Heuristic Algorithms for Combinatorial Optimization problems Ph.D. course in Computer Science

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Lesson 5: Exchange heuristics

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### Exchange algorithms

In Combinatorial Optimization every solution x is a subset of B

An exchange heuristic updates a current subset  $x^{(t)}$  step by step 1 start from a feasible solution  $x^{(0)} \in X$  found somehow (often by a constructive heuristic)

generate a family of feasible solutions by exchanging elements, i.e. add subsets A external to x<sup>(t)</sup> and delete subsets D internal to x<sup>(t)</sup>

$$x'_{A,D} = x \cup A \setminus D$$
 with  $A \subseteq B \setminus x$  and  $D \subseteq x$ 

use a selection criterium φ (x, A, D) to choose the subsets to exchange

$$(A^*, D^*) = \arg \min_{(A,D)} \varphi(x, A, D)$$

g perform the chosen exchange to generate the new current solution

$$x^{(t+1)} := x^{(t)} \cup A^* \setminus D^*$$

 if a termination condition holds, terminate; otherwise, go back to point 2

An exchange heuristic is defined by:

- 1) the pairs of exchangeable subsets (A, D) in every solution x,
  - i.e. the solutions generated by a single exchange starting from x
- **2** the selection criterium  $\varphi(x, A, D)$

Neighbourhood  $N: X \to 2^X$  is a function which associates to each feasible solution  $x \in X$  a subset of feasible solutions  $N(x) \subseteq X$ 

The situation can be formally described with a search graph in which

- the nodes represent the feasible solutions  $x \in X$
- the arcs connect each solution x to those of its neighbourhood N (x), moving elements into and out of x (they are often denoted as moves)

Every run of the algorithm corresponds to a path in its search graph

How does one define a neighbourhood and select a move?

#### Neighbourhoods based on distance

Every solution  $x \in X$  can be represented by its incidence vector

$$\xi_i(x) = \begin{cases} 1 & \text{if } i \in x \\ 0 & \text{if } i \in B \setminus x \end{cases}$$

Hamming distance between two solutions x and x' is the number of elements in which their incidence vectors differ

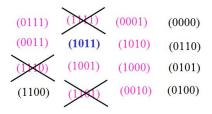
$$d_{H}(x, x') = \sum_{i \in B} |\xi_{i}(x) - \xi_{i}(x')|$$

Referring to the subsets,  $d_H(x, x') = |x \setminus x'| + |x' \setminus x|$ 

A typical definition of neighbourhood, with an integer parameter k, is the set of all solutions with a Hamming distance from x not larger than k

$$N_{H_k}(x) = \{x' \in X : d_H(x, x') \le k\}$$

The *KP* instance with  $B = \{1, 2, 3, 4\}$ , v = [5432] and V = 10, has 13 feasible solutions out of 16 subsets



since subsets {1,2,3,4}, {1,2,3} and {1,2,4} are unfeasible 10 subsets (pink) have Hamming distance  $\leq 2$  from  $x = \{1,3,4\}$  (blue) The neighbourhood  $N_{H_2}(x)$  consists of the 7 feasible subsets in pink  $N_{H_2}(x)$  excludes

- the 3 crossed subsets in pink because they are unfeasible
- the 5 subsets in black because their Hamming distance from x is > 2

## Neighbourhoods based on operations

Another common definition of neighbourhood is obtained defining

- a family  ${\mathcal O}$  of operations on the solutions of the problem
- the set of all solutions generated applying to x the operations of  $\mathcal{O}$  $N_{\mathcal{O}}(x) = \{x' \in X : \exists o \in \mathcal{O} : o(x) = x'\}$

Considering again the KP,  ${\cal O}$  can be defined as

- adding to x an element of  $B \setminus x$
- deleting from x at most an element ( "at most" to impose  $x \in N(x)$ )
- swapping one element of x with one of  $B \setminus x$

The resulting neighbourhood  $N_O$  is related to those defined by the Hamming distance, but does not coincide with any of them

$$N_{H_1} \subset N_{\mathcal{O}} \subset N_{H_2}$$

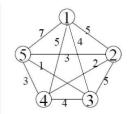
As the distance-based ones, these neighbourhoods can be parameterised considering sequences of k operations of O instead of a single one

$$N_{\mathcal{O}_k}(x) = \{x' \in X : \exists o_1, \ldots, o_k \in \mathcal{O} : o_k (o_{k-1} (\ldots o_1 (x))) = x'\}$$

## Distance and operation-based neighbourhoods

In general, an operation-based neighbourhood includes solutions with different Hamming distances from  $\boldsymbol{x}$ 

For the *TSP* one can define a neighbourhood  $N_{S_1}$  including the solutions obtained swapping two nodes in their visit order



The neighbourhood of solution x = (3, 1, 4, 5, 2) is:

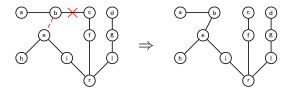
 $N_{S_1}(x) = \{(1,3,4,5,2), (4,1,3,5,2), (5,1,4,3,2), (2,1,4,5,3), (3,4,1,5,2), (3,5,4,1,2), (3,2,4,5,1), (3,1,5,4,2), (3,1,2,5,4), (3,1,4,2,5)\}$ 

If the two nodes are adjacent, the modified arcs are 3 + 3; otherwise, they are 4 + 4

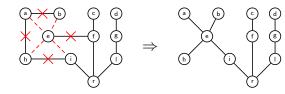
# Different neighbourhoods for the same problem: the CMST

Different ground sets yield different neighbourhoods

- In the CMST it is possible to set B = E or  $B = V \times T$ 
  - exchange edges: delete (b, c), add (b, e)



• exchange vertices: move *e* from subtree 2 to subtree 1, and recompute the two minimum spanning subtrees

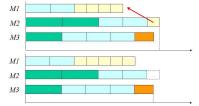


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# Different neighbourhoods for the same problem: the PMSP

For the *PMSP* it is possible to define

• the transfer neighbourhood  $N_{T_1}$ , based on the set  $T_1$  of all transfers of a task on another machine



 the swap neighbourhood N<sub>S1</sub>, based on the set S1 of the swaps of two tasks between two machines (one task for each machine)



#### An exchange heuristic can return the optimum only if every feasible solution can reach at least one optimal solution, that is there is a path from x to $X^*$ for every $x \in X$

Such a search graph is denoted as weakly connected to the optimum

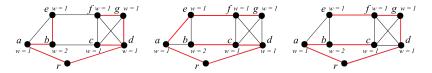
Since  $X^*$  is unknown, a stronger condition is often used: a search graph is strongly connected when it admits a path from x to y for every  $x, y \in X$ 

A good neighbourhood should guarantee some connectivity conditions

- in the *MDP*, neighbourhood  $N_{S_1}$  connects any pair of solutions with at most k swaps
- in the KP and the SCP, no neighbourhood N<sub>Sk</sub> gives that guarantee (feasible solutions can have any cardinality)
- the search graph becomes connected also in the *KP* and the *SCP* if swaps are combined with both additions and deletions

## Connectivity of the search graph

If feasibility is defined in a sophisticated way, exchanging, adding and deleting **single** elements can be insufficient to reach all solutions : the unfeasible subsets can break all paths between some feasible solutions



If V = 4, only three solutions are feasible, all with two subtrees:

- $x = \{(r, a), (a, b), (b, e), (r, d), (c, d), (d, g), (f, g)\}$
- $x' = \{(r, a), (a, e), (e, f), (r, d), (c, d), (b, c), (f, g)\}$
- $x'' = \{(r, a), (a, b), (b, c), (r, d), (d, g), (e, f), (f, g)\}$

The three solutions are mutually reachable only exchanging at least two edges at at time; exchanging only one yields unfeasible subsets

## Steepest descent (hill-climbing) heuristics

The simplest selection criterium  $\varphi(x, A, D)$  is the objective function It is used in nearly all exchange heuristics

When  $\varphi(x, A, D) = f(x \cup A \setminus D)$ , the heuristic moves from  $x^{(t)}$  to the best solution in  $N(x^{(t)})$ 

To avoid cyclic behaviour, only strictly improving solutions are accepted Consequently, the best known solution is the last visited one

Algorithm SteepestDescent $(I, x^{(0)})$   $x := x^{(0)};$ Stop := false; While Stop = false do  $\tilde{x} := \arg\min_{x' \in N(x)} f(x');$ If  $f(\tilde{x}) \ge f(x)$  then Stop := true; else  $x := \tilde{x};$ EndWhile; Return (x, f(x));

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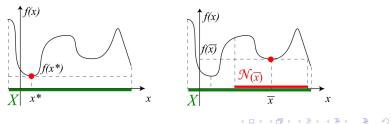
## Local and global optimality

A steepest descent heuristic terminates when it finds a locally optimal solution, that is a solution  $\bar{x} \in X$  such that

 $f(\bar{x}) \leq f(x)$  for each  $x \in N(x)$ 



A globally optimal solution is always also locally optimal, but the opposite is not true in general:  $X^* \subseteq \overline{X}_N \subseteq X$ 



13/72

#### Exact neighbourhood

Exact neighbourhood is a neighbourhood function  $N : X \to 2^X$  such that each local optimum is also a global optimum

 $\bar{X}_N = X^*$ 

Trivial case: the neighbourhood of each solution coincides with the whole feasible region  $(N(x) = X \text{ for each } x \in X)$ 

It is a useless neighbourhood: too wide to explore

The exact neighbourhoods are extremely rare

- exchange between edges for the Minimum Spanning Tree problem
- exchange between basic and nonbasic variables used by the simplex algorithm for Linear Programming

In general, the *steepest descent* heuristic does not find a global optimum Its effectiveness depends on the properties of search graph and of objective

# Properties of the search graph (1)

Some relevant properties for the effectiveness of an algorithm are

- the size of the search space |X|
- the connectivity of the search graph (as discussed above)
- the diameter of the search graph, that is the number of arcs of the minimum path between the two farthest solutions: larger neighbourhoods produce graphs of smaller diameter (but other factors exist: see the "smallworld" effect)

Consider neighbourhood  $N_{S_1}$  for the symmetric TSP on complete graphs

- the search space includes |X| = (n − 1)! solutions
- $N_{\mathcal{S}_1}$  (swap of two nodes) includes  $\binom{n}{2} = \frac{n(n-1)}{2}$  solutions
- the search graph is strongly connected and has diameter ≤ n − 2: every solution turns into another after at most n − 2 swaps
   For example, x = (1, 5, 4, 2, 3) becomes x' = (1, 2, 3, 4, 5) in 3 steps

 $x = (1, 5, 4, 2, 3) \rightarrow (1, 2, 4, 5, 3) \rightarrow (1, 2, 3, 5, 4) \rightarrow (1, 2, 3, 4, 5) = x'$ 

Other relevant properties

- the density of global optima (<sup>|X\*|</sup>/<sub>|X|</sub>) and local optima (<sup>|X<sub>N</sub>|</sup>/<sub>|X|</sub>): if the local optima are numerous, it is hard to find the global ones
- the distribution of the quality  $\delta(\bar{x})$  of local optima (SQD diagram): if local optima are good, it is less important to find a global one
- the distribution of the locally optimal solutions in the search space: if local optima are close to each other, it is not necessary to explore the whole space

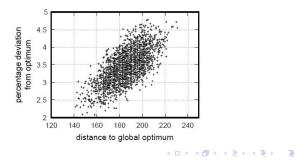
These indices would require an exhaustive exploration of the search graph In pratice, one performs a sampling and these analyses

- require very long times
- can be misleading, especially if the global optima are unknown

## Example: the TSP

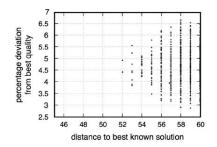
For the TSP on a complete symmetric graph with Euclidean costs

- the Hamming distance between local optima on average exceeds that between local and global optima: the global optima tend to concentrate in the middle of local optima
- the *FDC* diagram (*Fitness-Distance Correlation*) reports the quality δ(x̄) versus the distance from global optima d<sub>H</sub>(x̄, X\*): if they are correlated, better local optima are closer to the global ones



## Fitness-Distance Correlation

For the Quadratic Assignment Problem (QAP), the situation is different



If quality and closeness to the global optima are strongly correlated

- it is profitable to build good starting solutions, because they drive the search near a good local optimum
- it is better to intensify than to diversify

If the correlation is weak

- a good inizialization is less important
- it is better to diversify than to intensify

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## Landscape

The landscape is the triplet (X, N, f), where

- X is the search space, or the set of feasible solutions
- $N: X \to 2^X$  is the neighbourhood function
- $f: X \to \mathbb{N}$  is the objective function

It is the search graph with node weights given by the objective

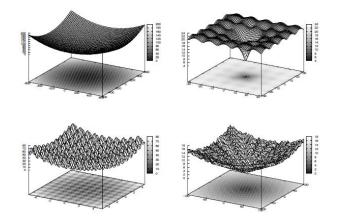


The effectiveness of steepest descent depends on the landscape

- smooth landscapes yield few local optima, possibly of good quality, hence to good results
- rugged landscapes yield several local optima of widespread quality, hence to bad results

## Different kinds of landscape

There is a great variety of landscapes, very different from one another



## Autocorrelation coefficient (1)

The complexity of a landscape can be empirically estimated

- 1 performing a *random walk* in the search graph
- 2 determining the sequence of values of the objective  $f^{(1)}, \ldots, f^{(t_{max})}$

 $\sum_{t=1}^{t=1} f^{(t)}$ 

- **3** computing the sample mean  $\bar{f} = \frac{\tilde{t=1}}{t_{\text{max}}}$
- 4 computing the empirical autocorrelation coefficient

$$r(i) = \frac{\sum_{t=1}^{t_{\max} - i} (f^{(t)} - \bar{f}) (f^{(t+i)} - \bar{f})}{\frac{t_{\max} - i}{\sum_{t=1}^{t_{\max}} (f^{(t)} - \bar{f})^2}}{\frac{t_{\max}}{t_{\max}}}$$

that relates the difference of the objective values in the solutions visited with the distance between these solutions along the walk

# Autocorrelation coefficient (2)

$$r(i) = \frac{\sum_{t=1}^{t_{\max} - i} (f^{(t)} - \bar{f}) (f^{(t+i)} - \bar{f})}{\frac{t_{\max} - i}{\sum_{t=1}^{t_{\max}} (f^{(t)} - \bar{f})^2}}{t_{\max}}}$$

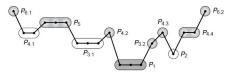
• r(0) = 1 (perfect correlation at 0 distance)

- in general r(i) decreases as the distance i increases
- if  $r(i) \approx 1$  in a large range of distances, the landscape is smooth:
  - the neighbour solutions have values close to the current one
  - there are few local optima
  - the steepest descent heuristic is effective
- if r (i) varies steeply, the landscape is rugged:
  - the neighbour solutions have values far from the current one
  - there are many local optima
  - the steepest descent heuristic is ineffective

#### Plateau

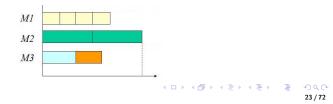
The search graph can be partitioned according to the objective value

• plateau of value *f* is each subset of solutions of value *f* that are adjacent in the search graph



Large plateaus complicate the choice of the solution: most neighbours are equivalent, and the choice ends up depending on the visit order An extremely uniform landscape is not an advantage!

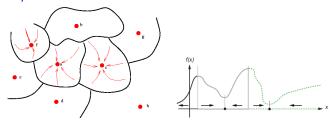
Example: all transfers and swaps between machines 1 and 3 leave the objective value unchanged (*most other moves worsen it*)



## Attraction basins

Alternatively, the search graph can be partitioned into:

• attraction basins of the locally optimal solutions  $\bar{x}$ , that are the subsets of solutions  $x^{(0)} \in X$  starting from which the *steepest descent* heuristic terminates in  $\bar{x}$ 



The steepest descent heuristic is

- effective if the attraction basins are few and large (especially if the global optima have larger basins)
- ineffective if the attraction basins are many and small (especially if the global optima have smaller basins)

# Complexity

Algorithm SteepestDescent  $(I, x^{(0)})$   $x := x^{(0)};$ Stop := false; While Stop = false do {  $t_{max}$  iterations }  $\tilde{x} := \arg\min_{x' \in N(x)} f(x);$ If  $f(\tilde{x}) \ge f(x)$  then Stop := true; else  $x := \tilde{x};$ EndWhile; Return (x, f(x));

#### The complexity of the steepest descent heuristic depends on

- 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 (x̃), which depends on how the search itself is performed, but usually only requires a standard complexity estimation

## The exploration of the neighbourhood

Two strategies to explore the neighbourhood are possible

- 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  $(\gamma_f(|B|, x))$

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 $(I, x^{(0)})$  $x := x^{(0)}$ : Stop := false; While Stop = false do $\{ \tilde{x} := \arg \min_{x' \in N(x)} f(x') \}$  $\tilde{x} := x$ : For each  $x' \in \tilde{N}(x)$  do If  $x' \in N(x)$  then If  $f(x') < f(\tilde{x})$  then  $\tilde{x} := x'$ ; Endlf: EndFor: If  $f(\tilde{x}) > f(x)$  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**  $\gamma_X$ : the time to evaluate their feasibility
- **3**  $\gamma_f$ : 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  $\phi_i$  for each element  $i \in A$ , added to x
- subtract  $\phi_i$  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), ...

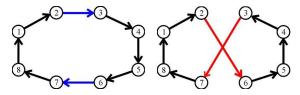
This update has two fundamental properties:

- 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?

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29 / 72

#### Evaluating or updating the objective: the quadratic case

The *MDP* has a quadratic objective function: computing it costs  $\Theta(n^2)$ Moving from x to  $x' = x \setminus \{i\} \cup \{j\}$  (neighbourhood  $N_{S_1}$ ), 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  $d_{ii} = 0$ 

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

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

Let us consider f(x)/2Evaluate 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

 $B \setminus x$ 

i

X

i

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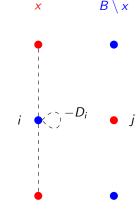
$$x \to x' = x \setminus \{i\} \cup \{j\}$$

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

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

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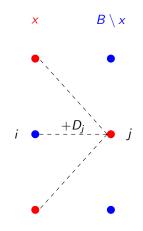
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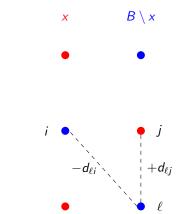
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- but the pair (i, j) is in excess

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

 $B \setminus x$ 

X

 $i - d_{ij}$ 



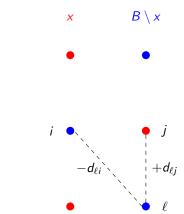
#### Update of the data structures:

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

For each element  $\ell \in B$ 

- *d*<sub>*li*</sub> disappears
- $d_{\ell j}$  appears

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



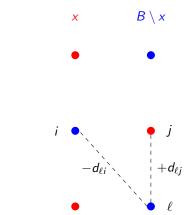
#### Update of the data structures:

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

For each element  $\ell \in B$ 

- *d*<sub>*li*</sub> disappears
- $d_{\ell j}$  appears

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



#### Update of the data structures:

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

For each element  $\ell \in B$ 

- *d*<sub>*li*</sub> disappears
- $d_{\ell j}$  appears

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

## Updating the objective function: nonlinear examples

Many nonlinear functions can be updated with similar tricks

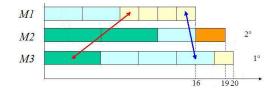
- save aggregated information on the current solution  $x^{(t)}$
- use it to compute f(x') efficiently for each  $x' \in N(x^{(t)})$
- update it when moving to the following solution  $x^{(t+1)}$

Using the transfer  $(N_{T_1})$  and swap  $(N_{S_1})$  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 exchange 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  $O(\log |M|))$

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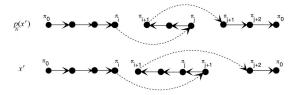
## Use of local auxiliary information

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

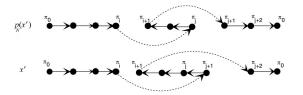
Consider the neighbourhood  $N_{\mathcal{R}_2}$  for the asymmetric *TSP*:

- 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



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#### Example: the asymmetric TSP



The variation of f(x) between two generic neighbour solutions is

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

but moving from exchange  $(s_i, s_j)$  to exchange  $(s_i, s_{j+1})$ 

- the first four terms change, but they can be checked in constant time
- the last two terms can be updated in constant time

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

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

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

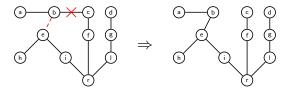
The feasibility test can be made efficient with techniques similar to the ones used for the objective evaluation

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

## Example: the CMSTP

Consider the swap neighbourhood  $N_{S_1}$  (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 ancestors of the receiving vertex e

## A general scheme of sophisticated exploration

The use of auxiliary information requires

1 the inizialization 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(I, x^{(0)})
x := x^{(0)}: GI := InitializeGI(): Stop := false:
While Stop = false do
  \tilde{x} := 0; \ \tilde{\delta} := 0; \ LI := InitializeLI()
   For each x' \in N(x) do
      If f(x') < f(\tilde{x}) then \tilde{x} := x';
      LI := UpdateLI(LI, x')
   EndFor:
   If f(\tilde{x}) > f(x)
      then Stop := true;
      else x := \tilde{x}; GI := UpdateGI(GI, \tilde{x})
   Fndlf
EndWhile:
Return (x, f(x));
```

## Partial saving of the neighbourhood (1)

When performing an operation  $o \in O$  on a solution  $x \in X$  the variation

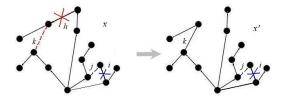
 $\delta f_o(x) = f(o(x)) - f(x)$ 

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

For example, consider the swap neighbourhood  $N_{S_1}$  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 effect of swap (i, j) depends only on the branches including *i* and *j*: it is the same in x and x' and is not affected by swap (h, k)

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

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# Partial saving of the neighbourhood (2)

There exists a subset of operations  $\tilde{\mathcal{O}} \subset \mathcal{O}$  such that

 $\delta f_{o}(x') = \delta f_{o}(x)$  for each  $o \in \tilde{\mathcal{O}}$  and for each x' = o(x)

- It is then advantageous to
  - compute and save δf<sub>o</sub> (x) for every o ∈ 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** recompute and save  $\delta f_o(x')$  only for  $o \in \mathcal{O} \setminus \tilde{\mathcal{O}}$ , that is remove the exchanges on modified branches, recompute their values, and retrieve  $\delta f_o(x')$  for all  $o \in \tilde{\mathcal{O}}$  (their values are still correct)
  - 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

- 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)

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# 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  $\phi_j$
  - delete only elements  $i \in x$  of high cost  $\phi_i$
- 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

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

## Very Large Scale Neighbourhood Search

Larger neighbourhoods yield in general larger attraction basins, so that

- the steepest descent heuristic becomes very effective
- but the exploration time is longer

The Very Large Scale Neighbourhood (VLSN) Search approaches have

- neighbourhoods exponential in |B| (or high-order polynomial)
- explored in low-order polynomial time

Two strategies allow to limit the computational time

- select a neighbourhood in which the objective can be optimized without an exhaustive exploration
- explore the neighbourhood heuristically and return a promising neighbour solution, instead of the best one

## Efficient visit of exponential neighbourhoods

The neighbourhoods based on operations can be easily parameterised

 $N_{\mathcal{O}_{k}}\left(x
ight)=\left\{x'\in X:x'=o_{k}\left(o_{k-1}\left(\ldots o_{1}\left(x
ight)
ight)
ight) ext{ with } o_{1},\ldots,o_{k}\in\mathcal{O}
ight\}$ 

and it would be nice to tune the number of operations k

- increasing k when necessary to improve the current solution x
- decreasing k when sufficient to improve the current solution x

The idea is to define a composite move as a set of elementary moves (that is a combinatorial optimisation problem!)

Finding the optimal solution in such neighbourhoods requires to solve an auxiliary problem, typically on a matrix or graph

- set packing: Dynasearch
- negative cost circuit: cyclic exchanges
- shortest path: ejection chains, order-and-split

Such auxiliary tools are usually defined improvement matrices or graphs

#### Combining elementary moves into composite ones

An operation  $o \in O$  usually modifies only some components of solution xOften only the modified components of x determine

- the feasibility of the new subset o(x)
- the variation of the objective function  $\delta f_o(x) = f(o(x)) f(x)$

Then, two operations  $o, o' \in \mathcal{O}$  that modify different components of x

• are compatible and commutable

$$o'(o(x)) = o(o'(x)) \in X$$

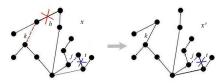
• have an overall effect independent from the order of application and easy to compute: for additive functions it is usually the sum

$$\delta f_{oo'}(x) = \delta f_{o'o}(x) = \delta f_o(x) + \delta f_{o'}(x)$$

The idea is to perform a whole set of moves combining their effects

## Examples of move combinations

• CMSTP: transfer or swap vertices between different subtrees (moves on overlapping subtrees could be unfeasible)



- VRP: transfer or swap nodes between different circuits (moves on overlapping circuits could be unfeasible)
- *TSP*: 2-opt exchanges operating on disjoint segments of the circuit (*arcs that define an exchange are removed/reversed in the others* 
  - moves (i, j) and (k, l) are compatible and can be applied in any order

moves (i, k) and (j, l) are incompatible, as (i, k) reverses (u<sub>j</sub>, u<sub>j+1</sub>)!

47 / 72

### Dynasearch

Let a composite move be a set of elementary moves with mutually independent effects on feasibility and the objective

The situation can be modelled with an improvement matrix A in which

- the rows represent the components of the solution (e.g., branches in the *CMSTP*, circuits in the *VRP*, circuit segments in the *TSP*)
- the columns represent the elementary moves o ∈ O:
   each one has a value equal to the objective improvement −δf<sub>o</sub>(x)
- if move *o* impacts on component *i*,  $a_{io} = 1$ ; otherwise  $a_{io} = 0$

Determine an optimum packing of the columns,

that is a subset of nonconflicting columns of maximum value

The Set Packing Problem is in general  $\mathcal{NP}$ -hard, but

- on special matrices it is polynomial (as in the matrix from the TSP)
- if each move modifies at most two components
  - the rows can be seen as vertices
  - the columns can be seen as edges
  - each packing of columns becomes a matching

and the maximum matching problem is polynomial

## Cyclic exchanges

In many problems

- a feasible solution is a partition of objects into components S<sup>(ℓ)</sup>, that is an assignment of objects to components (i, S<sub>i</sub>) (vertices or edges into branches for the CMSTP, nodes or arcs into circuits for the VRP, objects into containers in the BPP, etc...)
- the feasibility is associated to the single components
- the objective function is additive with respect to the components

$$f(x) = \sum_{\ell=1}^{r} f(S^{(\ell)})$$

In these problems, it is natural to define the set of operations  $\mathcal{T}_k$  which includes the transfers of k elements from their component to another and to derive from  $\mathcal{T}_k$  the neighbourhood  $N_{\mathcal{T}_k}$ 

- often the feasibility constraints forbid the simple transfers
- but the number of multiple transfers quickly grows with k

We want to find a subset of  $N_{\mathcal{T}_k}$  large, but efficient to explore

### The improvement graph

The improvement graph allows to describe sequences of transfers

- a node *i* corresponds to an element *i* of the current solution *x*
- an arc (i, j) corresponds to
  - the transfer of element *i* from its current component S<sub>i</sub> to the current component S<sub>j</sub> of element j
  - the deletion of element *j* from component *S<sub>j</sub>*
- the cost of arc  $c_{ij}$  corresponds to the (positive or negative) variation of the contribution of  $S_j$  to the objective

 $c_{ij} = f(S_j \cup \{i\} \setminus \{j\}) - f(S_j)$ 

with  $c_{ij} = +\infty$  if it is unfeasible to replace j with i in  $S_j$ 

A circuit in such a graph corresponds to a closed sequence of transfers

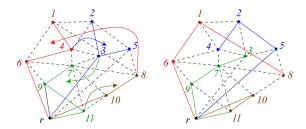
The cost of the circuit corresponds to the cost of the sequence

• but only if each node belongs to a different component

Find the minimum cost circuit satisfying this condition

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### Example: the CMSTP



(4, Rosso, Blu) (3, Blu, Verde) (11, Verde, Marrone) (8, Marrone, Rosso)

Consider the composite move (4, 3), (3, 11), (11, 8), (8, 4):

- vertex 4 moves into the blue branch to replace vertex 3
- vertex 3 moves into the green branch to replace vertex 11
- vertex 11 moves into the brown branch to replace vertex 8
- vertex 8 moves into the red branch to replace vertex 4 The cost variation for subtree  $S_j$  yields the cost of arc  $c_{ij}$ The weight of branch  $S_j$  varies by  $w_i - w_j$ : if unfeasible, forbid the arc

## Search for the minimum cost circuit (1)

The problem is actually  $\mathcal{NP}\text{-hard},$  but

- the constraint of visiting only once each component allows a rather efficient dynamic programming algorithm that grows partial paths (if the components are r, the circuit has at most r arcs)
- all partial paths of cost  $\geq 0$  can be neglected because
  - the total variation of the objective sums the effect of the single moves

$$\delta f_{o_{1},\ldots,o_{k}}\left(x\right)=\sum_{\ell=1}^{k}\delta f_{o_{\ell}}\left(x\right)$$

- every sequence of numbers with negative sum admits a cyclic permutation whose partial sums are all negative
   E. g., (+1, -2, +4, -10, +2) admits (-10, +2, +1, -2, +4)
- therefore, there is a cyclic permutation of the moves  $o_1, \ldots, o_k$

$$\delta f_{o_1,\ldots,o_k}\left(x\right) < 0 \Rightarrow \exists h : \delta f_{o_{(1+h)(\mathrm{mod}\ k)},\ldots,o_{(k+h)(\mathrm{mod}\ k)}}\left(x\right) < 0$$

that is, improving at each step

Moreover,

- there are heuristic polynomial algorithms for the problem
- there are polynomial algorithms to solve relaxations of the problem that neglect the constraint on the components, finding
  - a nonminimum negative circuit (Floyd-Warshall), if any exists
  - a circuit of minimum average cost (total cost / number of arcs)

If the cost of such relaxed solutions is

- positive, then no negative circuit exists
- negative, then the relaxed solution can be
  - optimal (if luckily they are feasible)
  - a starting point to generate a feasible heuristic solution

### Noncyclic exchange chains

It is also possible to create noncyclic transfer chains, so that the cardinality of the components can vary

It is enough to add to the improvement graph

- a source node
- a node for each component
- arcs from the source node to the nodes associated to the elements
- arcs from the nodes associated to the elements to the nodes associated to the components

#### Then, find the minimum cost path that

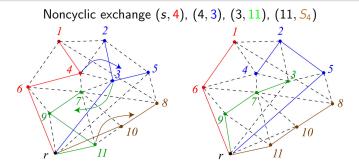
- starts from the source node
- ends in a component node (guaranteed by the topology)
- never visits two nodes associated to the same component

These paths correspond to open transfer chains in which

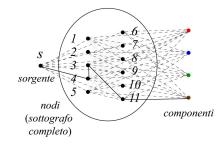
- a component loses an element
- zero or more components lose an element and acquire another one
- a component acquires an element

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## Example: the CMSTP



(4, Rosso, Blu) (3, Blu, Verde) (11, Verde, Marrone)



≣ ▶ ≣ •ીલ્ભ 55/72 The Order-first split-second method for partition problems

- builds a starting permutation of the elements
- partitions the elements into components in an optimum way under the additional constraint that elements of the same component be consecutive in the starting permutation

Of course, the solution depends on the starting permutation: it is reasonable to repeat the resolution for different permutations creating a two-level method

- 1 the upper level selects a permutation
- 2 the lower level computes the optimal partition for the permutation

*Problem: different permutations yield the same solution (the permutations are more numerous than the solutions)* 

# The auxiliary graph

Once again, we exploit an auxiliary graph

Given the permutation  $(s_1, \ldots, s_n)$  of the elements

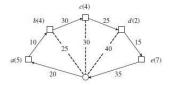
- each node *s<sub>i</sub>* corresponds to a element *s<sub>i</sub>* plus a fictitious node *s*<sub>0</sub>
- each arc  $(s_i, s_j)$  with i < j corresponds to a potential component  $S_{\ell} = (s_{i+1}, \ldots, s_i)$  formed by the elements of the permutation
  - from *s<sub>i</sub>* excluded
  - to s<sub>j</sub> included
- the cost  $c_{s_i,s_j}$  corresponds to the cost of the component  $f(S_\ell)$
- the arc does not exist if the component is unfeasible

Consequently

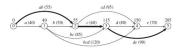
- each path from  $s_0$  a  $s_n$  represents a solution (partition of elements)
- the cost of the path coincides with the cost of the partition
- the graph is acyclic: finding the optimum path costs O(m) where m ≤ n(n-1)/2 is the number of arcs

## Example: the VRP

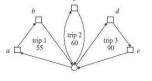
Given an instance of *VRP* with 5 nodes and capacity W = 10



the arcs corresponding to unfeasible paths (weight > W) do not exist, the costs of the arcs are the costs of the *TSP* solutions for  $\{d, s_{i+1}, \ldots, s_j\}$ 



The optimal path corresponds to three circuits:  $(d, s_1, s_2, d)$ ,  $(d, s_3, d)$ and  $(d, s_4, s_5, d)$ 

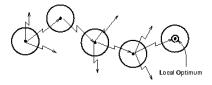


58 / 72

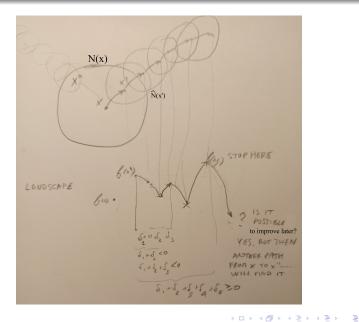
그 에 비행에 비행하는 비행이 가지 않는 것 같아.

In the VDS a composite move as sequence of elementary moves

- consider each solution x' in the basic neighbourhood  $N_{\mathcal{O}_1}(x)$
- from it, make a sequence of moves optimizing each elementary step, but allowing worsening moves and forbidding backward moves
- terminate when the current solution y becomes worse than x' or all moves are forbidden (the length k of the sequence is variable)
- return the best solution  $y^*$  found along the sequence



#### Variable Depth Search



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60 / 72

## Scheme of the Variable Depth Search

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

Given  $x^{(t)}$ , for each  $x' \in N(x^{(t)})$ , instead of evaluating only f(x')1 find a promising solution  $\tilde{y}$  in a neighbourhood  $\hat{N}(x') \subseteq N(x')$ 2 as long as  $\tilde{y}$  improves  $x^{(t)}$ , replace x' with  $\tilde{y}$  and go to 1 3 return the best solution  $y^*$  found during the whole process

{ Steepest descent } Compute f (x') { Variable Depth Search }  $y := x'; y^* := x'; \text{Stop} := false;$ While Stop = false do  $\tilde{y} := \arg\min_{y' \in \hat{N}(y)} f(y');$ If  $f(\tilde{y}) \ge f(x')$  then Stop := true; else  $y := \tilde{y};$ If  $f(\tilde{y}) < f(y^*)$  then  $y^* := \tilde{y};$ EndWhile; Compute  $f(y^*);$ 

It is a sort of roll-out mechanism for exchange algorithms

With respect to steepest descent exploration

- *VDS* finds a local optimum for each solution of the neighbourhood performing a sort of one-step *look-ahead*
- *VDS* admits worsenings along the sequence of elementary moves (but never with respect to the starting solution)
- VDS makes moves that increase the distance from the starting point to avoid cyclic behaviours (gradually restricting the neighbourhood)

In order to limit the computational effort

- the elementary moves use a reduced neighbourhood  $\hat{N} \subseteq N$
- $\hat{N}$  (elementary step) is explored with the *first-best* strategy
- *N* (basic neighbourhood) is explored with the *first-best* strategy

# Lin-Kernighan's algorithm for the symmetric TSP

Neighbourhood  $N_{\mathcal{R}_k}(x)$  includes the solutions obtained

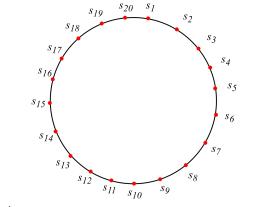
- deleting k arcs of x
- adding other k arcs that recreate a Hamiltonian circuit
- possibly inverting parts of the circuit (*leaving the cost unchanged*)

Lin-Kernighan's algorithm is a *VDS* with sequences of 2-opt exchanges: a *k*-opt exchange is equivalent to a sequence of (k - 1) 2-opt exchanges, where each deletes one of the two arcs added by the previous exchange

Then for each solution  $x' \in N_{\mathcal{R}_2}(x)$  obtained by exchange (i, j)

- evaluate the 2-opt exchanges that delete the added arc  $(s_i, s_{j+1})$  and each arc of  $x \cap x'$  to find the best exchange (i', j')
- if this improves upon x, perform exchange (i', j'), obtaining x''
- evaluate the exchanges that delete  $(s_{i'}, s_{j'+1})$  and each arc of  $x \cap x'' \dots$
- . . .
- if the best solution among  $x', x'', \ldots$  is better than x, accept it

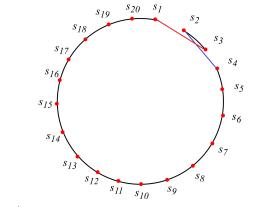
Explore all the solutions  $x' \in N_{\mathcal{R}_2}(x)$ , obtained with exchanges (i, j)



 $x = (s_1 \ \overline{s_2 \ s_3} \ s_4 \ s_5 \ s_6 \ s_7 \ s_8 \ s_9 \ s_{10} \ s_{11} \ s_{12} \ s_{13} \ s_{14} \ s_{15} \ s_{16} \ s_{17} \ s_{18} \ s_{19} \ s_{20})$ 

Let us focus on the exchange (1,3), that reverts  $(s_2,\ldots,s_3)$ 

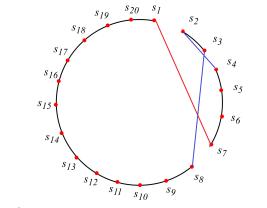
The exchange (1,3) replaces  $(s_1, s_2)$  and  $(s_3, s_4)$  with  $(s_1, s_3)$  and  $(s_2, s_4)$ 



 $x' = (s_1 \overline{s_3 s_2 s_4 s_5 s_6 s_7} s_8 s_9 s_{10} s_{11} s_{12} s_{13} s_{14} s_{15} s_{16} s_{17} s_{18} s_{19} s_{20})$ 

Search for the best exchange that removes  $(s_1, s_3)$  and an arc of  $x \cap x'$ Let us suppose that it is (1,7), which reverts  $(s_3, \ldots, s_7)$ 

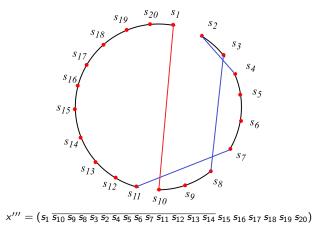
The exchange (1,7) replaces  $(s_1, s_3)$  and  $(s_7, s_8)$  with  $(s_1, s_7)$  and  $(s_3, s_8)$ 



 $x'' = (s_1 \,\overline{s_7 \, s_6 \, s_5 \, s_4 \, s_2 \, s_3 \, s_8 \, s_9 \, s_{10}} \, s_{11} \, s_{12} \, s_{13} \, s_{14} \, s_{15} \, s_{16} \, s_{17} \, s_{18} \, s_{19} \, s_{20})$ 

Search for the best exchange that removes  $(s_1, s_7)$  and an arc of  $x \cap x''$ Let us suppose that it is (1, 10), which reverts  $(s_7, \ldots, s_{10})$ 

The exchange (1, 10) replaces  $(s_1, s_7)$  and  $(s_{10}, s_{11})$  con  $(s_1, s_{10})$  and  $(s_7, s_{11})$ 

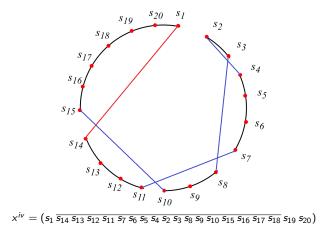


Search for the best exchange that removes  $(s_1, s_{10})$  and an arc of  $x \cap x'''$ 

Let us suppose that it is (1, 14), which reverts  $(s_{10}, \ldots, s_{14})$ 

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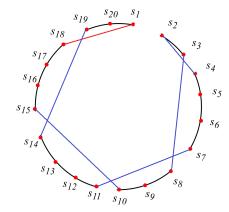
The exchange (1, 14) replaces  $(s_1, s_{10})$  and  $(s_{14}, s_{15})$  con  $(s_1, s_{14})$  and  $(s_{10}, s_{15})$ 



Search for the best exchange that removes  $(s_1, s_{14})$  and an arc of  $x \cap x^{i\nu}$ Let us suppose that it is (1, 18), which reverts  $(s_{14}, \ldots, s_{18})$ 

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The exchange (1,18) replaces  $(s_1,s_{14})$  and  $(s_{18},s_{19})$  con  $(s_1,s_{18})$  and  $(s_{14},s_{19})$ 



 $x^{\nu} = (s_1 \, s_{18} \, s_{17} \, s_{16} \, s_{15} \, s_{10} \, s_9 \, s_8 \, s_3 \, s_2 \, s_4 \, s_5 \, s_6 \, s_7 \, s_{11} \, s_{12} \, s_{13} \, s_{14} \, s_{19} \, s_{20})$ 

Search for the best exchange that removes  $(s_1, s_{18})$  and an arc of  $x \cap x^{\nu}$ Let us suppose that all exchanges yield solutions worst than x: terminate, returning the best solution found

#### Implementation details

- each step deletes an arc of the starting solution to avoid going back and one of the arcs added in the previous step to reduce complexity
- this imposes an upper bound on the length of the sequence
- stopping the sequence as soon as the solution is no longer better than the starting solution does not impair the result
  - the total variation of the objective sums the effect of the single moves

$$\delta f_{o_1,\ldots,o_k}\left(x\right) = \sum_{\ell=1}^k \delta f_{o_\ell}\left(x\right)$$

- every sequence of numbers with negative sum admits a cyclic permutation whose partial sums are all negative
- therefore, there is a cyclic permutation of the moves  $o_1, \ldots, o_k$

$$\delta f_{o_1,\ldots,o_k}\left(x\right) < 0 \Rightarrow \exists h : \delta f_{o_{(1+h)(\mathrm{mod}\ k)},\ldots,o_{(k+h)(\mathrm{mod}\ k)}}\left(x\right) < 0$$

that is, improving at each step

# Iterated greedy methods (destroy-and-repair)

Every exchange can be seen as a combination of addition and deletion

 $x' = x \cup A \setminus D$ 

with  $A = x' \setminus x$  and  $D = x \setminus x'$ 

However

- single swaps  $x' = x \cup \{j\} \setminus \{i\}$  can give bad or unfeasible results
- larger neighbourhoods can be inefficient
- in many problems the right cardinalities of A and D are unknown, because the solutions have nonuniform cardinality (e.g., KP, SCP...)
- A possible idea is to
  - **1** delete from x a subset  $D \subset x$  of cardinality  $\leq k$  (destroy heuristic)
  - 2 complete it with a constructive heuristic (repair heuristic)
- or, of course, the opposite
  - **1** add to x a set  $A \subset B \setminus x$  of cardinality  $\leq k$
  - 2 reduce it with a destructive heuristic

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Most of the time both subsets are chosen heuristically, not exhaustively

- tuning their size |A| and |D| with some parameter
- selecting promising elements based on their cost/value
- applying the first-best strategy (immediately accept any improving solution)

Usually both subsets are chosen in a randomised way

In this case, they are metaheuristics