



Nature Inspired Search and Optimisation

Advanced Aspects of Nature Inspired Search and Optimisation

Lecture 4: Stochastic Local Search algorithms

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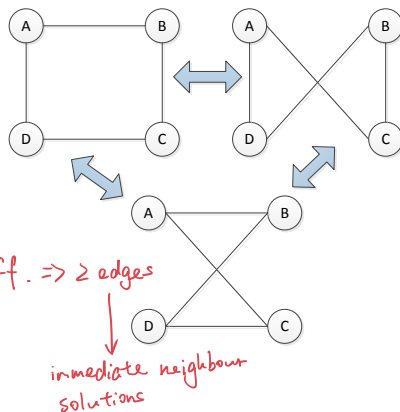
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Outline of Topics

- 1 2-Opt algorithm
- 2 Stochastic local search: basic ideas
 - Local search with random restart
 - Simulated Annealing
- 3 Conclusion

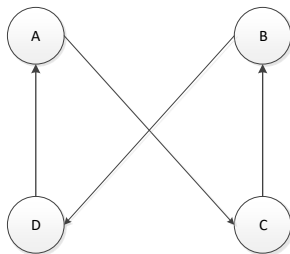
Let's take a look at some simple examples

- 2-3 cities: only one solutions
- 4 cities: 3 solutions
- **Question:** How those tours of the 4 cities TSP differ?
- Answer (Observation): **two immediate neighbour solutions can be two routes (cycles) only differ from two edges**
- Idea: **Swapping two edges** results in an **immediate neighbour** solution



2-Opt algorithm

- **Question:** Given a route, e.g., $A \rightarrow C \rightarrow B \rightarrow D \rightarrow A$, how to swap two edges?
- **Note:** if you can answer this question, you invent 2-Opt algorithm, a famous local search operator first proposed by Croes in 1958 [1] for solving the travelling salesman problem.



[1] G.A. Croes. A method for solving traveling-salesman problems. Operations Research. 1958



2-Opt algorithm

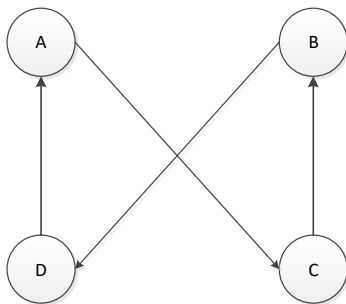
- Detailed swapping steps for swapping two edges, which result in an **immediate** neighbour solutions:
 - Step 1: **removal of two edges** from the current route, which results in two parts of the route.
 - Step 2: **reconnect by two other edges** to obtain a new solution

[1] G.A. Croes. A method for solving traveling-salesman problems. Operations Research. 1958

2-Opt algorithm

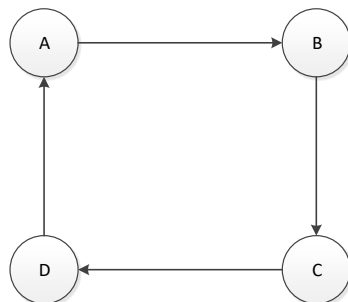
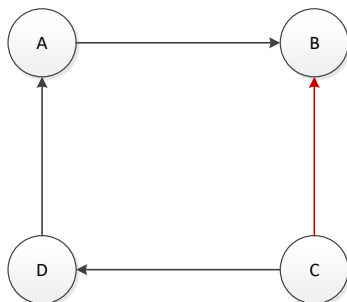
Suppose we have a route: $A \rightarrow C \rightarrow B \rightarrow D \rightarrow A$, let's see how to swap:

Step 1: removal of two edges from the current route, which results in two parts of the route



2-Opt algorithm

Step 2: reconnect by two other edges to obtain a new solution.

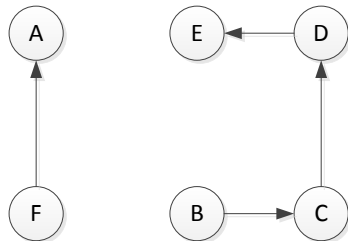
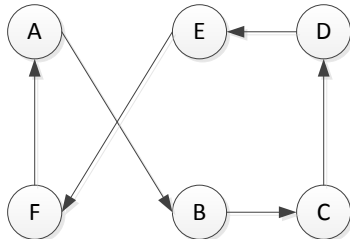


We need to reverse the order of one part of the solution, e.g., $C \rightarrow B$ in order to get an optimal route: $A \rightarrow B \rightarrow C \rightarrow D \rightarrow A$

2-Opt algorithm for 6 cities TSP

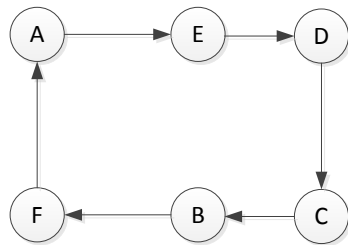
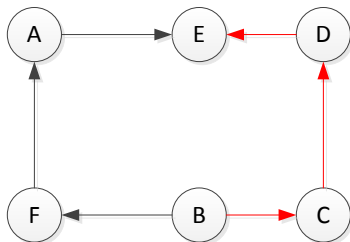
Suppose we have a route: $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow F \rightarrow A$, let's see how to swap:

Step 1: removal of two edges from the current route, which results in two parts of the tour



2-Opt algorithm for 6 cities TSP

Step 2: reconnect by two other edges to obtain a new solution



We need to **reverse the order** of $B \leftarrow C \leftarrow D \leftarrow E$ in order to get
 $A \rightarrow E \rightarrow D \rightarrow C \rightarrow B \rightarrow F \rightarrow A$

2-Opt algorithm: implementation

We observed 2-Opt essentially swap two cities, e.g., in the 6 cities TSP, 2-Opt swaps B and E, and then reverse the order of the route between them. We therefore have the following algorithm:

2-Opt algorithm

route := initial TSP solution

i, j := two cities for swapping

Step 1: take *route*[1] to *route*[*i* − 1] and add them in order to *newroute*

Step 2: take *route*[*i*] to *route*[*j*] and add them in **reverse** order to *newroute*

Step 3: take *route*[*j* + 1] to end and add them in order to new *newroute*

Output *newroute*

$$[a + \textcircled{b} + c]$$



Code demonstration

Let's run the hill-climbing with 2-opt algorithms

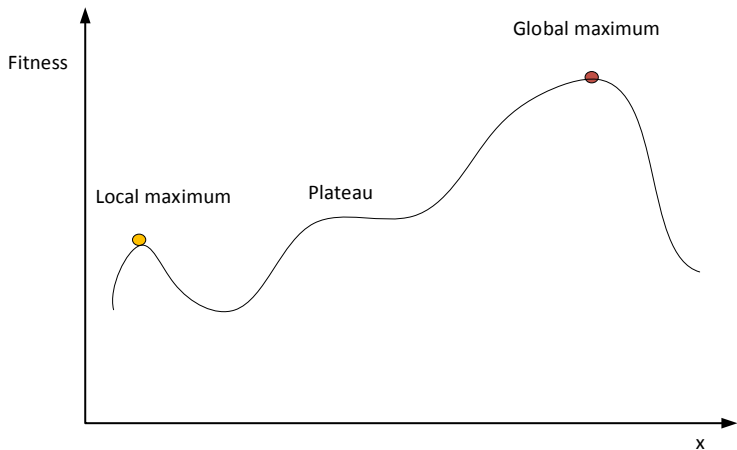
- **Simple hill climbing:** chooses the **first** better solution
- **Steepest ascent/descent hill climbing:** compares all neighbour solutions and chooses **the best** solution – greedy search

Why they cannot find the optimal solution of 10628?



Fitness landscape with global/local optima

Fitness landscape of a 1-dimensional optimisation (maximisation) problem





Randomised search vs Local search

- Randomised search:
 - **Good at exploration**, e.g., to search large unknown region of the search space
 - Not good at exploitation, e.g., to search small region around the current solution
 - Especially bad for problems where good solutions are just a small portion of all possible solutions
- Local search:
 - **Good at exploitation**: capable to find local optimum
 - Not good at exploration: **gets stuck into local optimum**
- Question: how to find global optimum?



Stochastic local search: Main idea

- Main idea: **escape** or **avoid** local optima
- How: Introduce randomness into local search algorithm to escape from local optima
- Escape strategies:
 - Random restart: simply restart the local search from a random initial solution
 - Applicable when:
 1. Number of local optima is small
 2. The cost for restarting the local search is cheap
 - Perform random non-improving step: randomly move **to a less fit neighbour** – Simulated Annealing (Explain later)



Hill climbing with random restart

Hill climbing with random restart

```
for  $k := 0$  to  $k_{\max}$ 
   $x_0 :=$  randomly generated initial solution
  terminationflag := false
   $x^i := x_0$ 
  while (terminationflag != true)
    Modify the current solution to a immediate neighbour one
    If  $f(v) < f(x_i)$  then  $x^i := v$ 
    If a termination criterion is met: terminationflag := true
  Store  $x^i$ 
Output  $x_{best} = \min(x^i, i = 1, \dots, k_{\max})$ 
```



Simulated Annealing

- Simulated Annealing: a generic heuristic algorithm for optimisation problems proposed by Kirkpatrick in 1983 [1]
- Your first Nature inspired algorithm: inspired by annealing in metallurgy:
 - *"heat treatment that alters a material to increase its ductility and to make it more workable"*
 - The real annealing:
 - Step 1: heating a material to above its critical temperature
 - Step 2: maintaining a suitable temperature
 - Step 3: cooling
 - In annealing: find a state of lower thermodynamic free energy for metal
 - In optimisation: find a solution to get to the minimum of an objective function

[1] S. Kirkpatrick, C. D. Gelatt Jr., M. P. Vecchi. Optimization by Simulated Annealing. Science. 1983



Generic Simulated Annealing algorithm for minimisation

```

 $x := x_0; e := f(x)$       // Initial solution, objective function value (energy).
 $x_{best} := x; x_{best} := x$   // Initial "best" solution
 $k := 0$       // Count evaluation number.
while ( $k < k_{max}$ )
     $T := temperature(t_0)$     // Temperature calculation.
     $x_{new} := neighbour(x)$     // Pick some neighbour.
     $e_{new} := f(x_{new})$       // Compute its objective function value.
    { if  $P(e, e_{new}, T) > R(0, 1)$  then      // Should we move to it?
         $x := x_{new}; e := e_{new}$       // Yes, change state.
    }
    if  $e_{new} < e_{best}$  then      // Is this a new best?
         $x_{best} := x_{new}; e_{best} := e_{new}$     // Save as 'best found'.
     $k := k + 1$  // Increase evaluation

```

Output x_{best}

$P := 1$ if $e_{new} < e$, and

$P := \exp\left(\frac{e - e_{new}}{T}\right)$ otherwise

Annealing schedule $temperature()$ defines how to decreased temperature from an initial temperature t_0 .



Simulated Annealing

- Without the analogue from metallurgy, SA algorithm is essentially a **stochastic local search** algorithm
- Main idea: Escape from local optima by a **random non-improving step**:

- Accepting better solutions with the probability of 1: $P := 1$ if $e_{new} < e$, i.e., e_{new} is better than e
- Accepting worse solutions with a certain probability:
 $P := \exp\left(\frac{e - e_{new}}{T}\right)$ if $e_{new} \geq e$, i.e., e_{new} is worse e

Handwritten notes for the probability formula:

$$+ \quad - \quad \downarrow \quad \uparrow$$

$$\frac{-5}{-5} \quad (-500)$$

$$\exp\left(\frac{-3}{100}\right) \sim 0.7 \rightarrow 1$$

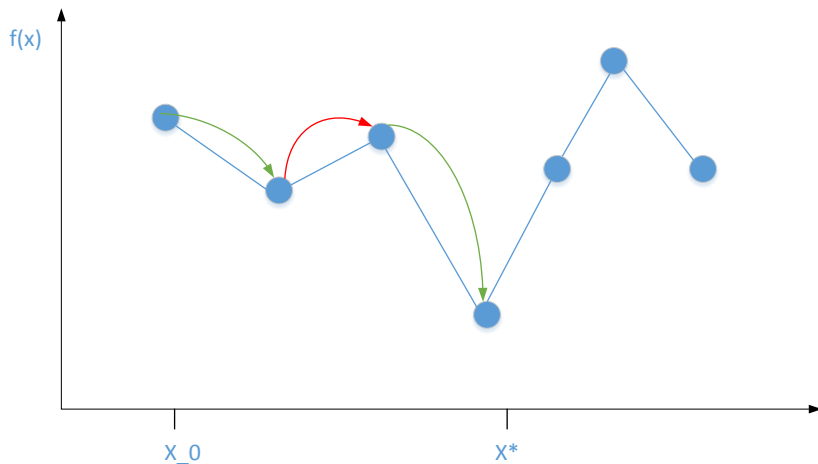
- This allows SA to explore more of the possible search space of solutions.
- T , which is determined by the **annealing schedule** $temperature()$, will decrease, so the probability of accepting worse solutions will **decrease**.
- Question:** what happen if $temperature()$ reaches 0?

Handwritten note:

$$T \text{ starts high} \rightarrow T \downarrow \quad P \downarrow$$



Search trajectory of simulated annealing





Wait!

- Main idea: escape or **avoid** local optima
- Algorithm uses the ‘avoiding’ strategy: **Tabu search**



Conclusion

- Local search algorithms is simple but can generate good solutions for many problems
- However, local search algorithms only focus on exploitation, which will lead to local optima
- Different stochastic local search algorithms use different strategies to escape or avoid local optima
- Stochastic local search algorithms usually produce better results using default parameters than local search
- However, tuning stochastic local search algorithms to get better results sometimes is difficult