



### A brief introduction to combinatorial optimization: The Traveling Salesman Problem

Simon de Givry



Find a tour with minimum distance, visiting every city only once

## Distance matrix (miles)

Distances	Camara	Caniço	Funchal	
Camara	0	15	7	
Caniço	15	0	8	
Funchal	7	8	0	
•••				



Find an order of all the markers with maximum likelihood

## 2-point distance matrix (Haldane)

Distances	M1	M2	M3	
M1	0	14	7	
M2	14	0	8	
M3	7	8	0	





 $\forall$ ,j,k distance(i,j) ? distance(i,k) + distance(k,j) =, $\leq$ 

Multi-point likelihood (with unknowns) ⇔ the distance between two markers depends on the order

## **Traveling Salesman Problem**

Complete graph Positive weight on every edge Symmetric case: dist(i,j) = dist(j,i) Triangular inequality: dist(i,j) ≤dist(i,k) + dist(k,j) Euclidean distance Find the shortest Hamiltonian cycle





### Total distance = xxx miles

## **Traveling Salesman Problem**

Theoretical interest

NP-complete problem

1993-2001: +150 articles about TSP in INFORMS & Decision Sciences databases

**Practical interest** 

Vehicle Routing Problem

Genetic/Radiated Hybrid Mapping Problem NCBI/Concorde, Carthagène, ...

### Variants

Euclidean Traveling Salesman Selection Problem Asymmetric Traveling Salesman Problem Symmetric Wandering Salesman Problem Selective Traveling Salesman Problem TSP with distances 1 and 2, TSP(1,2)K-template Traveling Salesman Problem Circulant Traveling Salesman Problem On-line Traveling Salesman Problem Time-dependent TSP The Angular-Metric Traveling Salesman Problem Maximum Latency TSP Minimum Latency Problem Max TSP Traveling Preacher Problem Bipartite TSP Remote TSP Precedence-Constrained TSP Exact TSP The Tour Cover problem



Introduction to TSP Building a new tour Improving an existing tour Finding the best tour

### Building a new tour





Nearest Neighbor heuristic



### Greedy (or multi-fragments) heuristic



### Savings heuristic (Clarke-Wright 1964)



Mean distance to the optimum

Savings:	11%
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Greedy:	12%
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Nearest Neighbor: 26%



Savings Tour

Optimal Tour

## Improving an existing tour



Which local modification can improve this tour?



Remove two edges and rebuild another tour convert a given sequence of markers







Remove three edges and rebuild another tour (7 possibilities) —Swap the order of two sequences of markers

## « greedy » local search

### 2-opt

<u>Note</u>: a finite sequence of « 2-change » can reach any tour, including the optimum tour

Strategy:

Select the best 2-change among N\*(N-1)/2 neighbors (2-move neighborhood)

Repeat this process until a fix point is reached (i.e. no tour improvement was made)



### Greedy local search

Mean distance to the optimum 9% 2-opt : 4% 3-opt : LK (limited k-opt) : 1% Complexity 2-opt :  $\sim N^3$  $\sim N^4$ 3-opt : LK (limited k-opt) : < N<sup>4</sup>?

## **Complexity** n = number of vertices

Algorithm	Complexity
A-TSP	(n-1)!
S-TSP	(n-1)! / 2
2-change	1
3-change	7
k-change	(k-1)! . 2 <sup>k-1</sup>
k-move	(k-1)! . 2 <sup>k-1</sup> . n! / (k! . (n-k)!)
	~ O( n <sup>k</sup> ) k << n
In practice:	o( n )
2-opt et 3-opt	~ O( n <sup>k+1</sup> )
In practice:	o( n <sup>1.2</sup> )
	time(3-opt) ~ 3 x time(2-opt)

### 2-opt implementation trick:



For each edge (uv), maintain the list of vertices w such that dist(w,v) < dist(u,v)

## Lin & Kernighan (1973)

- k-change :  $e_1 f_1, e_2 f_2, ...$ 
  - =>  $Sum_{i=1}^{k}(dist(e_i) dist(f_i)) > 0$
  - There is an order of i such that all the partial sums are positives:

$$S_{i} = Sum_{i=1}^{i}(dist(e_{i}) - dist(f_{i})) > 0$$

=> Build a valid increasing alternate cycle: xx '->yx ', yy' -> zy', zz' -> wz', etc. dist(f<sub>1</sub>)<dist(e<sub>1</sub>),dist(f<sub>1</sub>)+dist(f<sub>2</sub>)<dist(e<sub>1</sub>)+dist(e<sub>2</sub>),... + Backtrack on y and z choices + Restart (in maximization)



 ${x,y,z,w,..} ^{x',y',z',w',..} = 0$ 

y is among the 5 best neighbors of x', the same for z' and w



### Is this 2-opt tour optimum?



2-opt + vertex reinsertion



Local search & « meta-heuristics »

Tabu Search

Select the best neighbor even if it decreases the quality of the current tour

Forbid previous local moves during a certain period of time

List of tabu moves

Restart with new tours

When the search goes to a tour already seen Build new tours in a random way



# Experiments with CarthaGène N=50 K=100 Err=30% Abs=30%

Log-likelihood improvement of genetic maps with 50 markers on simulated data



### **Experiments - next**



## **Other meta-heuristics**

Simulated Annealing

- Local moves are randomly chosen
- Neighbor acceptance depends on its quality Acceptance process is more and more greedy
- **Genetic Algorithms** 
  - Population of solutions (tours)
  - Mutation, crossover,...
- Variable Neighborhood Search





Potential solutions

# Local Search

### Demonstration

### Finding the best tour





## Tree search

Complexity : n!/2 different orders

Avoid symmetric orders (first half of the tree)

Can use *heuristics* in choice points to order possible alternatives

Branch and bound algorithm

Cut all the branches which cannot lead to a better solution

Possible to combine local search and tree search



 $\leq$  linear programming relaxation of TSP, LB(I)/OPT(I)  $\geq$  2/3



### Christofides heuristic (1976)

 $=> A(I) / OPT(I) \leq 3/2$  (with triangular inequalities)

# Complexity

Complexity	Standard	Computer	Computer
	computer	100 times	1000 times
		faster	faster
Ν	N1	100*N1	1000*N1
N <sup>2</sup>	N2	10*N2	31,6*N2
N <sup>3</sup>	N3	4,64*N3	10*N3
2 <sup>N</sup>	N4	N4+6,64	N4+9,97
3 <sup>N</sup>	N5	N5+4,19	N5+6,29

## **Complete methods**

- 1954 : 49 cities
- 1971 : 64 cities
- 1975 : 100 cities
- 1977 : 120 cities
- 1980 : 318 cities
- 1987 : 2,392 cities
- 1994 : 7.397 cities
- 1998 : 13.509 cities
- 2001 : 15.112 cities (585936700 sec. ≈19 years of CPU!)