DM865 – Spring 2019

Heuristics and Approximation Algorithms

Construction Heuristics for Traveling Salesman Problem

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark

Outline

Outline

Aim of the Heuristic Part of the Course

To enable the student to solve discrete optimization problems
that arise in practical applications

Discrete and Combinatorial Optimization

- Discrete optimization emphasizes the difference to continuous optimization, solutions are described by integer numbers or discrete structures
- Combinatorial optimization is a subset of discrete optimization.
- Combinatorial optimization is the study of the ways discrete structures (eg, graphs) can be selected/arranged/combined: Finding an optimal object from a finite set of objects.
- Discrete/Combinatorial Optimization involves finding a way to efficiently allocate resources in mathematically formulated problems.

Discrete Optimization Problems

Discrete Optimization problems

They arise in many areas of
Computer Science, Artificial Intelligence, Operations Research...:

- allocating register memory
- planning, scheduling, timetabling
- Internet data packet routing
- protein structure prediction
- auction winner determination
- portfolio selection
- ...

Discrete Optimization Problems

Simplified models are often used to formalize real life problems

- finding models of propositional formulae (SAT)
- finding variable assignment that satisfy constraints (CSP)
- partitioning graphs or digraphs
- partitioning, packing, covering sets
- finding shortest/cheapest round trips (TSP)
- coloring graphs (GCP)
- finding the order of arcs with minimal backward cost
- ...

Example Problems

- They are chosen because conceptually concise, intended to illustrate the development, analysis and presentation of algorithms
- Although real-world problems tend to have much more complex formulations, these problems capture their essence

Elements of Combinatorial Problems

Combinatorial problems are characterized by an input,
i.e., a general description of conditions (or constraints) and parameters,
and a question (or task, or objective) defining
the properties of a solution.

They involve finding a grouping, ordering, or assignment
of a discrete, finite set of objects that satisfies given conditions.

Candidate solutions are combinations of objects or solution components that need not satisfy all given conditions. They can be partial solutions or complete solutions.

Feasible solutions are candidate solutions that satisfy all given conditions.

Optimal Solutions are feasible solutions that maximize or minimize some criterion or objective function.

Approximate solutions are feasible candidate solutions that are not optimal but good in some sense.

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

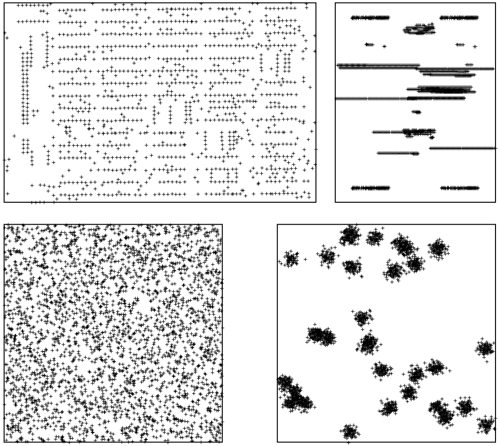
TSP: Benchmark Instances

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)

Outline

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 or Cachy cycle notation (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
  - Symmertic 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.
- $f(i; j_1, j_2, \ldots, j_k)$ length of a path of minimal length from i to 0 which passes exactly once through each of the remaining k unvisited cities $j_1, j_2, \ldots, j_k$
- $f(0; j_1, j_2, \ldots, j_n)$ is the solution to the problem

- Recursive relation

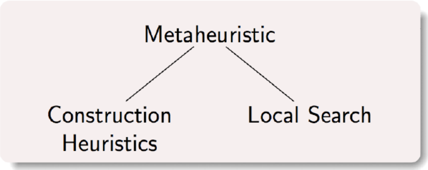
$$f(i; j_1, j_2, \ldots, j_k) = \min_{1 \le m \le k} \{d_{ij_m} + f(j_m; j_1, j_2, \ldots, j_{m-1}, j_{m+1}, \ldots, j_k)\}$$

- $f(i; j) = d_{ij} + d_{j0}$
- $f(i; j_1, j_2) = \min_{j_1, j_2} \{d_{ij_1} + f(j_1; j_2), d_{ij_2} + f(j_2; j_1)\}$
- $n2^n$ values $f(i; j_1, j_2, \ldots, j_k)$ 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 was a backward implementation. See wikipedia for a forward implementation and a numerical example

Heuristics

Get inspired by approach to problem solving in human mind
[A. Newell and H.A. Simon. "Computer science as empirical inquiry: symbols and search." Communications of the ACM, ACM, 1976, 19(3)]

- effective rules without theoretical support
- trial and error



Applications:

- Optimization
- But also in Psychology, Economics, Management [Tversky, A.; Kahneman, D. (1974). "Judgment under uncertainty: Heuristics and biases". Science 185]

Basis on empirical evidence rather than mathematical logic. Getting things done in the given time.

Outline

1. Combinatorial Optimization
2. Solution Approaches
3. TSP
4. Code Speed Up

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

Nearest Neighbor Heuristic

[Bentley, 1992]

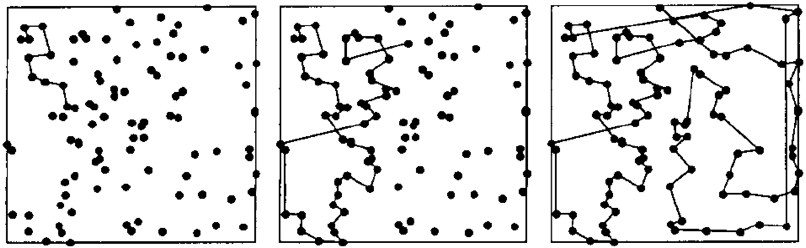


Figure 1. The Nearest Neighbor heuristic.

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

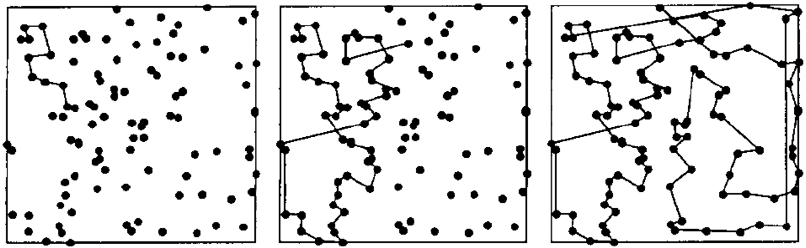


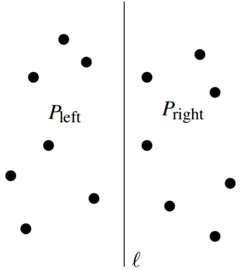
Figure 1. The Nearest Neighbor heuristic.

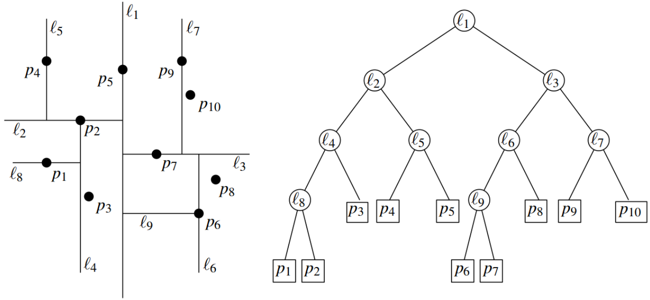
- In geometric instances: $NN < \frac{(\lceil \log N \rceil + 1)}{2} \cdot OPT$
- Double-Ended NN

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

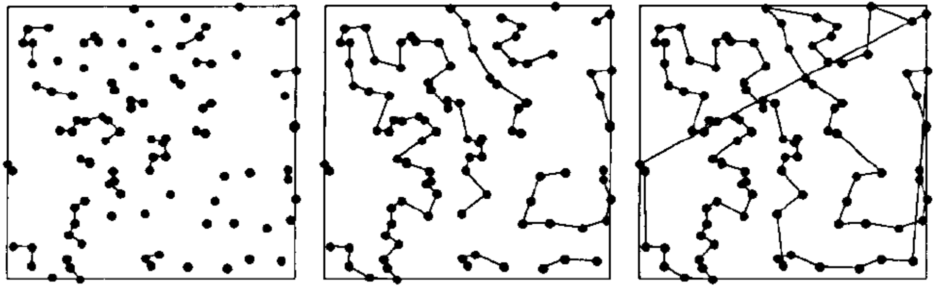


Figure 5. The Multiple Fragment heuristic.

Greedy Heuristic for TSP

[Bentley, 1992]

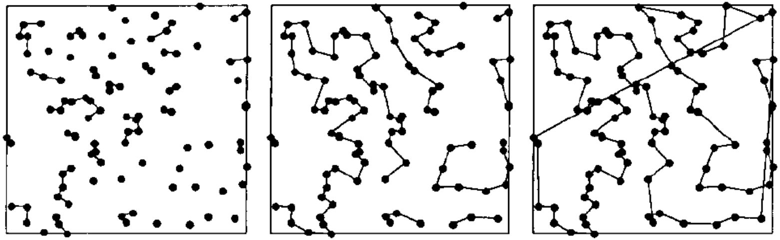


Figure 5. The Multiple Fragment heuristic.

- 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

Addition Heuristics

[Bentley, 1992]

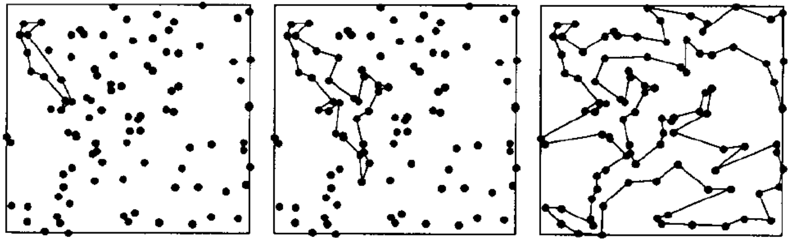


Figure 8. The Nearest Addition heuristic.

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]

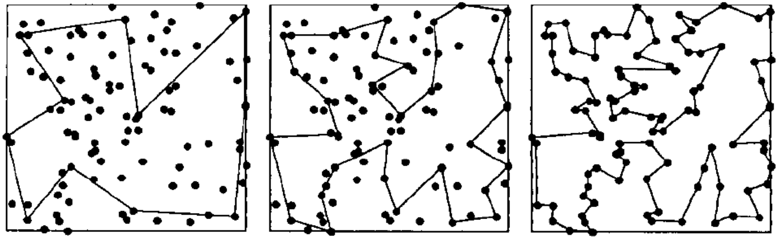


Figure 11. The Farthest Addition heuristic.

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

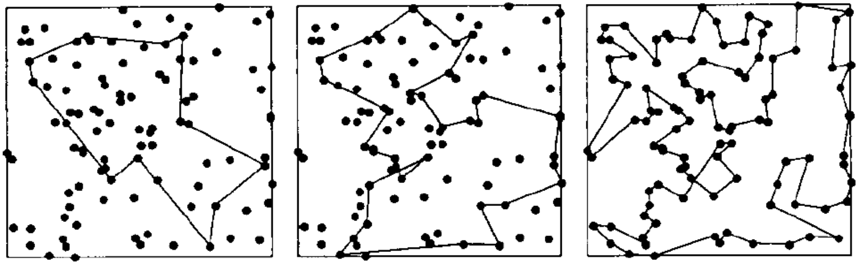
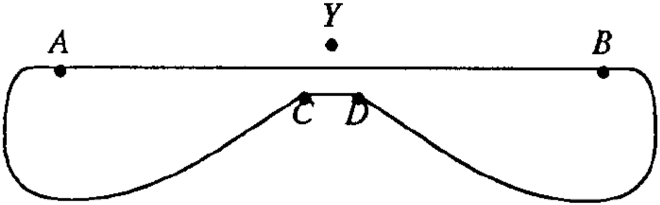


Figure 14. The Random Addition heuristic.

Insertion Heuristics

Motivation:

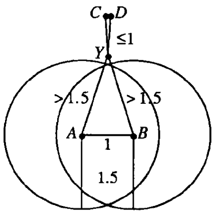


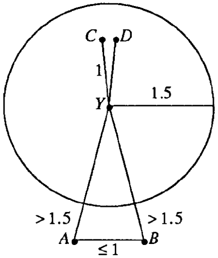
Theorem

Y not yet in tour
C nearest neighbor of Y
D neighbor of C in tour that minimize $C(Y, CD)$
The tour edges with minimal expansion is:

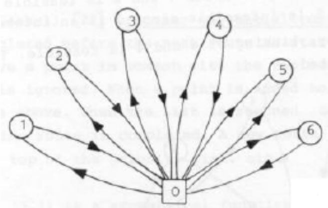
- *the nearest neigbhor edge CD*
- *the edge AB such that A is in $\texttt{NNBall}(Y, 1.5 \cdot e_{min})$, e_{min} shortest edge from Y*
- *the edge AB such that Y is in $\texttt{SphereOfInfluence}(A, 1.5 \cdot e_{max})$, e_{max} longest edge from A scale 1.5*

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





Saving Heuristic



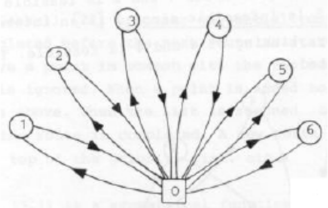
Clarke-Wright Saving Heuristic (1964)

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 $(0, i, \ldots, j, 0)$ determine s_{ki} and s_{jl}
3. merge with $(k, 0)$ or $(0, l)$

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

Minimum Spanning Tree Heuristics

[Bentley, 1992]

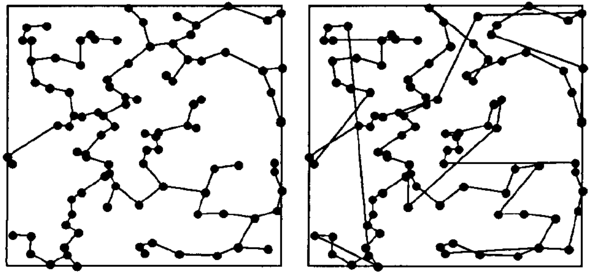


Figure 18. The Minimum Spanning Tree heuristic.

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]

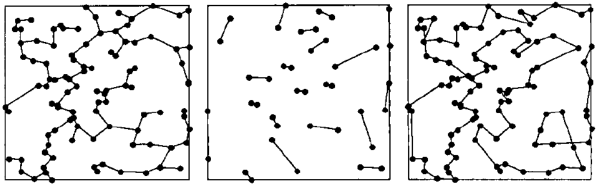


Figure 19. Christofides' heuristic.

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 and best known

Outline

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