H_k}(x) = \{x' \subseteq B : d(x', x) \leq k\} \supseteq N_{H_k}(x) = \tilde{N}_{H_k}(x) \cap X$$

$$\tilde{N}_{\mathcal{O}}(x) = \{x' \subseteq B : \exists o \in \mathcal{O} : o(x) = x'\} \supseteq N_{\mathcal{O}}(x) = \tilde{N}_{\mathcal{O}}(x) \cap X$$

(*Examples: KP, BPP, SCP, CMSTP...*)

If it is not possible to avoid *a priori* the unfeasible subsets, one must

- test the feasibility of each element of $\tilde{N}(x)$ to obtain $N(x)$
- for the feasible elements, evaluate the cost

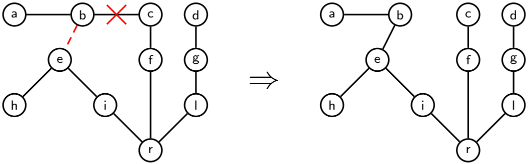
The feasibility test can be made efficient with techniques similar to the ones used for the objective evaluation

Example: update in constant time the total volume of a subset in the KP

Example: the *CMSTP*

Consider the swap neighbourhood $N_{\mathcal{S}_1}$ (add one edge, delete another)

- if the two edges are in the same branch, the solution remains feasible
- if they are in different branches, one loses weight, the other acquires it: the variation is equal to the weight of the subtree transferred



If each vertex saves the weight of its appended subtree, to test feasibility compare this weight with the residual capacity of the receiving branch (*the weight appended to b with the residual capacity of the left branch*)

Once the best exchange is performed, the information must be updated in time $O(n)$ visiting the old ancestors from c and the new ones from e

A general scheme of sophisticated exploration

The use of auxiliary information requires

1. the inizialisation of suitable data structures
   - partly local, i. e., related to neighbour solutions
   - partly global, i. e., related to the current solution
2. their update between subsequent solutions or iterations

Algorithm SteepestDescent$\left(I, x^{(0)}\right)$

$x := x^{(0)}$; $GI :=$ InitialiseGI(x); Stop $:=$ *false*;

While Stop $=$ *false do*

  $\tilde{x} := 0$; $\tilde{\delta} := 0$; $LI :=$ InitialiseLI$(\tilde{x})$

  For each $x' \in N(x)$ *do*

    $f(x') :=$ Estimate$(f(x), LI, GI)$;

    If $f(x') < f(\tilde{x})$ *then* $\tilde{x} := x'$;

    $LI :=$ UpdateLI(LI, x')

  EndFor;

  If $f(\tilde{x}) \geq f(x)$

    then Stop $:=$ *true*;

    else $x := \tilde{x}$; $GI :=$ UpdateGI$(GI, \tilde{x})$

  EndIf

EndWhile;

Return $(x, f(x))$;

Partial saving of the neighbourhood (1)

When performing an operation $o \in \mathcal{O}$ on a solution $x \in X$ sometimes

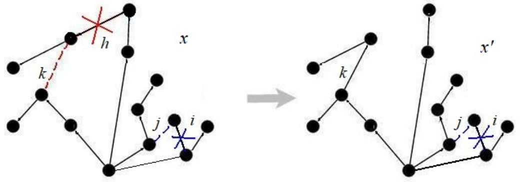
- the feasibility of the resulting solution $o(x)$
- the variation of the objective $\delta f_o(x) = f(o(x)) - f(x)$

depend only on a part of x (possibly, very small)

For example, consider the swap neighbourhood $N_{\mathcal{S}_1}$ for the *CMST*:

- add an edge $k \in B \setminus x$
- delete an edge $h \in x$

Two branches are involved: one acquires a subtree, the other loses it



The feasibility of swap (i, j) depends on the branches including i and j: it is the same in x and x' and is not affected by swap (h, k)

$$\delta f_{i,j}(x) = \delta f_{i,j}(x')$$

Partial saving of the neighbourhood (2)

For each operation $o \in \tilde{\mathcal{O}} \subset \mathcal{O}$ and for each $x' = o(x)$

- $o(x')$ is feasible if and only if $o(x)$ is feasible
- $\delta f_o(x') = \delta f_o(x)$

It is then advantageous to

1. compute and save $\delta f_o(x)$ for every $o \in \mathcal{O}$, that is
   keep the set of feasible exchanges and their associated values δf
2. perform the best operation o^*, and generate a new solution x'
3. retrieve $\delta f_o(x')$ for all $o \in \tilde{\mathcal{O}}$ (*their values are still correct*)
   and recompute and save $\delta f_o(x')$ only for $o \in \mathcal{O} \setminus \tilde{\mathcal{O}}$, that is
   recompute only the values of the exchanges on the modified branches
4. go back to point 2

If the branches are numerous, $|\mathcal{O} \setminus \tilde{\mathcal{O}}| \ll |\mathcal{O}|$ and the saving is very strong

It is typical of problems whose solution is a partition

Trade-off between efficiency and effectiveness

The complexity of an exchange heuristic depends on three factors

1. number of iterations
2. cardinality of the visited neighbourhood
3. computation of the feasibility and cost for the single neighbour

The first two factors are clearly conflicting:

- a small neighbourhood is fast to explore, but requires several steps to reach a local optimum
- a large neighbourhood requires few steps, but is slow to explore

The optimal trade-off is somewhere in the middle: a neighbourhood

- large enough to include good solutions
- small enough to be explored quickly

but it is hard to identify, because

- efficiency quickly worsens as size increases
- the resulting solution also changes with the neighbourhood (large neighbourhoods have better local optima)

Fine tuning of the neighbourhoods

It is also possible to define a neighbourhood N and tune its size

- explore only a promising subneighbourhood $N' \subset N$

  For example, if the objective function is additive, one can

  - add only elements $j \in B \setminus x$ of low cost ϕ_j
  - delete only elements $i \in x$ of high cost ϕ_i

- terminate the visit after finding a promising solution

  For example, the first-best strategy stops the exploration at the first solution better than the current one

$$\text{If } f(\tilde{x}) < f(x) \text{ then } x := \tilde{x}; \text{ Stop} := \text{true};$$

The effectiveness depends on the objective

- if the cost of some elements influences very much the objective, it is worth taking it into account, fixing of forbidding them

and on the structure of the neighbourhood

- if the landscape is smooth, the first improving solution approximates well the best solution of the neighbourhood: it is better to stop
- if the landscape is rugged, the best solution of the neighbourhood could be much better: it is better to go on