Introduction to Metaheuristics

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EU/ME Meeting: From Metaheuristics to Quantum Approches

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Table of Content

1. Introduction

Reference Book for this Presentation

- É. D. Taillard
  Design of Heuristic Algorithms for Hard Optimization
  with Python Codes for the Travelling Salesman Problem
  Springer, 2023
  Open Access
- To lighten the slides, the references are grouped at the end

Definition of Metaheuristics

Set of building blocks for designing a heuristic algorithm

- Problem Modelling (not specific to metaheuristics!)
  - Classification, simulation
  - Mono vs multi-objective optimization
  - Problem decomposition
- Solution Building
- Solution Improvement
  - Sub-problem optimization
  - Matheuristics
  - POPMUSIC
- Learning
  - Construction Learning: Artificial Ant Colony
  - Improvement Learning: Tabu Search
  - Learning with Solutions: Genetic Algorithms, Scatter Search, Particle Swarm

Combinatorial Optimization

Simple vs Hard Problems

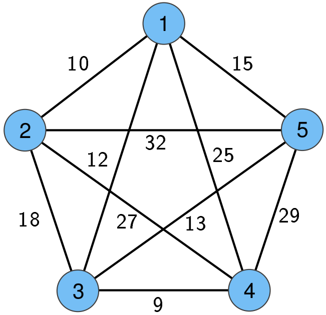
Polynomially Solvable $\in P$

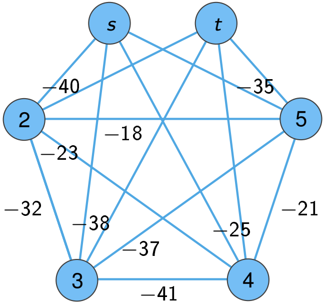
- Shortest Path
  - Exponential number of solutions
  - Efficient algorithms: Jarník, Dijkstra, Bellman-Ford

Intractable $\in$ NP-hard

- Elementary Shortest Path
  - No polynomial algorithm known

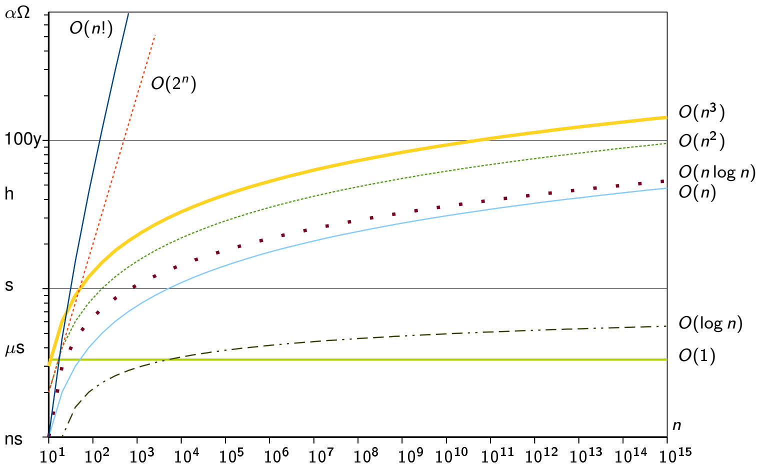
Travelling Salesman Problem (TSP) $\propto$ Elementary Shortest Path





- Data: n cities, distance matrix $D = (d_{ij})$
- Solution: Permutation π of the n cities
- Objective: $\min_\pi \sum_{i=1}^{n-1} d_{\pi_i \pi_{i+1}} + d_{\pi_n \pi_1}$

Computational Complexity

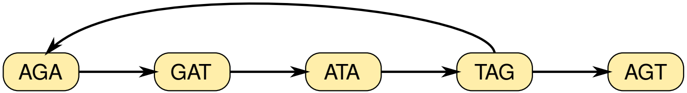


Importance of Problem Modelling: de Bruijn Graphs

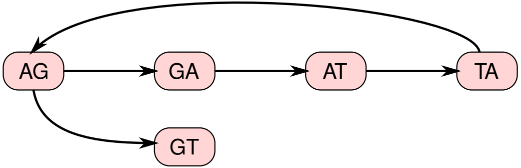
Sequence to discover: AGATAGT; Detected 3-nucleoids AGA, GAT, ATA, TAG, AGT

Nodes ≡ detected 3-nucleotids

Hamiltonian path



Directed edges ≡ detected 3-nucleotids



Eulerian path

Quantum computing forces us to imagine new ways of modelling problems

2. Constructive methods

Kruskal Algorithm for Minimum Spanning Tree

Input : A network with set E of edges
Weight $w(e) \quad \forall e \in E$
Result : Minimum Spanning Tree T

```
R ← E                                        // Edges that can be potentially added to T
while R ≠ ∅ do
    Choose e′ ∈ R minimizing w(e′)
    T ← T ∪ e′                               // Include e′ in the partial tree T
    Remove from R the edges that cannot be added any more to T (degree 3, cycle)
```

Greedy Constructive Method

Input : A trivial partial solution s (generally $\varnothing$); set E of elements constituting a solution; incremental cost function $c(s, e)$

Result : Complete solution s

$R \leftarrow E$ // Elements that can be potentially added to s

while $R \neq \varnothing$ **do**

  Choose $e' \in R$ optimizing $c(s, e')$

  $s \leftarrow s \cup e'$ // Include e' in the partial solution s

  Remove from R the elements that cannot be added any more to s

Greedy Constructive Method

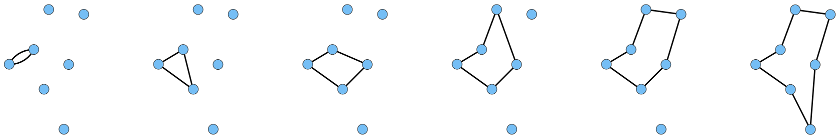
- Build a solution element by element
- At each step, choose the element that is the most appropriate
- Never change a choice

Kruskal's algorithm is a Greedy method

Provides the best possible solution to the minimum spanning tree in polynomial time

Least Cost Insertion for the TSP

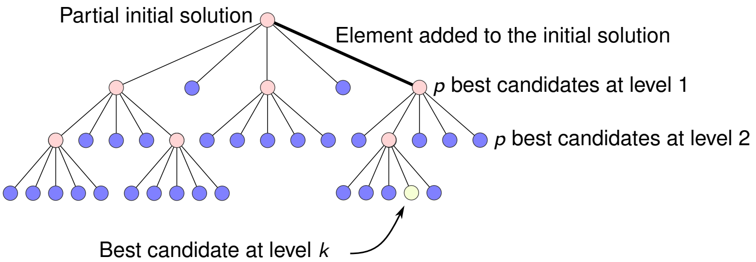
- Start from a partial tour containing a single city
- Element e à to add: a city
- Incremental cost: Minimum detour to add e to the partial tour
- Choose the city with the lowest incremental cost



Seems to work not too bad for the TSP

Beam Search

- Avoid a myopic choice by examining k forward insertions
- Avoid exponential explosion by keeping only the p best candidate at each level
- $c(s, e)$: Best candidate at level k



3. Local Search

Bellman-Ford Algorithm for Shortest Path

Data : Directed network $R = (V, E, w)$ given with an arc list, a starting node s

Result : Immediate predecessor $pred_j$ of j on a shortest path from s to j with its length λ_j, $\forall j \in V$, or: warning message of the existence of a negative length circuit

forall $i \in V$ **do**
- $\lambda_i \leftarrow w(s, i)$ (∞ if arc $(i, j) \notin E$)
- $pred_i \leftarrow s$

$k \leftarrow 0$ // Step counter

$continue \leftarrow true$ // At least one λ modified at last step

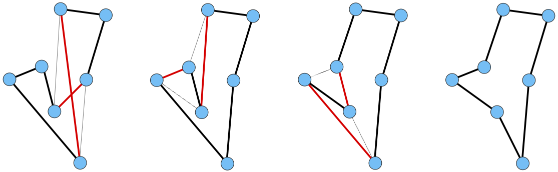
while $k < |V|$ *and continue* **do**
- $continue \leftarrow false$
- $k \leftarrow k + 1$
- **forall** *arc* $(i, j) \in E$ // Check if a better path can be identified
- **do**
  - **if** $\lambda_j > \lambda_i + w(i, j)$ // Improvement found: modify the solution
  - **then**
    - $\lambda_j \leftarrow \lambda_i + w(i, j)$
    - $pred_j \leftarrow i$
    - $continue \leftarrow true$

if $k = |V|$ **then**
- Warning: there is a negative length circuit that can be reached from s

Local search

Bellman-Ford works fine for finding shortest paths

- It's a local improvement technique, like the Simplex algorithm
- Start with a solution obtained with a simple method
- Improve it with local modifications



Successive improvements of a travelling salesman problem solution with a 2-opt local search
Two edges are replaced by two others whose sum of lengths is smaller

Local Search Frame: Best Improvement

Input : Solution s, neighbourhood specification $N(\cdot)$, fitness function $f(\cdot)$ to minimize.
Result : Improved solution s

```
repeat
    end ← true
    best_neighbour_value ← ∞
    forall s' ∈ N(s) do
        if f(s') < best_neighbour_value then A better neighbour is found
            best_neighbour_value ← f(s')
            best_neighbour ← s'

    if best_neighbour_value < f(s) then Move to the improved solution
        s ← best_neighbour
        end ← false
until end
```

Pareto Local Search for Multi-Objective Optimization

Neighbourhood_evaluation

Input : Solution s; neighbourhood $N(\cdot)$ objective functions $\overrightarrow{f}(\cdot)$

Result : Approximation of Pareto set P completed with neighbours of s

forall $s' \in N(s)$ **do**

    `Update_Pareto`$(s', \overrightarrow{f}(s'))$

Update_Pareto

Input : Solution s, objective values $\overrightarrow{v}$

Result : Updated Pareto set P

if $P = \varnothing$ *or* $(s, \overrightarrow{v})$ *dominates a solution of* P **then**

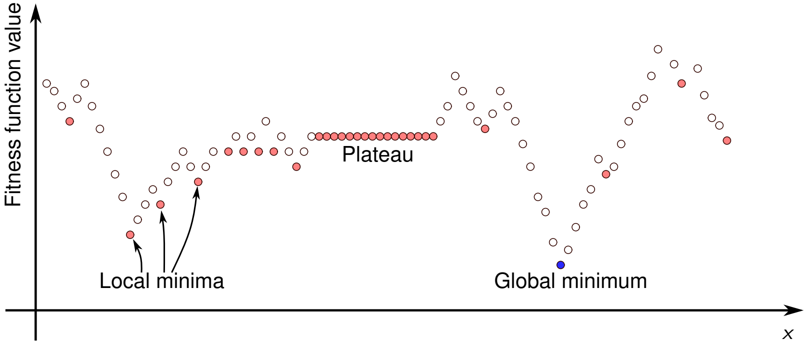
    From P, remove all the solutions dominated by $(s, \overrightarrow{v})$

    $P \leftarrow P \cup (s, \overrightarrow{v})$

    `Neighbourhood_evaluation`(s)

Local, global minimum, plateau

- A local search stops in a *local optimum*, not necessarily the (*global optimum*)
- The quality of a local optimum depends on starting solution and neighbourhood definition

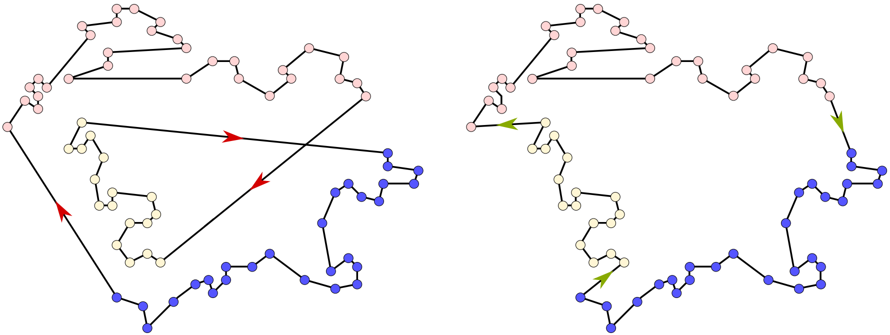


Neighbourhood: modify x by 1 unit

TSP 3-opt move

Replace 3 edges by 3 others

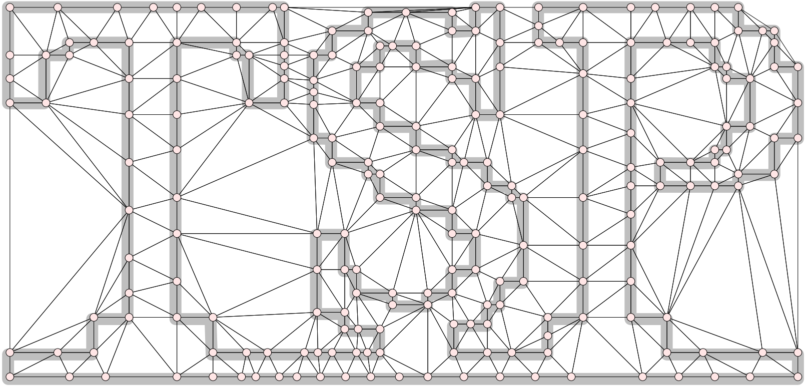
$(i \rightarrow s_i), (j \rightarrow s_j), (k \rightarrow s_k)$ replaced by: $(i \rightarrow s_j), (j \rightarrow s_k), (k \rightarrow s_i)$
Respect the edge orientation on the other edges (not the case for 2-opt)



Limitation of Neighbourhood Size: Candidate List

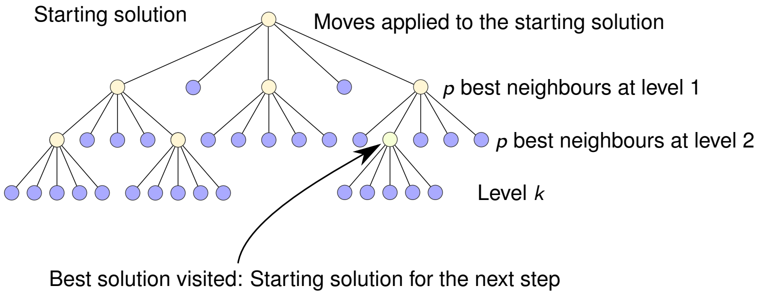
Idea: select a subset of potentially interesting neighbour solutions

Example for the Euclidean TSP: keep only the edges of the Delaunay triangulation

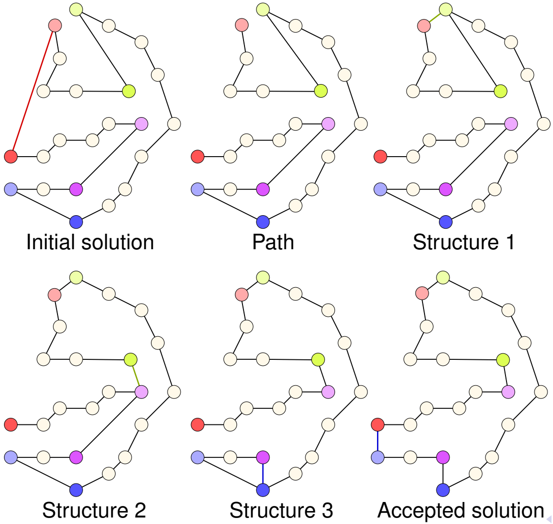


Neighbourhood extension: Filter and Fan

Idea: Similar to Beam Search, but for a Neighbourhood

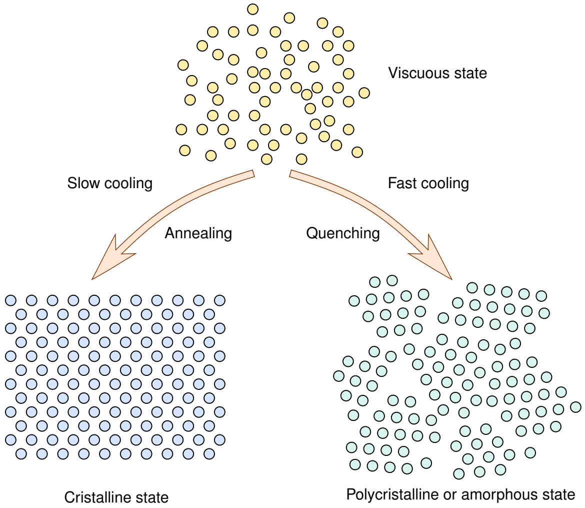


Ejection Chain: Lin-Kernighan Neighbourhood



4. Randomized Methods

Annealing and Quenching Physical Process



Simulated Annealing: Randomized Local Search

Input : Initial solution s; fitness function f to minimize; neighbourhood structure $N(\cdot)$, parameters T_{init}, $T_{end} < T_{init}$ and $0 < \alpha < 1$

Result : Modified solution s

$T \leftarrow T_{init}$

while $T > t_{end}$ **do**

  Randomly generate $s' \in N(s)$

  $\Delta = f(s') - f(s)$

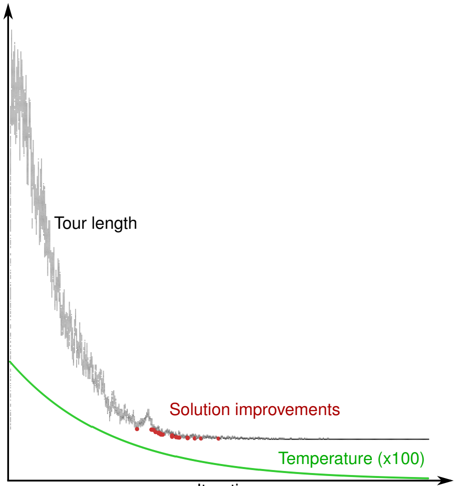
  Randomly generate $0 < u < 1$

  if $\Delta < 0$ *or* $e^{-\Delta/T} > u$ **then** m is accepted

    $s \leftarrow s'$

  $T \leftarrow \alpha \cdot T$

Evolution TSP Tour Length



Greedy Randomized Adaptive Search Procedure (GRASP)

Input : Set E of elements constituting a solution; incremental cost function $c(s, e)$; fitness function f to minimize, parameters I_{max} and $0 \leqslant \alpha \leqslant 1$, improvement method *local_search*

Result : Complete solution s^*

```
f* ← ∞
for I_max iterations do
    Initialize s to a trivial partial solution
    R ← E                                         // Elements that can be added to s
    while R ≠ ∅ do
        Find c_min = min_{e∈R} c(s, e) and c_max = max_{e∈R} c(s, e)
        Choose randomly, uniformly e′ ∈ R such that c_min ⩽ c(s, e′) ⩽ c_min + α(c_max − c_min)
        s ← s ∪ e′                                // Include e′ in the partial solution s
        Remove from R the elements that cannot be added any more to s
    s′ ← local_search(s)                          // Find the local optimum associated with s
    if f* > f(s′) then
        f* ← f(s′)
        s* ← s′
```

5. Metaheuristic Learning Techniques

Construction Learning: Artificial Ants

Simplified Idea: GRASP with Learning

- Compute a statistics τ_e for each element e constituting a potential solution (artificial pheromone)
  - Running average depending on the number of times e appears in previously generated solutions, fitness, ...
  - MAX-MIN Ant System: maintain $\tau_{min} \leqslant \tau_e \leqslant \tau_{max}$
- Instead of choosing any element e such that $c_{min} \leqslant c(s, e) \leqslant c_{max}$, choose e with a probability depending on τ_e and $c(s, e)$
- Add parameters for balancing a priori interest $c(s, e)$ and a posteriori interest τ_e
- Other options: several solutions built in parallel, choice of solutions used to update τ

MAX-MIN Ant System

Input : Set E of elements constituting a solution; incremental cost function $c(s, e) > 0$; fitness function f to minimize, parameters I_{max}, m, α, β, τ_{min}, τ_{max}, ρ and improvement method $a(\cdot)$

Result : Solution s^*

- $f^* \leftarrow \infty$
- **for** $\forall e \in E$ **do**
  - $\tau_e \leftarrow \tau_{max}$
- **for** I_{max} *iterations* **do**
  - **for** $k = 1 \dots m$ **do**
    - Initialize s as a trivial, partial solution
    - $R \leftarrow E$ // Elements that can be added to s
    - **while** $R \neq \varnothing$ **do** Build a new solution
      - Randomly choose $e \in R$ with a probability proportional to $\tau_e^\alpha \cdot c(s, e)^\beta$ // Ant colony formula
      - $s \leftarrow s \cup e$
      - From R, remove the elements that cannot be added any more to s
    - $s_k \leftarrow a(s)$ // Find the local optimum s_k associated with s
    - **if** $f^* > f(s_k)$ **then** Update the best solution found
      - $f^* \leftarrow f(s_k)$
      - $s^* \leftarrow s_k$
  - **for** $\forall e \in E$ **do** Pheromone trail evaporation
    - $\tau_e \leftarrow (1 - \rho) \cdot \tau_e$
  - $s_b \leftarrow$ best solution from $\{s_1, \dots, s_m\}$
  - **for** $\forall e \in s_b$ **do** Update trail, maintaining it between the bounds
    - $\tau_e \leftarrow max(\tau_{min}, min(\tau_{max}, \tau_e + 1/f(s_b)))$

Local Search Learning: Tabu Search

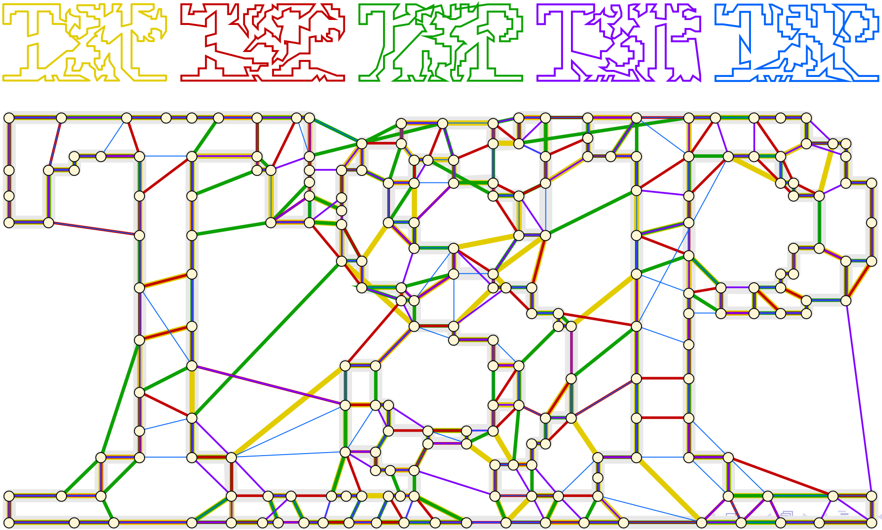
- Local search with best move policy
- Allow degrading moves
- Use a memory to avoid visiting cyclically a subset of solutions
  - Forbid to come back to a solution already visited (the solution is *tabu*)
  - Forbid to perform the reverse of a move recently used
  - Penalize frequently performed moves
  - Force the use of moves never performed for a long time
- A lot of other strategies suggested in original work (aspiration, candidate list, oscillations, . . .)

Tabu Search

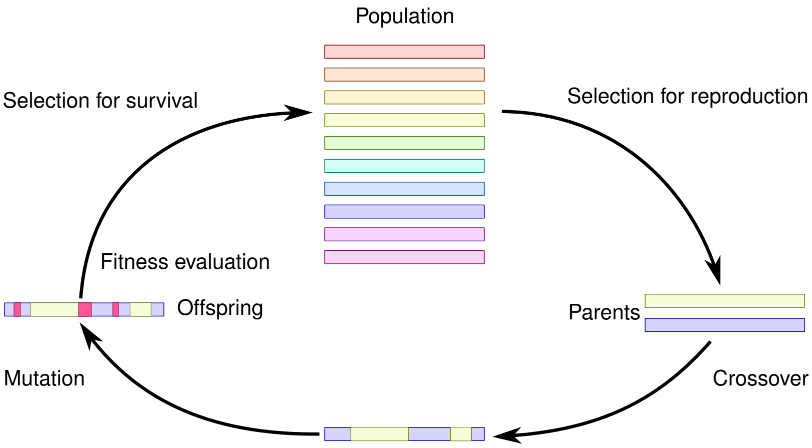
Input : Solution s, neighbourhood $N(\cdot)$, fitness function $f(\cdot)$ to minimize, parameters I_{max}, d
Result : Improved solution s^*

$s^* \leftarrow s$
for I_{max} *iterations* **do**
    $best\_neighbour\_value \leftarrow \infty$
    forall $s' \in N(s)$ *(such that s' is not marked as taboo)* **do**
        if $f(s') < best\_neighbour\_value$ **then**
            $best\_neighbour\_value \leftarrow f(s')$
            $best\_neighbour \leftarrow s'$
    if $best\_neighbour\_value < \infty$ **then**
        Mark s (or the reverse of the move from s to s') as taboo for the next d iterations
        $s \leftarrow s'$
        if $f(s) < f(s^*)$ **then**
            $s^* \leftarrow s$
    else
        Error message: d too large: no move allowed!

Population Learning



Generational Loop in an Evolutionary Algorithm



Population Management Principles

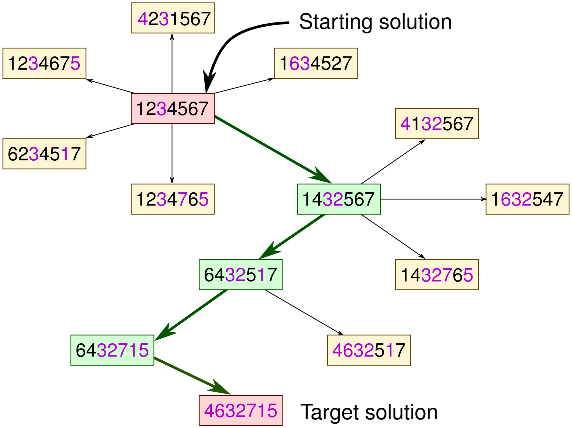
- Keep a subset of elite solutions in the population
- Introduce a diversity measure between solutions and keep solutions as scattered as possible in the population
- Exploitation of the population
  - Mix 2 solutions: genetic crossover
  - Mix several solutions: scatter search
  - Apply a local search to the new created solutions
  - Go from a starting solution to a target solution using a neighbourhood: path relinking

Getting an Offspring

Depends on the problem, but technically possible!

Getting an Offspring: Scatter Search Extension

Exploiting a Population of Solutions: Path Relinking



GRASP with Path Relinking

Input : GRASP procedure (with local search LS and parameter $0 \leqslant \alpha \leqslant 1$), parameters I_{max} and μ

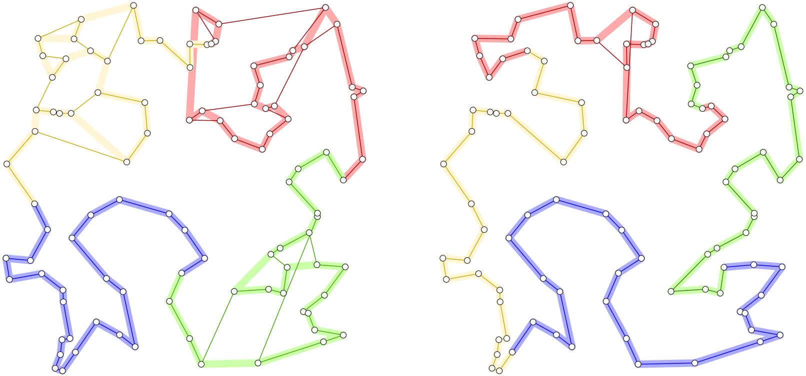
Result : Population P of solutions

$P \leftarrow \varnothing$
while $|P| < \mu$ **do**
  $s \leftarrow GRASP(\alpha, \mathtt{LS})$
  if $s \notin P$ **then**
    $P \leftarrow P \cup s$
for I_{max} *iterations* **do**
  $s \leftarrow GRASP(\alpha, \mathtt{LS})$
  Randomly draw $s' \in P$
  Apply a path relinking between s and s'; identify the best solution s'' on the path
  if $s'' \notin P$ *and s'' is strictly better than a solution of P* **then**
    s'' replaces the most different solution of P which is worse than s''

6. Decomposition Methods

Improvement of a TSP Tour

Decompose the tour into sub-paths containing approximately r cities
Optimize each sub-path with a good quality method (matheuristics: with an exact method)
Restart by considering overlapping sub-paths



POPMUSIC Frame

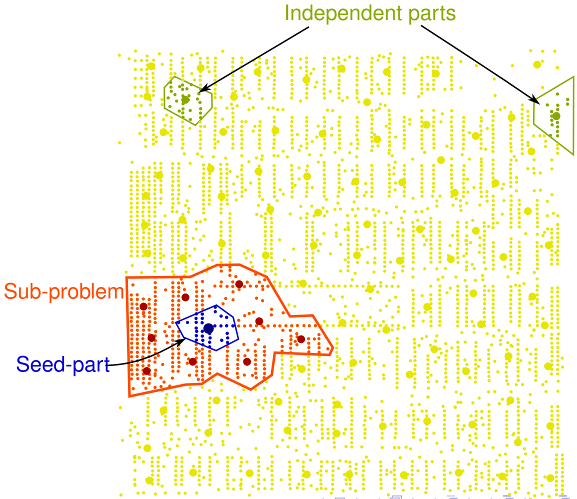
Input : Initial solution s composed of q disjoint parts $s_1, \dots, s_q$; sub-problem improvement method, parameter r

Result : Improved solution s

```
U = {s_1, ..., s_q}
while U ≠ ∅                                   // Natural stopping criterion
 do
    Select s_g ∈ U // s_g: Seed part
    Build a sub-problem R composed of the r parts of s the closest to s_g
    Tentatively optimize R
    if R is improved then
        Update s
        From U, remove the part no longer belonging to s
        In U, insert the parts composing R
    else R not improved
        Remove s_g from U
```

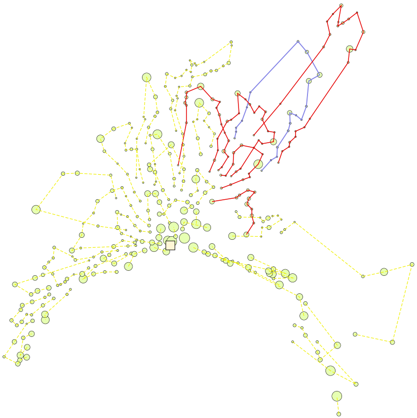
POPMUSIC for Centroid Clustering

- Optimizing 2 cluster well separated cannot improve the solution
- Choose a seed-cluster and the r centres that are the closest
- Optimize these r clusters independently
- Restart with other seed-clusters



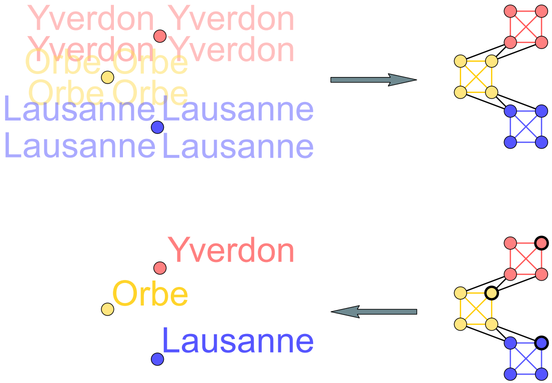
POPMUSIC for the Vehicle Routing Problem

- The customers of a tour is a part
- A subproblem is a VRP with r tours



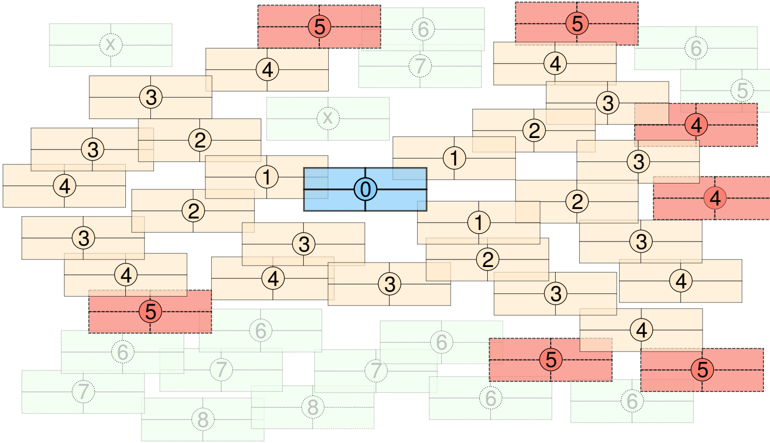
Map Labelling as a Stable Set Problem

- Create as many node as there are possible label positions for the object
- Connect 2 incompatible nodes by an edge (only 1 label for each object, no overlapping labels)



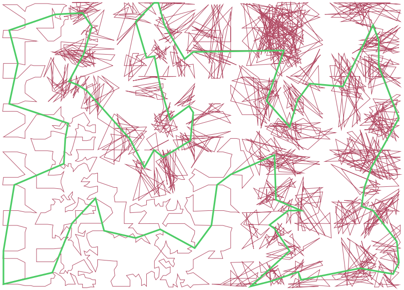
POPMUSIC Map Labelling

- A part is an object to label (here: 4 possible positions for the label of an object)
- Two objects are at distance 1 if their labels overlap
- Here: 0 is the seed object
- A sub-problem contains 25 objects
    - Labels of red ones taken into consideration but cannot be moved
    - Green ones are ignored



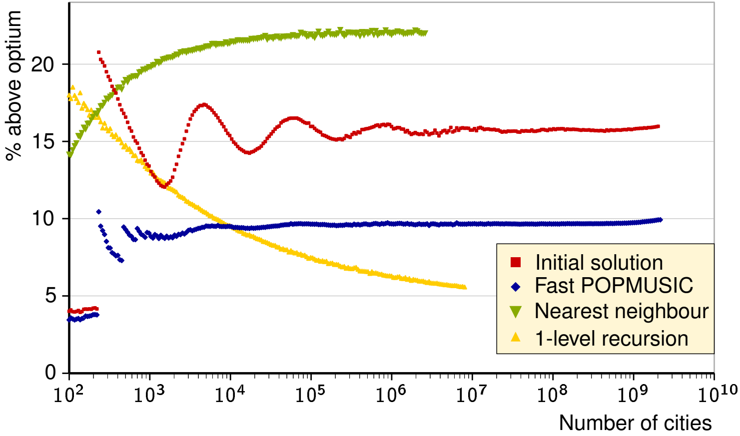
POPMUSIC for the TSP: Empirical Complexity in $O(n^{1.57})$

- Select a sample of $O(n^{0.56})$ cities
- Find a good tour on the sample with Lin-Kernighan neighbourhood
- Group all the cities into a number of clusters equals to the sample
- Optimize the tour with 2-opt neighbourhood by considering 2 successive clusters at a time
- Re-optimize the tour with POPMUSIC (all subsets of 50 successive cities are LK optimum)



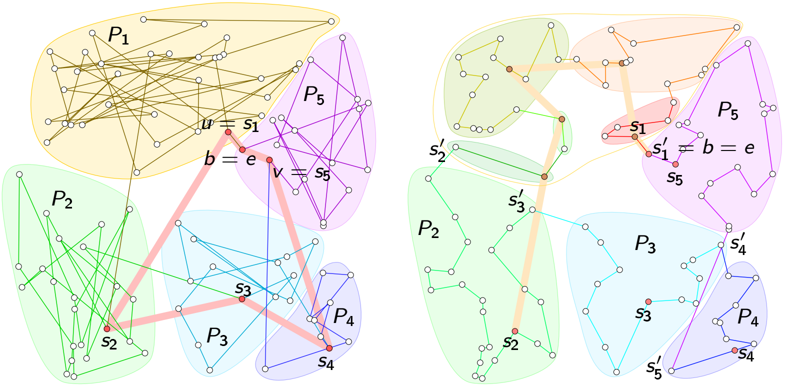
Solution Quality for the TSP with toroidal distances

Fast POPMUSIC: Initial solution obtained recursively, $2 \times n/225$ sub-problem optimization
The Lin-Kernighan method used to optimize sub-path produces solutions 4% above optimum

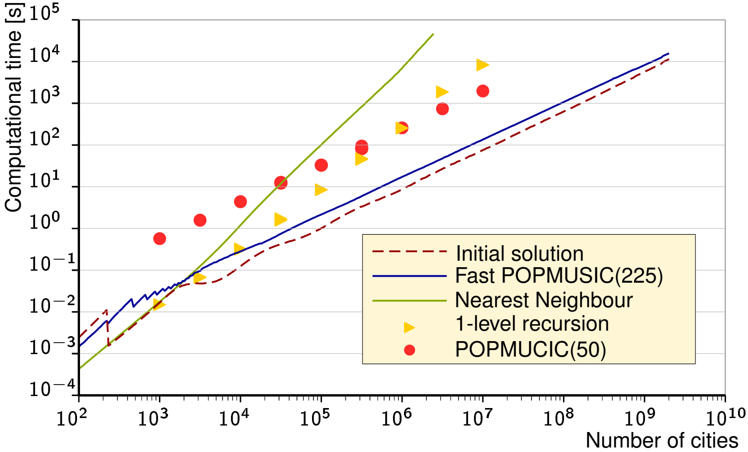


Getting an Appropriate Initial Solution in Linearithmic Time

- Create a tour on a sample of r cities
- Insert the remaining cities in any order, but next to the closest city of the sample
- If the path between 2 cities of the sample has too many cities: decompose it recursively
- Else, optimize the path with a good method (exact, Lin-Kernighan, . . .)



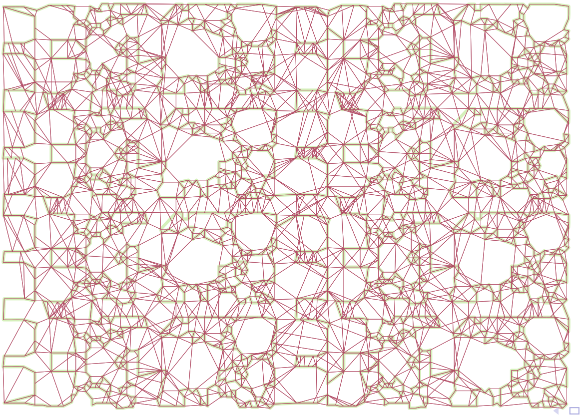
POPMUSIC Empirical Complexity



Union 20 POPMUSIC Solutions

Optimum solution in green

Method now included in LKH solver for filtering the potential edges retained



Research Perspectives

- Use of TSP edge filtering for limiting the neighbourhood size for other problems
- Opportunity to test quantum programming for optimizing small sub-problems
  - Drawback: sub-problem optimization is empirically not the most complex part
  - Getting an appropriate initial solution with low computational effort
- Application to other problems
  - Simple adaptation not working for the quadratic assignment problem
  - Not working at all for instances with completely random data?
- Study on the contribution of parameters and options in heuristics
- Merging machine learning and metaheuristics

Questions ?

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