Heuristic Algorithms

Master's Degree in Computer Science/Mathematics

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Extensions of the basic constructive scheme

The basic scheme of constructive algorithms can be enhanced using

1. a more effective construction graph
   - add more than one element to the current subset x
   - add elements to x, but also remove elements from x
2. a more sophisticated selection criterium, such as
   - a regret-based function that estimates potential future losses associated with element i
   - a look-ahead function that estimates the final value of the objective obtained adding i to x

Extensions of the construction graph

The constructive algorithm adds one element at a time to the solution

It is possible to generalize this scheme with algorithms that at each step

1. add more than one element: the selection criterium $\varphi_A(B^+, x)$ identifies a subset $B^+ \subseteq B \setminus x$ to add, instead of a single element i
2. add elements, but also remove a smaller number of elements: the selection criterium $\varphi_A(B^+, B^-, x)$ identifies a subset $B^+ \subseteq B \setminus x$ to add and a subset $B^- \subseteq x$ to remove, with $|B^+| > |B^-|$

These algorithms build an acyclic construction graph on the search space, so that they never revisit any subset

The fundamental problem is to define a family $\Delta_A^+(x)$ of subset pairs such that optimising the selection criterium is a polynomial problem

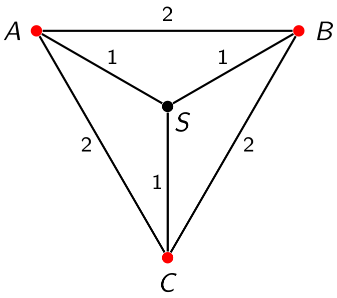
$$\min_{(B^+,B^-)\in\Delta_A^+(x)} \varphi_A\left(B^+, B^-, x\right)$$

that is

- subsets efficiently optimisable (minimum paths,...)
- subsets of limited size (e. g., $|B^+| = 2$ and $|B^-| = 1$)

The Steiner Tree Problem (*STP*)

Given an undirected graph $G = (V, E)$, a cost function $c : E \to \mathbb{N}$ on the edges and a subset of special vertices $U \subset V$, find a tree connecting at minimum cost all special vertices



The minimum tree spanning the special vertices is not necessarily optimal (*and it might not even exist*)

The *Distance Heuristic* (*DH*) for the *STP*

A basic constructive algorithm could adopt the same search spaces as

- Kruskal's algorithm: the set of all forests
- Prim's algorithm: the set of all trees including a (special) vertex

but adding one edge at a time

- returns solutions with redundant edges, therefore expensive
- has a hard time distinguishing useful and redundant edges

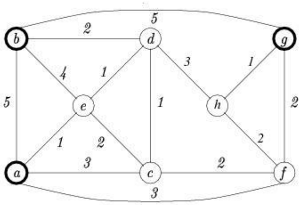
The *Distance Heuristic* adopts as search space $\mathcal{F}$
the collection of all trees including a given special vertex v_1 (*as in Prim*)

It iteratively adds a path B^+ between x and a special vertex
instead of a single edge, so that

- x remains a tree
- x spans a new special vertex
- the minimum cost path can be computed efficiently at each step

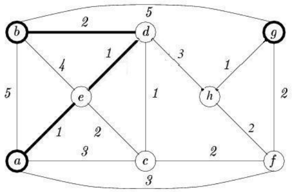
It terminates when all special vertices are spanned by x

Example



- start with a single special vertex a: $x := \emptyset$ (degenerate tree)
- add the closest special vertex (b) through path (a, e, d, b): $x = \{(a, e), (e, d), (d, b)\}$
- add the closest special vertex (g) through path (g, h, d): $x = \{(a, e), (e, d), (d, b), (g, h), (h, d)\}$
- all special vertices are in the solution: terminate

Example



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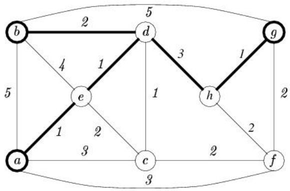

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- all special vertices are in the solution: terminate

  (*this time, the solution is optimal*)

The *Distance Heuristic* algorithm is 2-approximated

It is equivalent to computing a minimum spanning tree on a graph with

- vertices reduced to the special vertices
- edges corresponding to the minimum paths

Counterexample to optimality

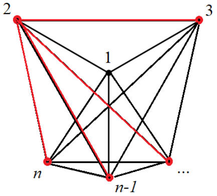
Consider a complete graph $G = (V, E)$ with $U = V \setminus \{1\}$ and cost

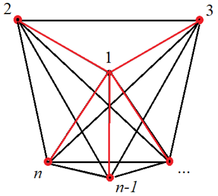
$$c_{uv} = \begin{cases} (1+\epsilon)M & \text{for } u \text{ or } v = 1 \\ 2M & \text{for } u, v \in U \end{cases}$$

(M *is just used to obtain integer costs for any* ϵ)

The *DH* returns a star spanning the special vertices: $f_{\mathrm{DH}} = (n-2) \cdot 2M$

The optimal solution is a spanning star centred in 1: $f^* = (n-1) \cdot (1+\epsilon)M$





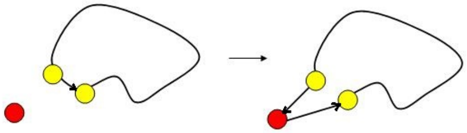
The approximation ratio is $\rho_{DH} = \dfrac{f_{\mathrm{DH}}}{f^*} = \dfrac{n-2}{n-1} \cdot \dfrac{2}{1+\epsilon} < 2$

and converges to 2 as n increases and ϵ decreases

Insertion algorithms for the *TSP*

Several heuristic algorithms for the *TSP* define the search space $\mathcal{F}_A$ as the set of all circuits of the graph including a given node; a circuit

- cannot be obtained from another one by adding a single arc
- can be obtained adding two arcs (i, k), (k, j) and removing one (i, j)



1. Start with a zero-cost self-loop on node 1: $x^{(0)} = \{(1, 1)\}$

   It is not very different from an empty set
2. Select a node k to be added and an arc (i, j) to be removed
3. If the circuit does not visit all nodes, go back to point 2; otherwise terminate

Such a scheme never visits again the same solution and builds a feasible solution in $n - 1$ steps (*each step adds a new node*)

Insertion algorithms for the *TSP*

The selection criterium $\varphi_A(B^+, B^-, x)$ must choose an arc and a node; there are $(n - |x|)|x| \in O(n^2)$ alternatives

- $|x|$ possible arcs (s_i, s_{i+1}) to remove
- $n - |x|$ possible nodes k to add through the arcs (s_i, k) and (k, s_{i+1})

The *Cheapest Insertion* (*CI*) heuristic uses as a selection criterium

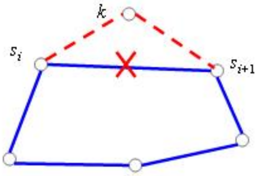
$$\varphi_A(B^+, B^-, x) = f(x \cup B^+ \setminus B^-)$$

Objective function $f(x)$ is additive, hence extensible to the whole of $\mathcal{F}_A$

Since $f(x \cup B^+ \setminus B^-) = f(x) + c_{s_i,k} + c_{k,s_{i+1}} - c_{s_i,s_{i+1}}$

$$\arg \min_{(B^+,B^-)} \varphi_A(B^+, B^-, x) = \arg\min_{i,k} \left(c_{s_i,k} + c_{k,s_{i+1}} - c_{s_i,s_{i+1}}\right)$$

The computational cost of evaluating φ_A decreases from $\Theta(n)$ to $\Theta(1)$



Cheapest Insertion heuristic for the *TSP*

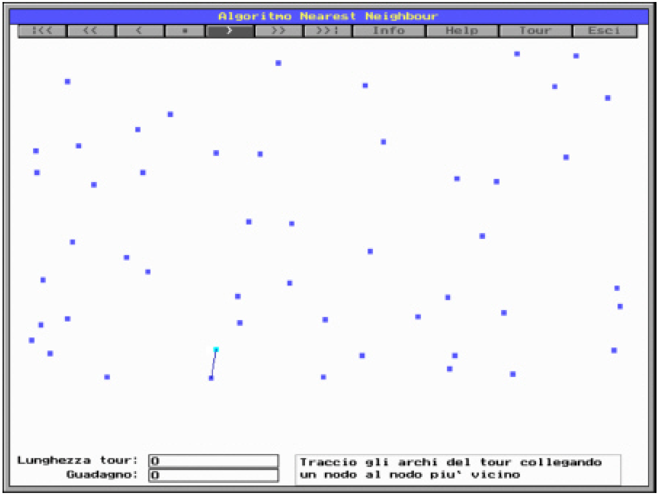
Algorithm *Cheapest Insertion*

1. start with a zero-cost self-loop on node 1: $x^{(0)} = \{(1,1)\}$
   It is also like starting with a single node
2. select the arc $(s_i, s_{i+1}) \in x$ and the node $k \notin N_x$ such that $(c_{s_i,k} + c_{k,s_{i+1}} - c_{s_i,s_{i+1}})$ is minimum
3. if the circuit does not visit all nodes, go back to point 2; otherwise terminate

It is not exact, but 2-approximated, under the triangle inequality

An example

Start with a single node (as in the *NN* heuristic)

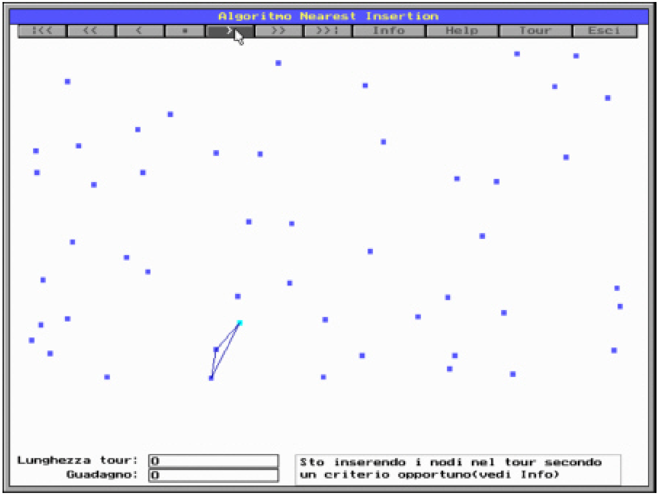


Lunghezza tour: 0
Guadagno: 0

Traccio gli archi del tour collegando un nodo al nodo piu' vicino

An example

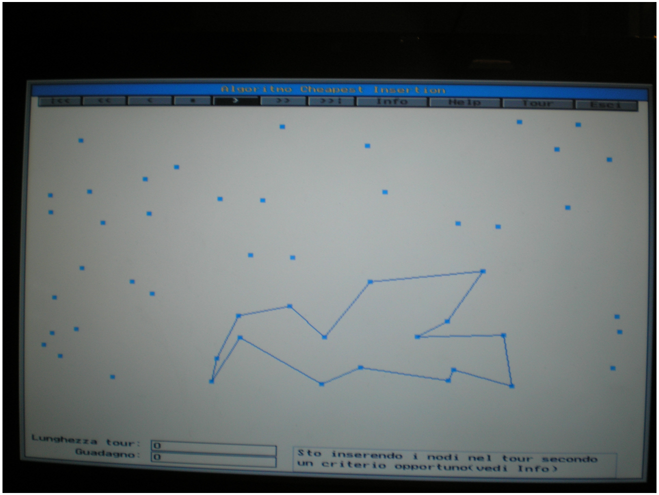
Create a circuit (instead of a path)



Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

Add at each step the node that minimally increases the circuit cost



Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

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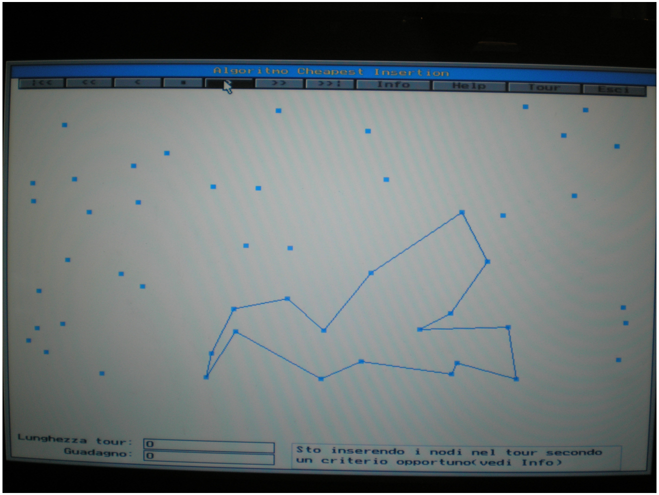
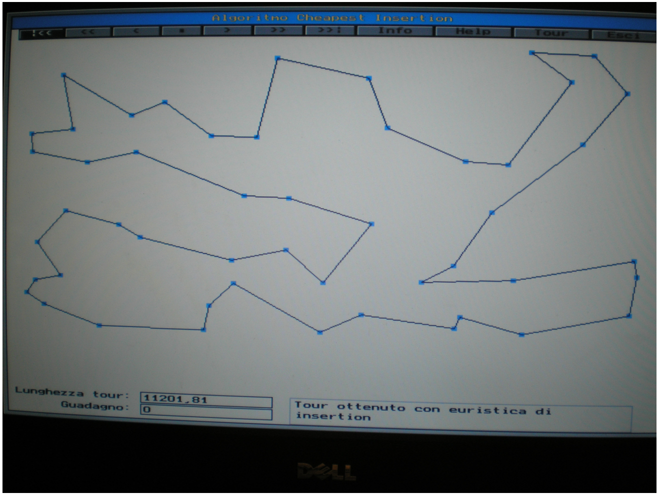


Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

Terminate when the circuit visits all nodes



Lunghezza tour: 11201,81
Guadagno: 0

Tour ottenuto con euristica di insertion

Cheapest Insertion heuristic for the *TSP*

The *CI* algorithm performs $n - 1$ steps: at each step t

- it evaluates $(n - t)\, t$ node-arc pairs
  - each evaluation requires constant time
  - each evaluation possibly updates the best move
- it performs the best addition/removal
- it decides whether to terminate

The overall complexity is $\Theta\left(n^3\right)$

It can be reduced to $\Theta\left(n^2 \log n\right)$ collecting in a *min-heap* the insertion costs for each external node: each of the n steps

- selects the best insertion in $O(n)$ time and performs it
- creates two new insertions and removes one for each external node; updating each of the $O(n)$ heaps takes $O(\log n)$ time

Nearest Insertion heuristic for the *TSP*

Algorithm *Cheapest Insertion* tends to select nodes close to circuit x: minimising $c_{s_i,k} + c_{k,s_{i+1}} - c_{s_i,s_{i+1}}$ implies that $c_{s_i,k}$ and $c_{s_{i+1},k}$ are small

To accelerate, one can decompose criterium φ_A into two phases

Algorithm *Nearest Insertion* (*NI*)

1. start with a zero-cost self-loop on node 1: $x^{(0)} = \{(1,1)\}$
2. Add criterium: select the node k nearest to circuit x

$$k = \arg \min_{\ell \notin N_x} \left(\min_{s_i \in N_x} c_{s_i,\ell} \right)$$

3. Delete criterium: select the arc (s_i, s_{i+1}) that minimises f

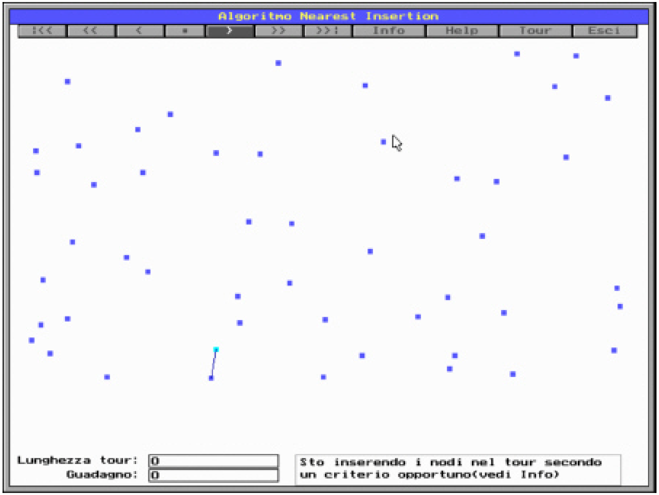
$$(s_i, s_{i+1}) = \arg \min_{(s_i,s_{i+1}) \in x} \left(c_{s_i,k} + c_{k,s_{i+1}} - c_{s_i,s_{i+1}} \right)$$

4. If the circuit does not visit all nodes, go back to point 2; otherwise terminate

It is not exact, but 2-approximated, under the triangle inequality

An example

Start with a single vertex (as in *NN* and *CI*)

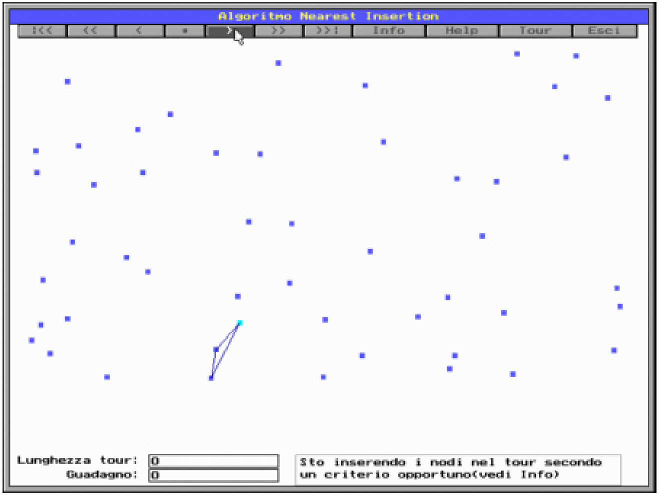


Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

Create a circuit (as in *CI*)

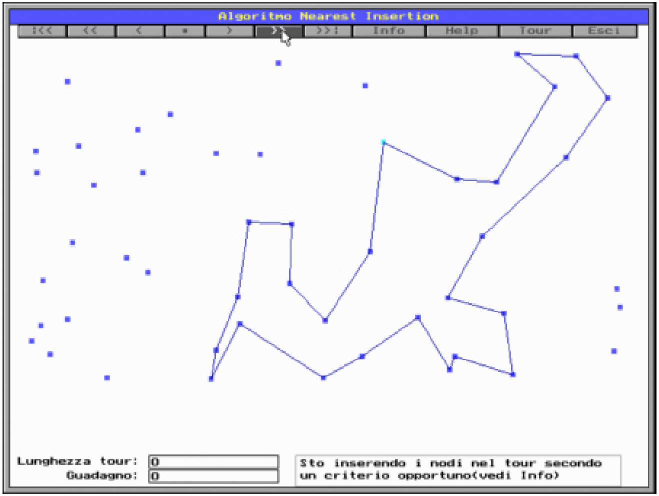


Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

The circuit grows differently, always adding the closest node, even if this increases the cost more than another node

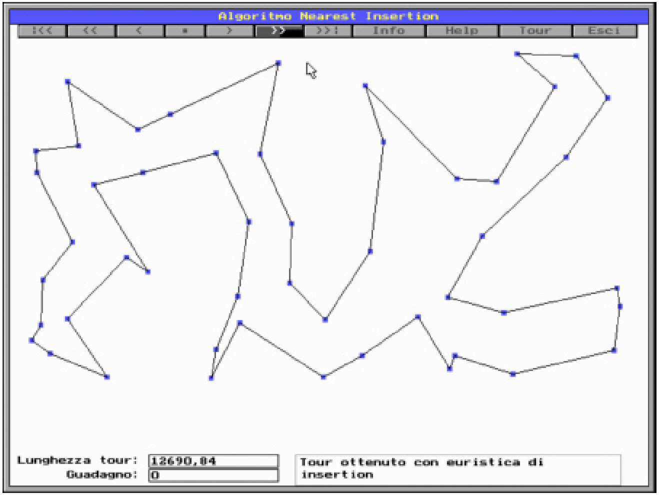


Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

Terminate when the circuit visits all nodes



Lunghezza tour: 12690,84
Guadagno: 0

Tour ottenuto con euristica di insertion

Nearest Insertion heuristic for the *TSP*

The *NI* algorithm performs $n-1$ steps: at each step t

- it evaluates the distance of $(n-t)$ nodes from the circuit, each one in $\Theta(t)$ time
- it selects the node at minimum distance
- it evaluates the removal of t arcs, each one in $\Theta(1)$ time
- it performs the best addition/removal
- it decides whether to terminate

The overall complexity is $\Theta\left(n^3\right)$

It can be reduced to $\Theta\left(n^2\right)$ collecting in a vector for each external node the closest internal node: each of the $n-1$ steps

- selects the closest node in $O(n)$ time
- finds the insertion point in $O(n)$ time
- inserts the node creating a new internal node for each external node, which possibly becomes the closest saved in the vector; each of the $O(n)$ updates takes $O(1)$ time

Farthest Insertion heuristic for the *TSP*

The choice of the closest node to the cycle is natural, but misleading: since all nodes must be visited, it is preferable to service in the best way the most problematic ones (i. e., the farthest ones)

Algorithm *Farthest Insertion* (*FI*)

1. start with a zero-cost self-loop on node 1: $x^{(0)} = \{(1,1)\}$
2. Add criterium: select the node k farthest from cycle x

$$k = \arg\max_{\ell \notin N_x} \left(\min_{s_i \in N_x} c_{s_i,\ell} \right)$$

(*the node that is farthest from the closest node of the cycle*)

3. Delete criterium: select the arc (s_i, s_{i+1}) minimising

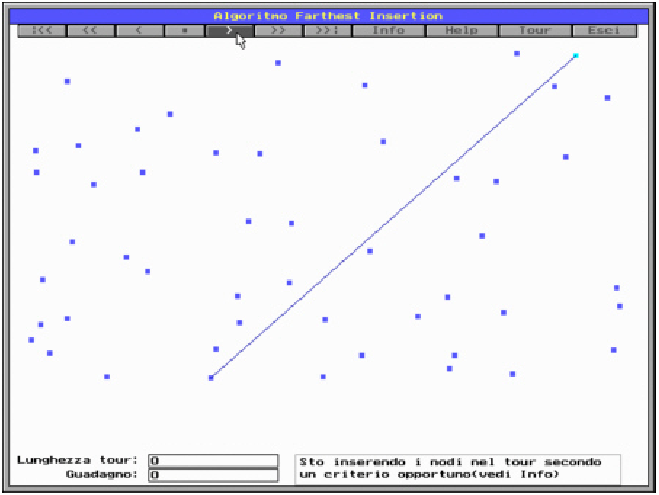
$$(s_i, s_{i+1}) = \arg\min_{(s_i,s_{i+1}) \in x} \left(c_{s_i,k} + c_{k,s_{i+1}} - c_{s_i,s_{i+1}} \right)$$

4. If the circuit does not visit all nodes, go back to point 2; otherwise terminate

It is log n-approximated under the triangle inequality, hence worse than the previous ones in the worst-case (but often experimentally better)

An example

Start reaching immediately the farthest node

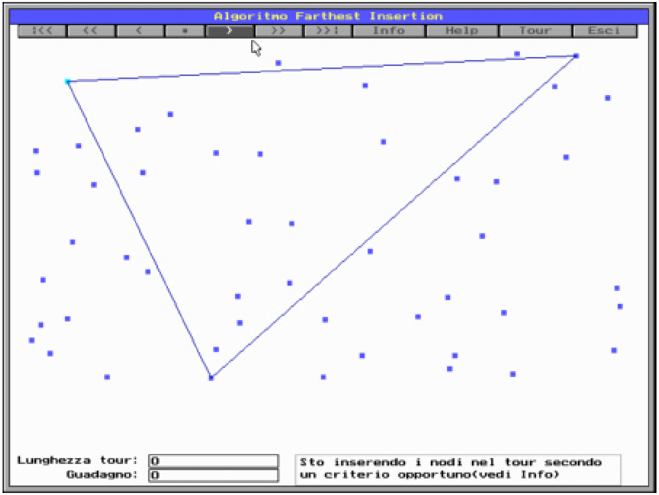


Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

And go on like that

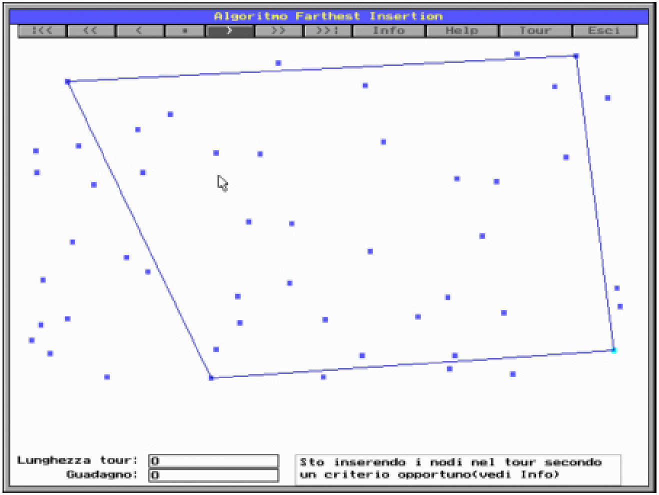


Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

But always inserting these nodes in the best possible way

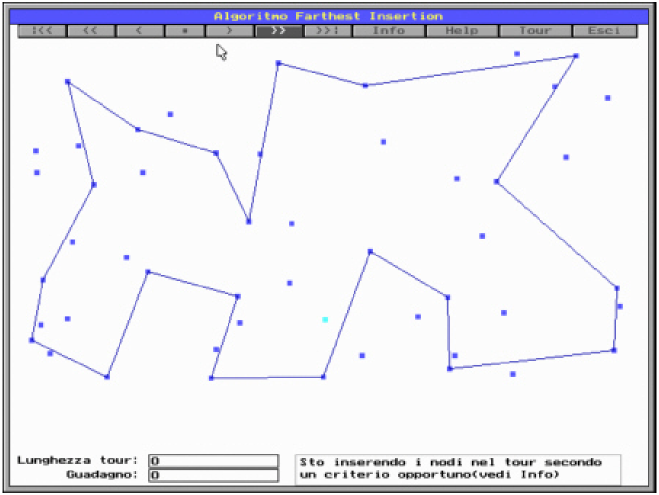


Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

The circuit grows more regularly, with much less crossings and twists

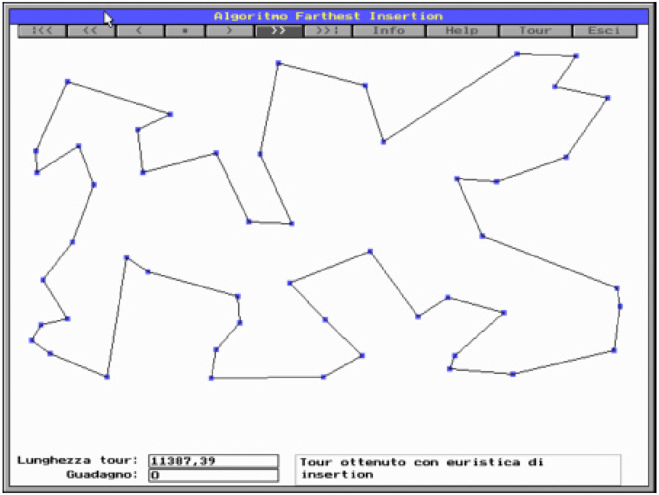


Lunghezza tour: 0
Guadagno: 0

Sto inserendo i nodi nel tour secondo un criterio opportuno(vedi Info)

An example

Terminate when the circuit visits all nodes



Lunghezza tour: 11387,39
Guadagno: 0

Tour ottenuto con euristica di insertion

Farthest Insertion heuristic for the *TSP*

The *FI* algorithm performs $n - 1$ steps: at each step t

- it evaluates the distance of $(n - t)$ nodes from the circuit, each one in $\Theta(t)$ time
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The overall complexity is $\Theta\left(n^3\right)$

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The basic scheme of constructive algorithms can be enhanced using

1. a more effective construction graph
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2. a more sophisticated selection criterium, such as
   - a regret-based function that estimates potential future losses associated with element i
   - a look-ahead function that estimates the final value of the objective obtained adding i to x

Regret-based constructive heuristics

Decisions taken in early steps can severely restrict the feasible choices in later steps due to the constraints of the problem

- *BPP*: all objects must be put into a container, but early assignments could make some containers unavailable for later objects
- *TSP*: all nodes must be visited, but early routing decisions could make the visit of later nodes more expensive
  (*even impossible, if the graph is noncomplete*)
- *CMST*: all vertices must be linked to the root through a subtree, but early links could make some subtrees unavailable for later vertices

The selection criterium can take it into account implicitly

- *BPP*: the Decreasing First-Fit heuristic assigns the larger objects first
- *TSP*: the Farthest Insertion heuristic visits the farther nodes first

Some selection criteria aim explicitly to leave larger sets of good choices

Regret criterium

A typical regret-based heuristic consists in

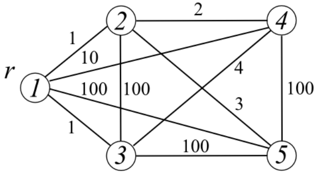
- partitioning $\Delta_A^+(x)$ into disjoint classes of choices
  (*the assignments of each object, the edges incident in each vertex*)
- compute a basic selection criterium for all choices
- compute for each class the regret, i. e. the difference between
  - the second-best choice or
  - the average of the other choices (possibly weighted)

  and the best choice in order to estimate the damage incurred by postponing the best choice until it becomes impossible
- choose the best choice of the class for which the regret is maximum

This is effective when a single choice per class must be taken

Example

Consider the *CMSTP* and ground set $B = V \times T$ (*(vertex,subtree) pairs*)
Let the weights be uniform ($w_v = 1$ for all $v \in V$) and capacity $W = 2$



Let the search space $\mathcal{F}$ include all partial solutions

The greedy algorithm puts vertex 2 in subtree 1, vertex 3 in subtree 2;
then vertex 4 in subtree 1 and finally vertex 5 in subtree 2:
$c(x) = 1 + 1 + 2 + 100 = 104$

The regret algorithm puts vertex 2 in subtree 1; now:

- the regret of vertex 3 is the difference $c(3,3) - c(3,2) = 1 - 1 = 0$
- the regret of vertex 4 is the difference $c(4,2) - c(4,1) = 10 - 2 = 8$
- the regret of vertex 5 is the difference $c(5,2) - c(5,1) = 100 - 3 = 97$

The algorithm puts vertex 5 in subtree 1
Then, it proceeds putting vertices 2 and 4 in subtree 2:
$c(x) = 1 + 3 + 1 + 4 = 9$

Roll-out heuristics

They are also known as single-step look-ahead constructive heuristics and were proposed by Bertsekas and Tsitsiklis (1997)

Given a basic constructive heuristic A

- start with an empty subset: $x^{(0)} = \emptyset$
- at each step t
  - extend the subset in each feasible way: $x^{(t-1)} \cup \{i\}, \forall i \in \Delta_A^+(x)$
  - apply the basic heuristic to each extended subset and compute the resulting solution $x_A(x^{(t-1)} \cup \{i\})$
  - use the value of the solution as the selection criterium to choose $i^{(t)}$

$$\varphi_A(i, x) = f\left(x_A(x^{(t-1)} \cup \{i\})\right)$$

- terminate when $\Delta_A^+(x)$ is empty

Try every feasible move, look at the result, go back and choose the move

The result of the roll-out heuristic dominates that of the basic heuristic (*under very general conditions*)

The complexity remains polynomial, but is much larger:
in the worst case, $T_{\mathrm{ro}(A)} = |B|^2 \, T_A$

Example: roll-out for the *SCP*

$$\begin{array}{c|ccccc|} c & 25 & 6 & 8 & 24 & 12 \end{array}$$

$$A \quad \begin{array}{|ccccc|} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{array}$$

1. start with the empty subset: $x^{(0)} = \emptyset$
2. for each column i, apply the constructive heuristic starting from subset $x^{(0)} \cup \{i\} = \{i\}$
   - for $i = 1$, obtain $x_A(\{1\}) = \{1\}$ of cost $f(x_A(\{1\})) = 25$
   - for $i = 2$, obtain $x_A(\{2\}) = \{2,3,5,4\}$ of cost $f(x_A(\{2\})) = 50$
   - for $i = 3$, obtain $x_A(\{3\}) = \{3,2,5,4\}$ of cost $f(x_A(\{3\})) = 50$
   - for $i = 4$, obtain $x_A(\{4\}) = \{4,2,5\}$ of cost $f(x_A(\{4\})) = 43$
   - for $i = 5$, obtain $x_A(\{5\}) = \{5,2,3,4\}$ of cost $f(x_A(\{5\})) = 50$
3. the best solution is the first one, therefore $i^{(1)} = 1$
4. all rows are covered: the algorithm terminates

Generalised roll-out heuristics

The scheme can be generalised

- applying several basic heuristics $A^{[1]}, \dots, A^{[\ell]}$
- increasing the number of look-ahead steps,
  i. e., using $x^{(t-1)} \cup B^+$ with $|B^+| > 1$

The result improves and the complexity worsens further

The overall scheme does not change significantly

- start from the empty subset: $x^{(0)} = \emptyset$
- at each step t
  - for each possible extension $B^+ \in \Delta_A^+(x^{(t-1)})$
    apply each basic algorithm $A^{[l]}$ starting from $x^{(t-1)} \cup B^+$
  - the selection criterium is $\min_l f_{A^{[l]}}(x^{(t-1)} \cup B^+)$
  - use the value of the best solution as the selection criterium for $i^{(t)}$

$$\varphi_A(i, x) = \min_{l=1,\dots,\ell} f\left(x_A(x^{(t-1)} \cup \{i\})\right)$$

- when $\Delta_A^+(x)$ is empty, terminate

Destructive heuristics

It is an approach exactly complementary to the constructive one

- start with the full ground set: $x^{(0)} := B$
- remove an element at a time, selected
  - so as to remain within the search space $\mathcal{F}_A$

$$\Delta_A^+(x) = \{i \in x : x \setminus \{i\} \in \mathcal{F}_A\}$$

  - maximizing a selection criterium $\varphi_A(i, x)$ (usually a cost reduction)
- terminate when $\Delta_A^+(x) = \emptyset$ (there is no way to remain in $\mathcal{F}_A$)

A destructive heuristic (for a minimisation problem) can be described as

```
Algorithm Stingy(I)
x := B; x* := B;
If x ∈ X then f* := f(x) else f* := +∞;
While Δ_A^+(x) ≠ ∅ do
    i := arg max_{i ∈ Δ_A^+(x)} φ_A(i, x);
    x := x \ {i};
    If x ∈ X and f(x) < f* then x* := x; f* := f(x);
Return (x*, f*);
```

It is optimal for the Minimum Spanning Tree Problem!

Why are they less used?

When the solutions are much smaller than the ground set ($|x| \ll |B|$) a destructive heuristic

- requires a larger number of steps
- is more likely to make a wrong decision at an early step
- sometimes requires more time to evaluate $\Delta_A^+(x)$ and $\varphi_A(i,x)$

When a constructive heuristic returns redundant solutions, it is useful to append a destructive heuristic at its end as a post-processing phase

This auxiliary destructive heuristic

- starts from the solution x of the constructive heuristic, instead of B
- adopts as a search space the feasible region:

$$\mathcal{F}_A = X \Rightarrow \Delta_A^+(x) = \{i \in x : x \setminus \{i\} \in X\}$$

- adopts as the selection criterium the objective function:

$$\varphi_A(i,x) = f(x \setminus \{i\})$$

- terminates after very few steps

Constructive/destructive heuristic for the *SCP*

$$\begin{array}{c|cccc|}
c & 6 & 8 & 24 & 12
\end{array}$$

$$A \quad \begin{array}{|cccc|}
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{array}$$

1. The constructive heuristic selects, in order, columns 1, 2, 4 and 3
   (*each one covers new rows*)
2. The solution is redundant: column 2 can be removed
   (*the following columns also cover already covered rows*)
3. The auxiliary destructive heuristic removes column 2 and provides the optimal solution $x^* = \{1, 3, 4\}$
   (*columns* 1, 3 *and* 4 *are essential to cover rows* 1, 2, 5 *and* 6)

Summary about constructive and destructive algorithms

Constructive and destructive algorithms

1. are intuitive
2. are simple to design, analyze and implement
3. are very efficient (low-order polynomials)

$$T_A(n) \in O\left(n\left(T_{\Delta_A^+}(n) + T_{\varphi_A}(n)\right)\right)$$

   where

   - $T_{\Delta_A^+}(n)$ is the cost to identify $\Delta_A^+(x)$
   - $T_{\varphi_A}(n)$ is the cost to evaluate $\varphi_A(i,x)$ for each $i \in \Delta_A^+(x)$
   - the selection of $\arg\min \varphi_A(i,x)$ and update of x (and auxiliary data structures) are dominated

4. have a strongly variable effectiveness
   - on some problems they guarantee an optimal solution
   - on other problems they provide an approximation guarantee
   - on most problems they provide solutions of extremely variable quality, often scarse
   - on some problems they cannot even guarantee a feasible solution

It is fundamental to study the problem before the algorithm

When are they used?

Constructive and destructive algorithm are used

1. when they provide the optimal solution
2. when the execution time must be very short
   (e.g., for on-line problems: schedulers, on-call services, . . .)
3. when the problem has a huge size or requires heavy computations
   (e.g., some data are obtained by simulation)
4. as component of other algorithms, for example as
   - starting phase for exchange algorithms
   - basic procedure for recombination algorithms