DM841

Discrete Optimization — Heuristics

Construction Heuristics for Traveling Salesman Problem

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark

Outline

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1. Travelling Salesman Problem
2. Solution Approaches
3. TSP
4. Code Speed Up

Traveling Salesman Problem

Traveling Salesman Problem

Given: a weighted complete graph
Output: an Hamiltonian cycle of minimum total weight.

- http://www.math.uwaterloo.ca/tsp/
- “platform for the study of general methods that can be applied to a wide range of discrete optimization problems”
- arranging school bus routes to pick up the children in a school district.
- scheduling of service calls at cable firms
- delivery of meals to homebound persons
- scheduling of stacker cranes in warehouses
- scheduling of a machine to drill holes in a circuit board or other object
- routing of trucks for parcel post pickup

General vs Instance

General problem *vs* problem instance:

General problem $\mathcal{P}$:

- Given *any* set of points X in a square, find a shortest Hamiltonian cycle
- *Solution:* Algorithm that finds shortest Hamiltonian cycle for any X

Problem instantiation π:

- Given a specific set of points π in the square, find a shortest Hamiltonian cycle
- *Solution:* Shortest Hamiltonian cycle for π

Problems can be formalized on sets of problem instances Π (instance classes)

Traveling Salesman Problem

Types of TSP instances:

- Complete vs incomplete graphs
- Symmetric: For all edges uv of the given graph G, vu is also in G, and $w_{uv} = w_{vu}$.
  Otherwise: asymmetric.
- Metric TSP: symmetric + triangle inequality ($w_{ij} \leq w_{ik} + w_{kj}$)
  - Euclidean: Vertices = points in an Euclidean space,
    weight function = Euclidean distance metric.
  - Geographic (metric TSP): Vertices = points on a sphere,
    weight function = geographic (great circle) distance.

Alternatively, these features can become part of the general problem description and exploited in the development of the solution algorithm

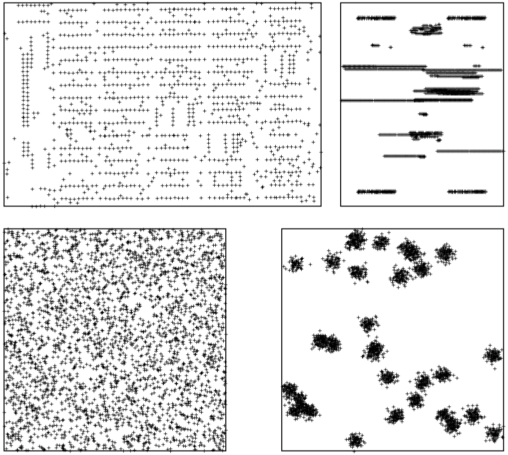
TSP: Benchmark Instances

Instance classes

- Real-life applications (geographic, VLSI)
- Random Euclidean
- Random Clustered Euclidean
- Random Distance

Available at the TSPLIB (more than 100 instances upto 85.900 cities)
and at the 8th DIMACS challenge

TSP: Instance Examples



Complete Algorithms and Lower Bounds

Reference Results

- Branch & cut algorithms (Concorde: http://www.math.uwaterloo.ca/tsp/concorde)
  - cutting planes + branching
  - use LP-relaxation for lower bounding schemes
  - effective heuristics for upper bounds

Solution times with Concorde

Instance	Computing nodes	CPU time (secs)
att532	7	109.52
rat783	1	37.88
pcb1173	19	468.27
fl1577	7	6705.04
d2105	169	11179253.91
pr2392	1	116.86
rl5934	205	588936.85
usa13509	9539	ca. 4 years
d15112	164569	ca. 22 years
s24978	167263	84.8 CPU years

- Lower bounds: (within less than one percent of optimum for random Euclidean, up to two percent for TSPLIB instances)

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Enumeration

Good way to start approaching a problem:

- Make a small example and a drawing of the problem
- Represent a solution: decision variables, data structures.
  For the TSP: permutation as array of all different values corresponds to cycle notation, alternative notation: Cauchy's notation or (node images)
- Enumerate all possible solutions and determine the optimal solution
- For TSP: solution representation is a permutation of vertices, construct all possible permutations by, for example, tree search.
  Consider which parts of the tree can be spared.
  - Rotating permuations: keep starting node fixed
  - Symmetric permuations

  Overall complexity $O((n-1)!/2)$

Held Karp Algorithm: Dynamic Programming

- Consider the problem as a multistage decision problem.
- fix the origin at some city, say 0 (wlog).
- Suppose that at a certain stage of an optimal tour starting at 0 one has reached a city i and there remain k cities $j_1, j_2, \ldots, j_k$ to be visited before returning to 0.
- Principle of Optimality for the tour being optimal, the path from i through $j_1, j_2, \ldots, j_k$ in some order and then to 0 must be of minimum length (if not the entire tour could not be optimal, since its total length could be reduced by choosing a shorter path from i through $j_1, j_2, \ldots, j_k$ to 0).
- $f(i; \{j_1, j_2, \ldots, j_k\}; 0)$ length of a path of minimal length from i to 0 which passes exactly once through each of the remaining k unvisited cities $j_1, j_2, \ldots, j_k$
- $f(0; \{j_1, j_2, \ldots, j_n\}; 0)$ is the solution to the problem

- Recursive relation

$$f(i;\{j_1,j_2,\ldots,j_k\};0)=\min_{1\le m\le k}\{d_{ij_m}+f(j_m;\{j_1,j_2,\ldots,j_{m-1},j_{m+1},\ldots,j_k\};0)\}$$

- $f(i;\{j\};0)=d_{ij}+d_{j0}$
- $f(i;\{j_1,j_2\};0)=\min_{j_1,j_2}\{d_{ij_1}+f(j_1;\{j_2\};0),d_{ij_2}+f(j_2;\{j_1\};0)\}$
- $n2^n$ values $f(i;j_1,j_2,\ldots,j_k;0)$; to calculate
each value costs up to n operations if previous values available
Overall time complexity: $O(n^2 2^n)$; memory usage $O(n2^n)$.
- This is a backward implementation. See wikipedia for a forward implementation and a numerical example

Outline

Construction Heuristics for TSP

Construction heuristics specific for TSP

- Heuristics that Grow Fragments
  - Nearest neighborhood heuristics
  - Double-Ended Nearest Neighbor heuristic
  - Multiple Fragment heuristic (aka, greedy heuristic)
- Heuristics that Grow Tours
  - Nearest Addition
  - Farthest Addition
  - Random Addition
  - Nearest Insertion
  - Farthest Insertion
  - Random Insertion
  - Clarke-Wright savings heuristic
- Heuristics based on Trees
  - Minimum spanning tree heuristic
  - Christofides' heuristics
  - Fast recursive partitioning heuristic

Heuristics that grow fragments

Nearest Neighbor Heuristic

[Bentley, 1992]

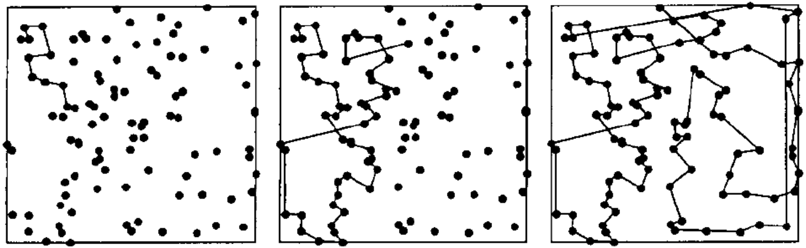


Figure 1. The Nearest Neighbor heuristic.

NN (Flood, 1956)

1. Randomly select a starting node
2. Add to the last node the closest node until no more nodes are available
3. Connect the last node with the first node

Running time $O(N^2)$

Nearest Neighbor Heuristic

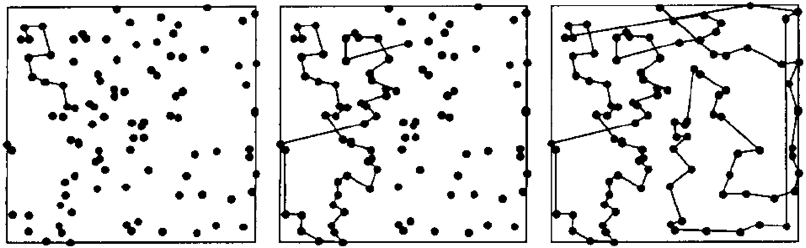


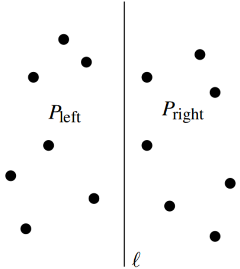
Figure 1. The Nearest Neighbor heuristic.

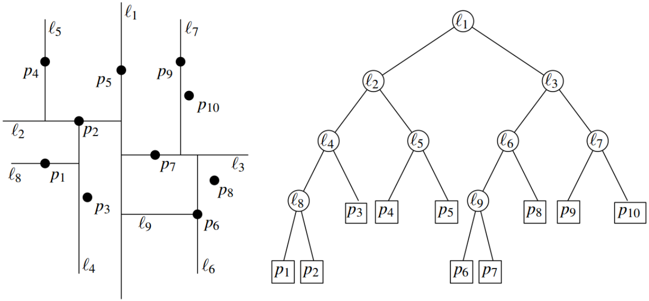
- In geometric instances: $NN < \frac{(\lceil \log N \rceil + 1)}{2} \cdot OPT$
- Double-Ended NN

Nearest Neighbor Heuristic

```
Build(PtSet)
Perm[1]:=StartPt
DeletePt(Perm[1])
for i:=2 to N do
    Perm[i]:=NN(Perm[i-1])
    DeletePt(Perm[i])
```

Data Structure: *k*d-tree





Data Structure: *kd*-tree

- Construction in $O(n \log n)$ time and $O(n)$ space
- Range search: reports the leaves from a split node.
- `Delete(PointNum)` amortized constant time
- `NearestNeighbor(PointNum)` bottom-up search
  visit nodes + compute distances
  $A + BN^C$, $A > 0, B < 0, -1 < C < 0$ (expected constant time) if no deletions happened and data uniform
- `FixedRadiusNearestNeighbor(PointNum, Radius, function)`
- `BallSearch(PointNum, function)` ball centered at point
- `SetRadius(PointNum, float Radius)`
- `SphereOfInfluence(PointNum, float Radius)` ball centered at point with given radius

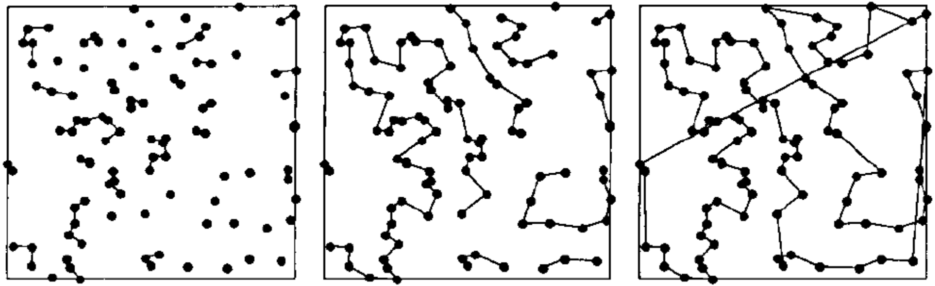


Figure 5. The Multiple Fragment heuristic.

Greedy Heuristic for TSP

[Bentley, 1992]

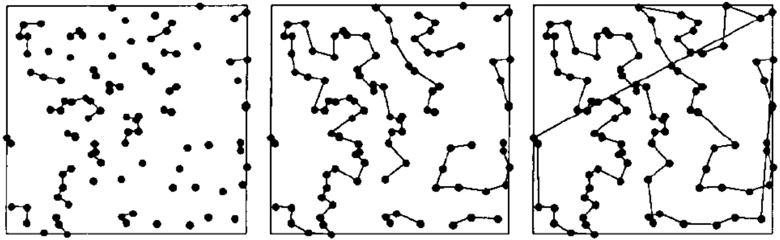


Figure 5. The Multiple Fragment heuristic.

- Add the cheapest edge provided it does not create a cycle.
- $O(\sqrt{N})$ approximation

Greedy Heuristic: Implementation Details

- Array `Degree` num. of tour edges
- K-d tree for nearest neighbor searching (only eligible nodes)
- Array `NNLink` containing index to nearest neighbor of i not in the fragment of i
- Priority queue (heap) with nearest neighbor links
- Array `Tail` link to the other tail of current fragments.

Important Elements

- Exploit the locality inherent in the problem to solve it (NN search, Fixed-radius search, ball search)
- Search time modelled by a function $A + BN^C$
- Number of searches
- Priority queue of links to nearest neighbors

Heuristics that grow tours

Cross product of	Variable selection	Value selection Expansion rule
	Nearest	Addition
	Farthest	Insertion
	Random	

Addition Heuristics

[Bentley, 1992]

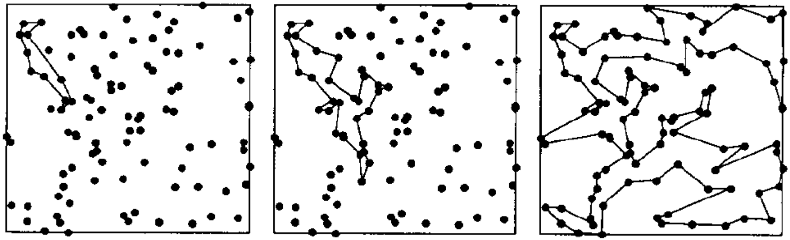


Figure 8. The Nearest Addition heuristic.

NA

1. Select a node and its closest node and build a tour of two nodes
2. Insert in the tour the closest node v until no more node are available

Tour maintained as a double lined list
Running time $O(N^3)$

Addition Heuristics

[Bentley, 1992]

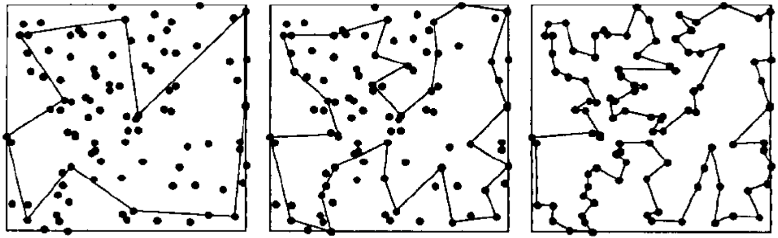


Figure 11. The Farthest Addition heuristic.

FA

1. Select a node and its farthest and build a tour of two nodes
2. Insert in the tour the farthest node v until no more node are available

FA is more effective than NA because the first few farthest points sketch a broad outline of the tour that is refined after.

Running time $O(N^3)$

Addition Heuristics

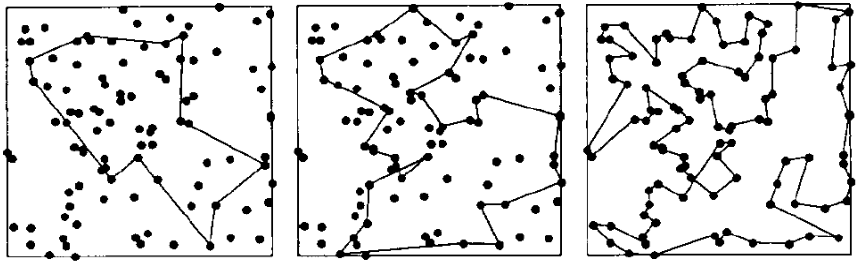
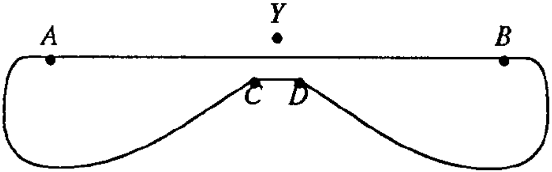


Figure 14. The Random Addition heuristic.

Insertion Heuristics

Motivation:



- A and B are far from Y relative to the distance from Y's nearest neighbor
- Y is near to A relative to the length of the edge AB.

Nearest Neighbor-ball at a point Y with scale S is a ball centered at Y with radius S times the distance from Y to its nearest neighbor among the points in the tour (eg, $D(Y, C)$).

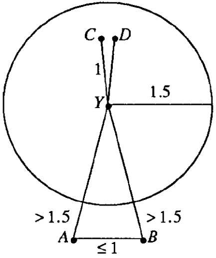
Sphere of influence at tour vertex A with scale S is a ball centered at A with radius S times the length of the longer edge adjacent to A (eg, $D(A, B)$).

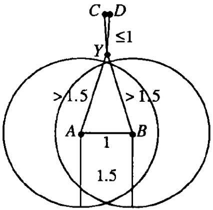
Theorem

Y not yet in tour
C nearest neighbor of Y
D neighbor of C in tour that minimize $C(Y, CD)$
There exists an edge AB such that $C(Y, AB) < C(Y, CD)$ only if one of the following is true:

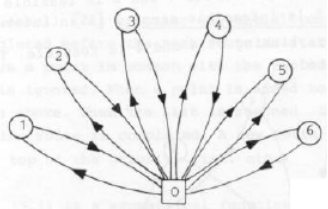
- *$D(A, B) \leq D(Y, C)$ and A or B is in Y's nearest-neighbor-ball with scale 1.5*
- *$D(A, B) \geq D(Y, C)$ and Y is in A or B's sphere of influence with scale 1.5*

Proof: $C(Y, CD) \leq 2D(Y, C)$





Saving Heuristic



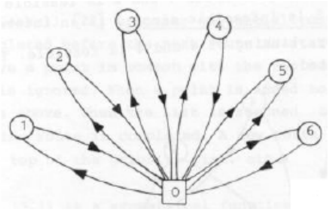
Clarke-Wright Saving Heuristic (1964)

1. Start with an initial allocation of one vehicle to each customer (0 is the depot for VRP or any chosen city for TSP)

Sequential:

2. consider in turn route $(0, i, \dots, j, 0)$
   determine savings s_{ki} and s_{jl} ($s_{ki} = c_{0k} + c_{0i} - c_{ki}$)
3. merge with the cheapest of $(k, 0)$ and $(0, l)$

Saving Heuristic



Clarke-Wright Saving Heuristic (1964)

1. Start with an initial allocation of one vehicle to each customer (0 is the depot for VRP or any chosen city for TSP)

Parallel:

2. Calculate saving $s_{ij} = c_{0i} + c_{0j} - c_{ij}$ and order the saving in non-increasing order
3. scan s_{ij}
   merge routes if i) i and j are not in the same tour ii) neither i and j are interior to an existing route [iii) vehicle and time capacity are not exceeded]

Heuristics based on trees

Minimum Spanning Tree Heuristics

[Bentley, 1992]

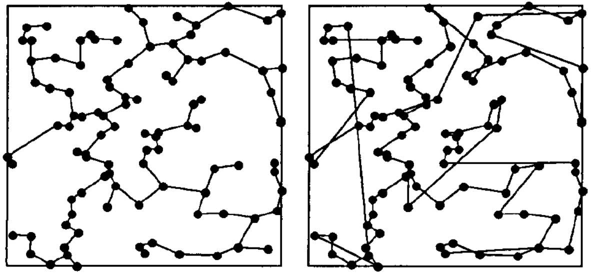


Figure 18. The Minimum Spanning Tree heuristic.

1. Find a minimum spanning tree $O(N^2)$
2. Append the nodes in the tour in a depth-first, inorder traversal

Running time $O(N^2)$
$A = MST/OPT \leq 2$

Christofides' Heuristic

[Bentley, 1992]

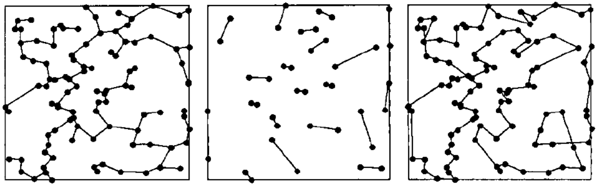


Figure 19. Christofides' heuristic.

1. Find the minimum spanning tree T. $O(N^2)$
2. Find nodes in T with odd degree and find the cheapest perfect matching M in the complete graph consisting of these nodes only. Let G be the multigraph of all nodes and edges in T and M. $O(N^3)$
3. Find an Eulerian walk (each node appears at least once and each edge exactly once) on G and an embedded tour. $O(N)$

Running time $O(N^3)$

$A = CH/OPT \leq 3/2$ tight, the best known is just an $\epsilon > 10^{-36}$ better

(metric TSP cannot be approximated with a ratio better than $\frac{220}{219}$ unless P=NP).

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Where do speedups come from?

Where can maximum speedup be achieved?
How much speedup should you expect?

Code Tuning

- Caution: proceed carefully! Let the optimizing compiler do its work!
  - optimizing flags
  - just-in-time-compilation: it converts code at runtime prior to executing it natively, for example bytecode into native machine code. (module `numba` https://www.ibm.com/developerworks/community/blogs/jfp/entry/Fast_Computation_of_AUC_ROC_score?lang=en)
- Caching, memoization (`@functools.lru_cache(None)`)
- Profiling (module `cProfile`)

- Expression Rules: Recode for smaller instruction counts.
- Loop and procedure rules: Recode to avoid loop or procedure call overhead.
- Hidden costs of high-level languages
- String comparisons: proportional to length of the string, not constant
- Object construction / de-allocation: very expensive
- Matrix access: row-major order $\neq$ column-major order
- Exploit algebraic identities
- Avoid unnecessary computations inside the loops

Where Speedups Come From?

McGeoch reports conventional wisdom, based on studies in the literature.

- Concurrency is tricky: bad -7x to good 500x
- Classic algorithms: to 1trillion and beyond
- Data-aware: up to 100x
- Memory-aware: up to 20x
- Algorithm tricks: up to 200x
- Code tuning: up to 10x
- Change platforms: up to 10x