中山大學
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Lecture 15
Optimization Algorithms (II)

Algorithm Design

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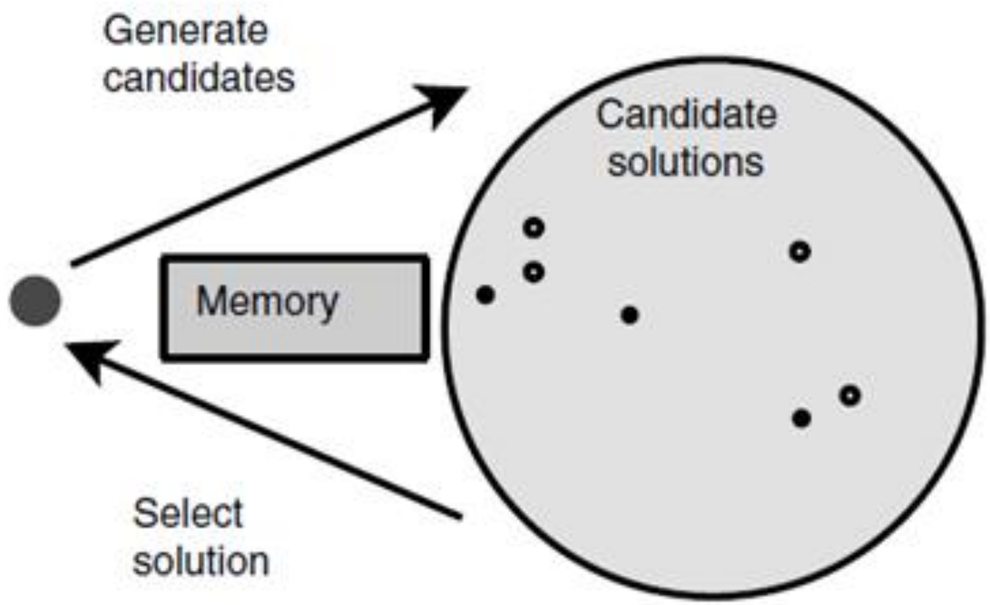
Single-Solution Based Metaheuristics

- Common Concepts
- Local Search
- Simulated Annealing
- Tabu Search
- Iterated Local Search
- Variable Neighborhood Search
- GRASP

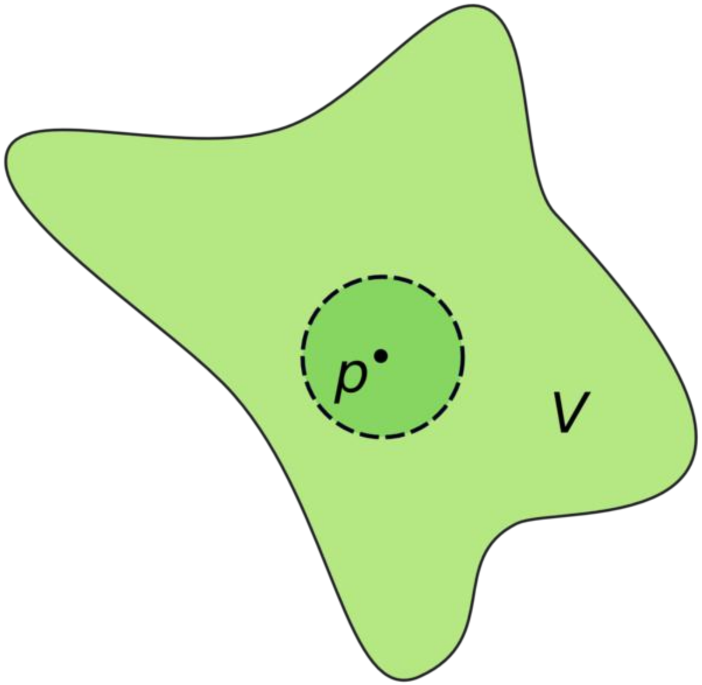
Common Concepts

- Single-metaheuristics iteratively apply the ***generation*** and ***replacement*** procedure from the current single solution.



Common Concepts

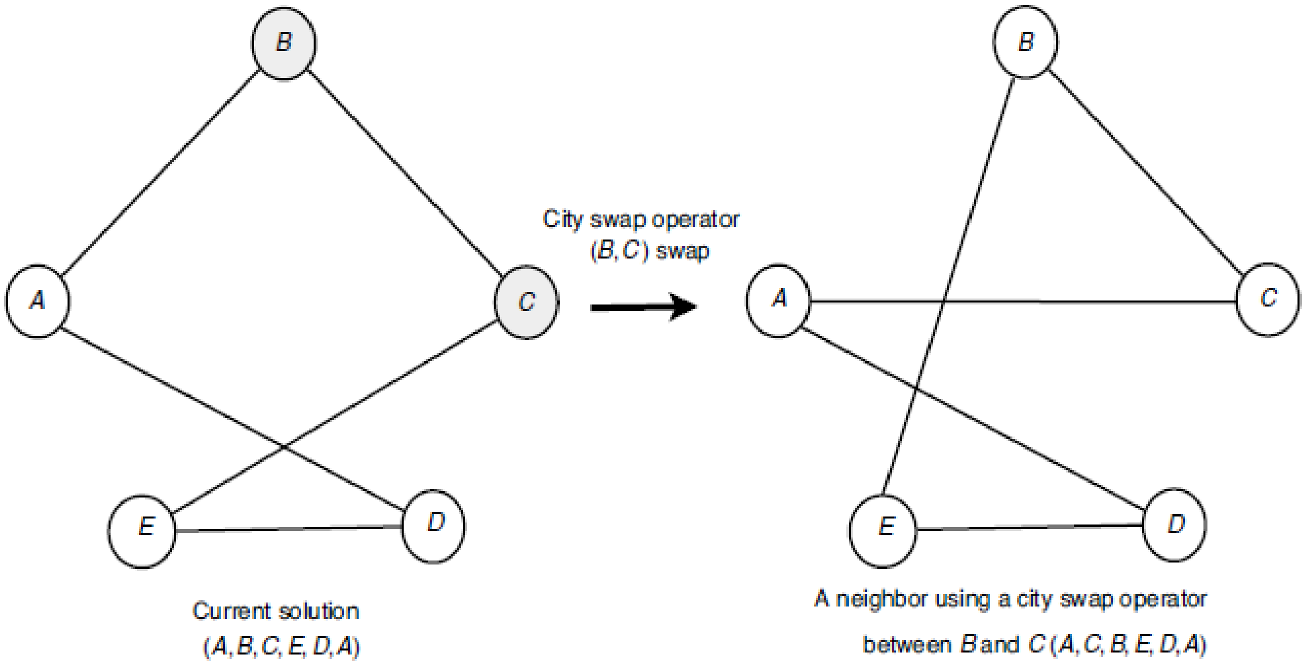
- **Neighborhood**
  - plays a crucial role in the performance of a single-metaheuristic.



  - A solution in the neighborhood is called a ***neighbor***.
  - A neighbor *s'* is generated by modifying the current solution *s*.
  - The area of the neighborhood is relied on the ***operator*** employed. (operators can be regarded the ways or rules of modifying *s*.)

Neighborhood Operators

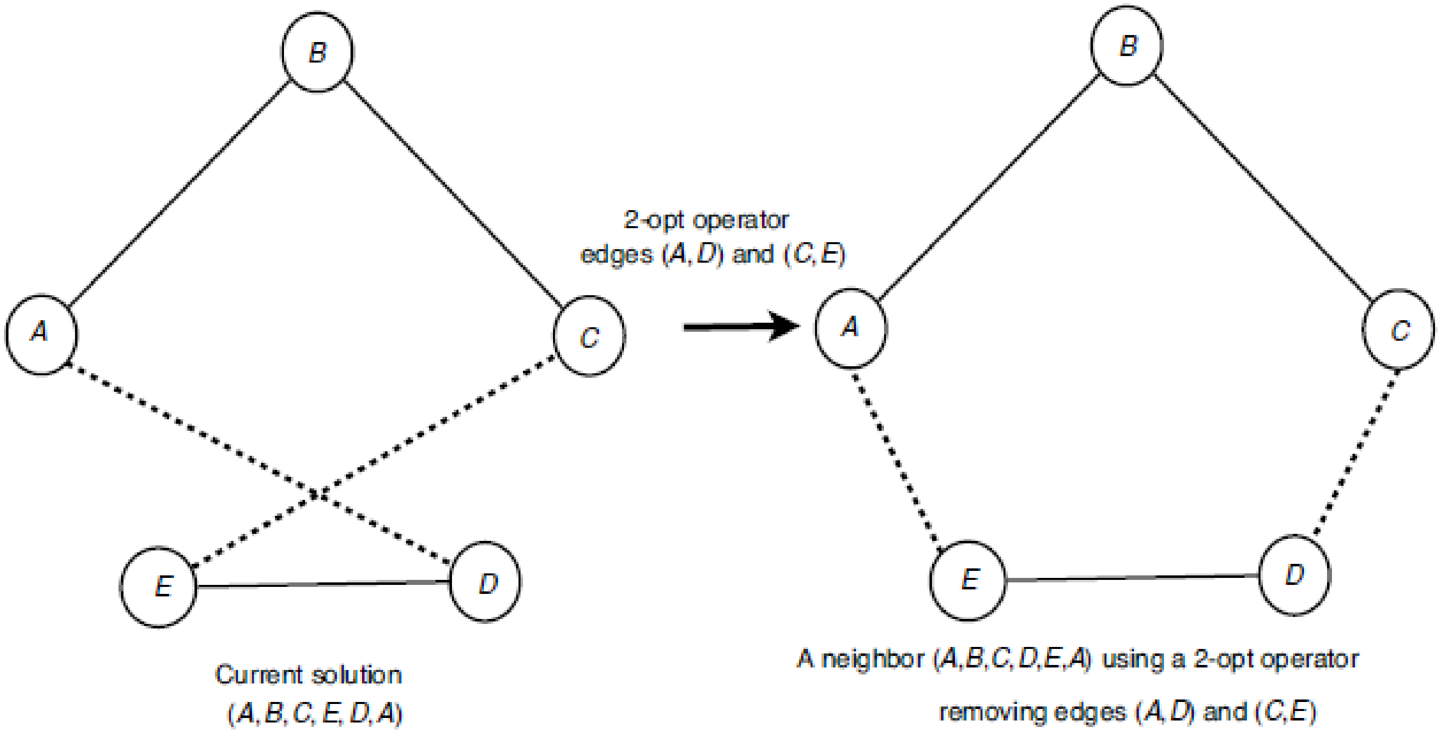
- For permutation problems, such as the TSP, single machine scheduling problem and *N* queens problem, the **exchange operator** (swap operator) may be used.



The size of this neighborhood is $n(n-1)/2$, where n is the number of cities.

Neighborhood Operators

- **2-opt operator**

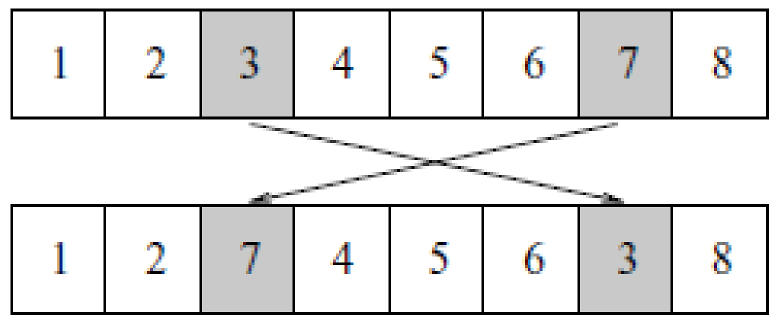


The size of the neighborhood for the 2-opt operator is [(n(n-1)/2) - n]; All pairs of edges are concerned except the adjacent pairs.

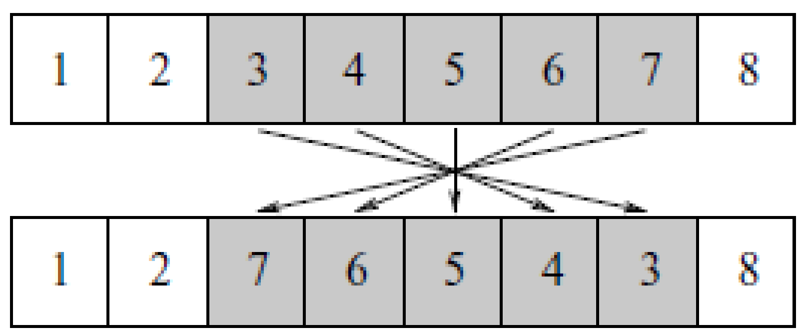
Neighborhood Operators

Insertion operator

Exchange operator



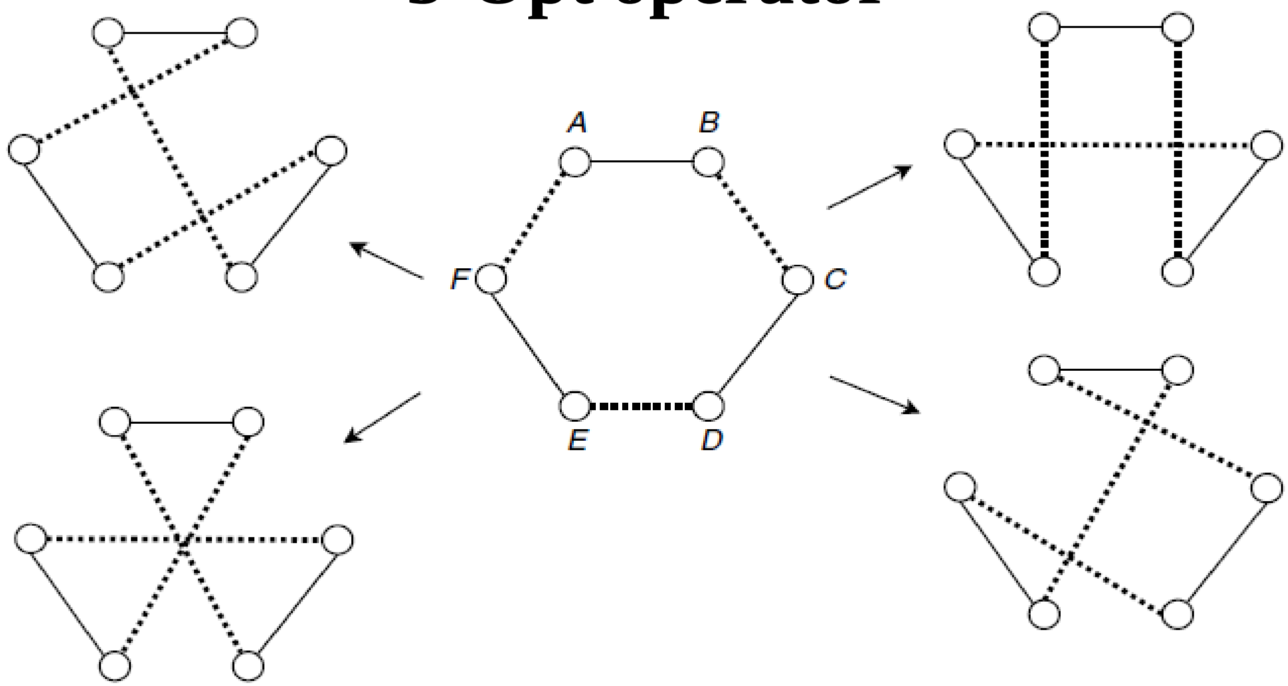
Inversion operator



Neighborhood Operators

- Another widely used operator is the k-opt operator, where k edges are removed from the solution and replaced with other k edges.
- The time complexity for 2-opt, 3-opt and 4-opt is $O(n^2)$, $O(n^3)$ and $O(n^4)$.

3-Opt operator



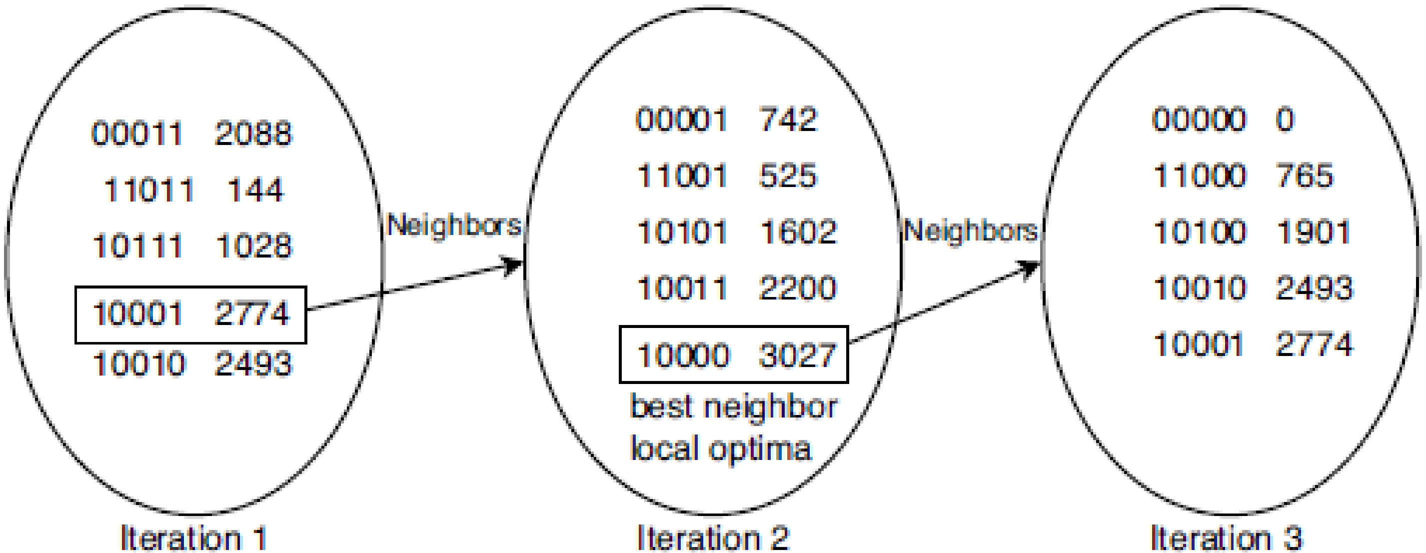
3-opt operator for the TSP. The neighbors of the solution (A,B,C,D,E,F) are (A,B,F,E,C,D), (A,B,D,C,F,E), (A,B,E,F,C,D), and (A,B,E,F,D,C).

Local Search (局部搜索)

- It is also called *hill climbing*, *descent*, *iterative improvement*, and so on.
- It is likely the oldest and simplest metaheuristic method.
- It starts at a given initial solution.
- At each iteration, the heuristic ***replace***s the current solution by a neighbor that ***improve***s the objective function.
- It stops when all candidate neighbors are worse than the current solution, i.e., a local minimum is reached.

LS Example

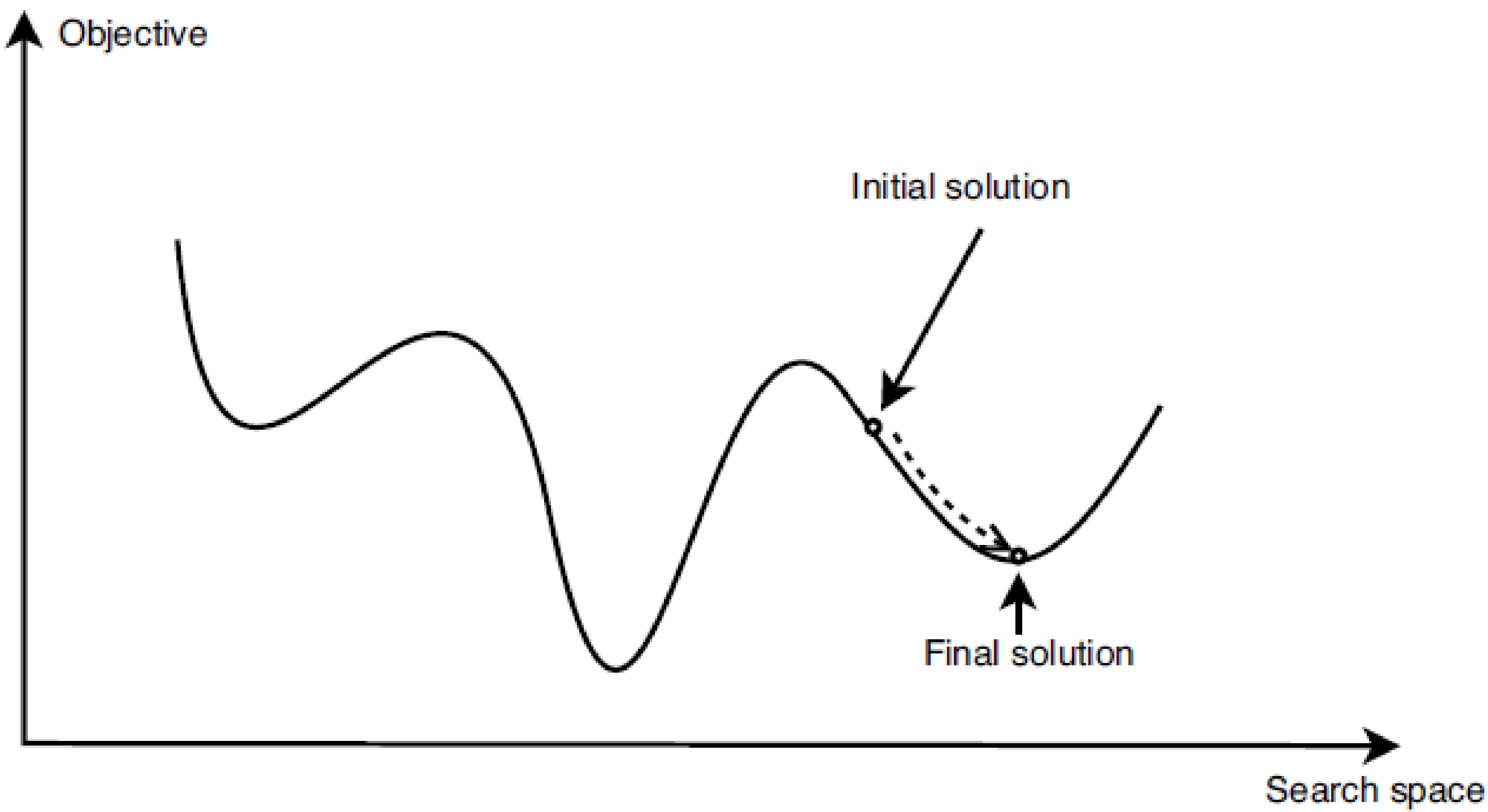
- Maximize $x^3 - 60x^2 + 900x$, x is discrete



- Local search process using a binary representation of solutions, a flip move operator, and the best neighbor selection strategy.
- The global optimal solution is $f([01010]_2) = f(10) = 4000$, while the final local optimal found is s = [10000], starting from the solution s0=[10001)]

Questions

- How to generate a set of neighbors?
- How to select a neighbor?



How LS Works

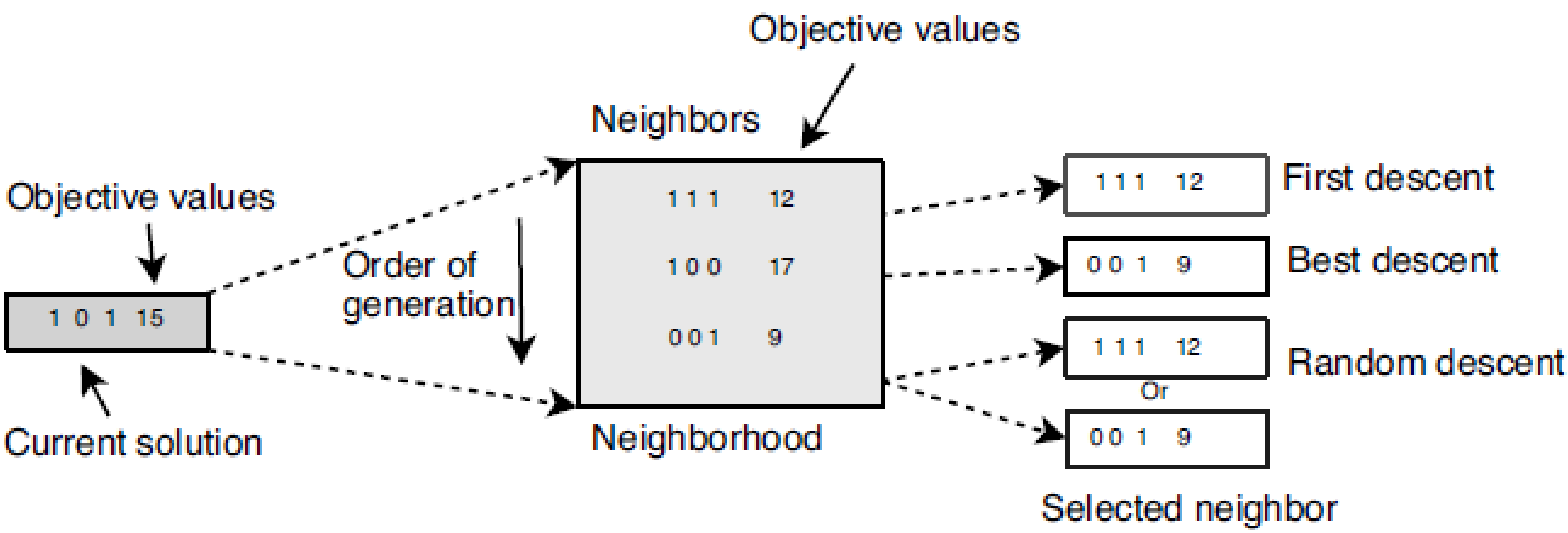
- LS may be seen as a descent walk in the graph $G=(S, V)$ representing the search space.
  - S represents the set of all feasible solutions.
  - V represents the neighborhood relation.
  - Each edge (i, j) in the graph will connect any neighboring s_i and s_j.
  - For a given solution s, the number of associated edges will be $|N(s)|$.

Template of a local search algorithm.

$s = s_0$; /* Generate an initial solution s_0 */
While not Termination_Criterion **Do**
  Generate $(N(s))$; /* Generation of candidate neighbors */
  If there is no better neighbor **Then** Stop ;
  $s = s'$; /* Select a better neighbor $s' \in N(s)$ */
Endwhile
Output Final solution found (local optima).

How LS Works

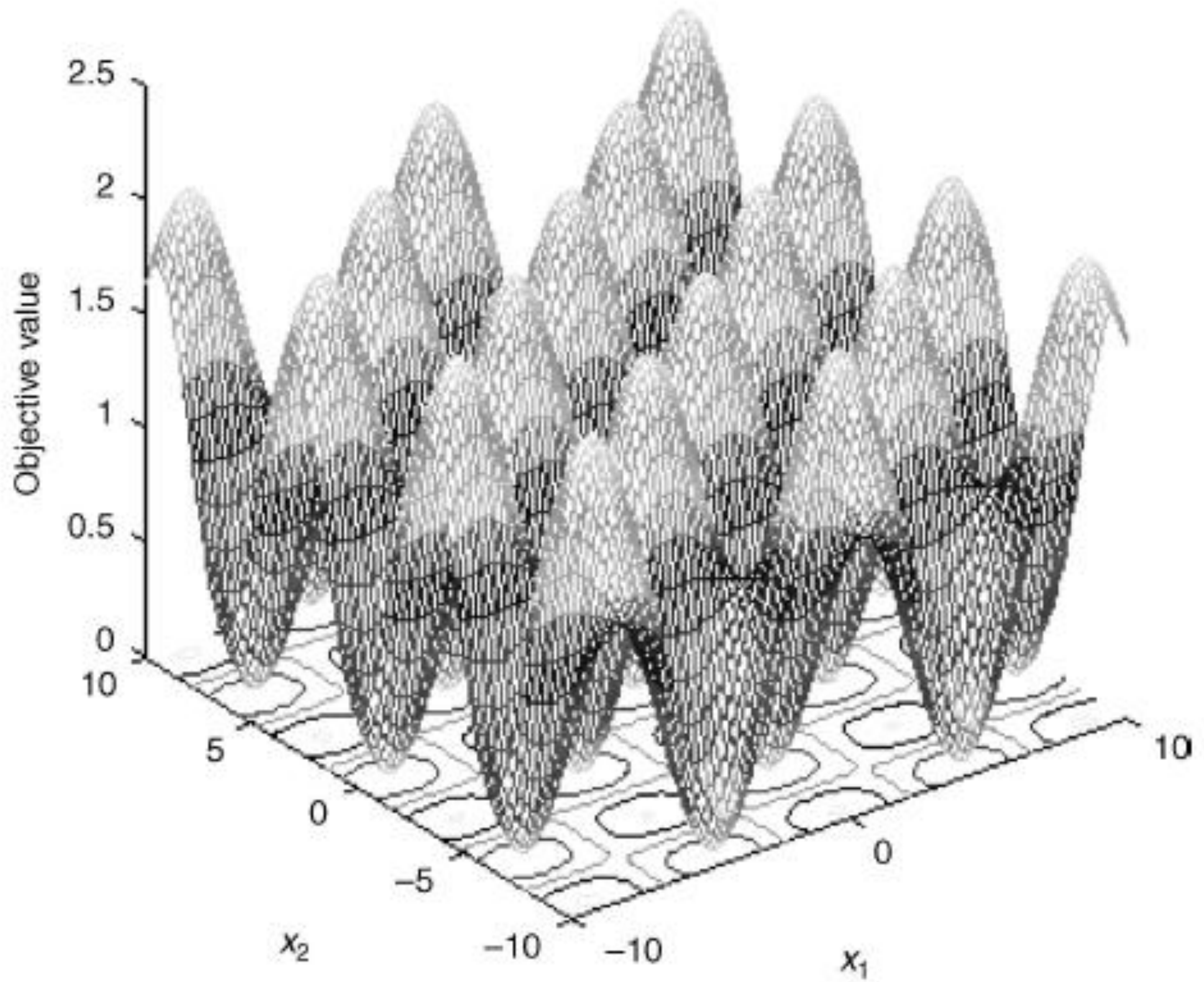
- **Selection of the Neighbor**
  - Best improvement (steepest descent)
  - First improvement
  - Random selection



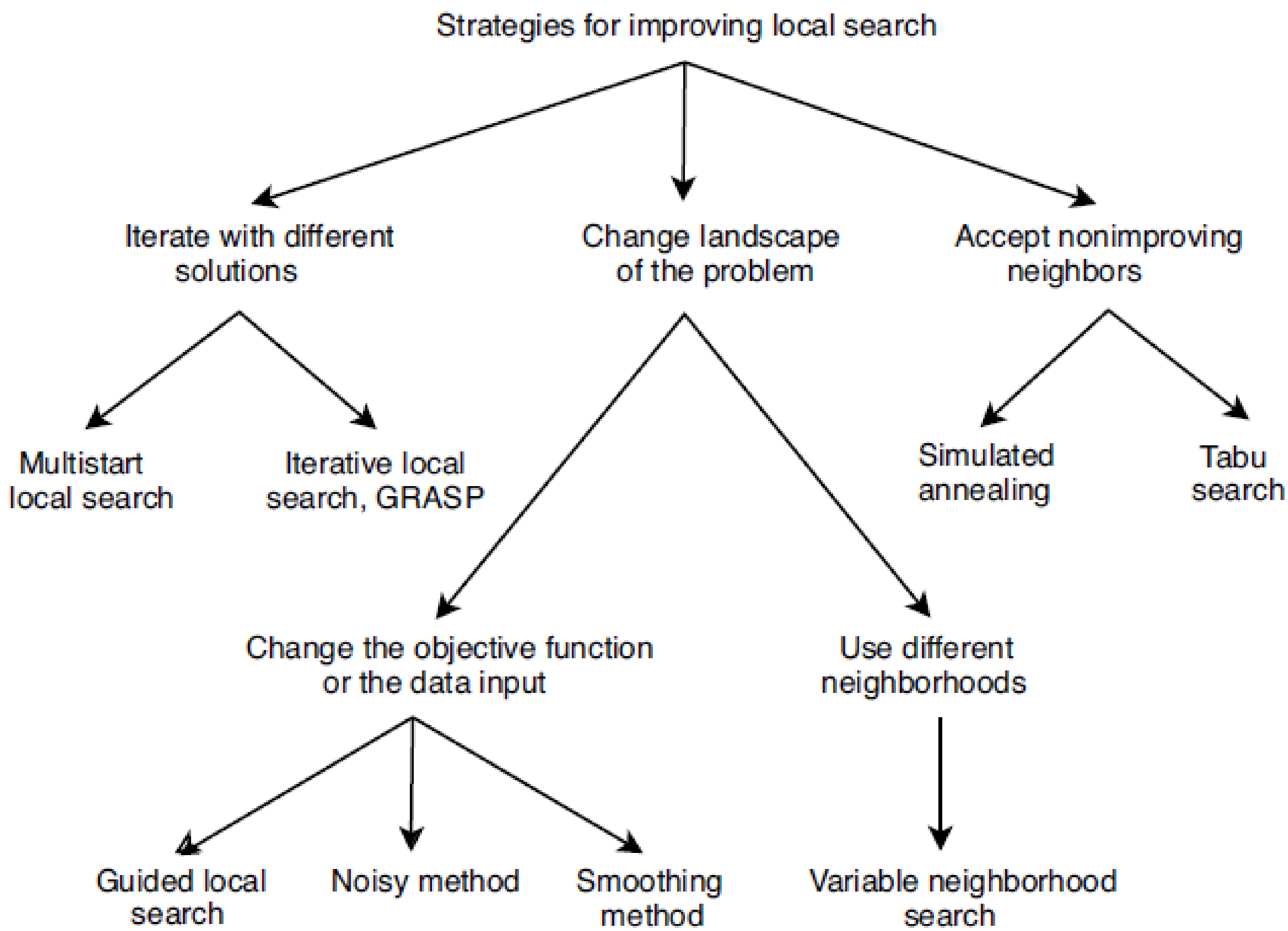
How LS Works

- Escaping from Local Optima
  - The LS is very sensitive to the initial solution.
  - No means to estimate the gap between the local optimum and the global optimum.
  - The number of iterations performed may not be known in advance.
  - Even if the LS runs very quickly, its worst case complexity is *exponential*.
  - Local search works well if there are not too many local optima.

Highly Multimodal Function

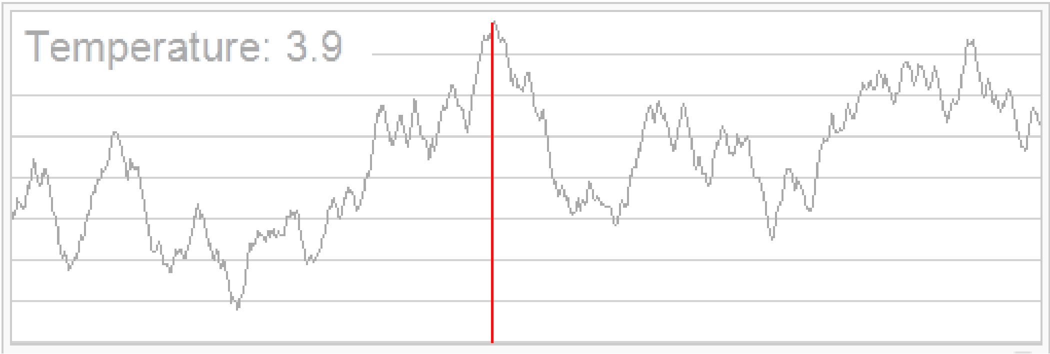


How to avoid local optima



Simulated Annealing (SA)

- In the pioneering works, SA has been applied to graph partitioning and VLSI design.
- Simple and efficient in solving combinatorial optimization problems.
- It has been extended to deal with continuous optimization problems.
- SA is based on the principles of statistical mechanics whereby the annealing process requires heating and then slowly cooling a substance to obtain a strong crystalline structure.



Description of SA

- At each iteration, a random neighbor s' is generated.
- Moves that improve the cost function are always accepted.
- Otherwise, the neighbor is selected with a given probability: (important!)

$$P(\Delta E, T) = e^{-\frac{f(s')-f(s)}{T}}$$

- Temperature *T* determines the probability of accepting non-improving solutions (How?).
- At a particular level of temperature, many trials are explored. Once an equilibrium state (what is this?) is reached, the temperature is gradually decreased according to a cooling schedule (why do so?).

SA Algorithm

Template of simulated annealing algorithm.

Input: Cooling schedule.
$s = s_0$; /* Generation of the initial solution */
$T = T_{max}$; /* Starting temperature */
Repeat
  Repeat /* At a fixed temperature */
    Generate a random neighbor s' ;
    $\Delta E = f(s') - f(s)$;
    If $\Delta E \leq 0$ **Then** $s = s'$ /* Accept the neighbor solution */
    Else Accept s' with a probability $e^{\frac{-\Delta E}{T}}$;
  Until Equilibrium condition
  /* e.g. a given number of iterations executed at each temperature T */
  $T = g(T)$; /* Temperature update */
Until Stopping criteria satisfied /* e.g. $T < T_{min}$ */
Output: Best solution found.

SA Example

- Maximize $f(x) = x^3 - 60x^2 + 900x + 100$, where x is discrete.
- A solution is represented as a string of 5 bits.
- The global maximum of this function is 01010 (x= 10, $f(x)$ = 4100).
- The first scenario starts from the solution 10011 (x=19, $f(x)$ = 2399) with an initial temperature T_0 equal to 500.
- The second scenario starts from the same solution 10011 with an initial temperature T_0 equal to 100.
- The initial temperature is not high enough and the algorithm gets stuck by local optima.

SA Example

First Scenario $T = 500$ and Initial Solution (10011)

T	Move	Solution	f	Δf	New Neighbor Solution
500	1	00011	2287	112	00011
450	3	00111	3803	<0	00111
405	5	00110	3556	247	00110
364.5	2	01110	3684	<0	01110
328	4	01100	3998	<0	01100
295.2	3	01000	3972	16	01000
265.7	4	01010	**4100**	<0	01010
239.1	5	01011	4071	29	01011
215.2	1	11011	343	3728	01011

Second Scenario: T = 100 and Initial Solution (10011). When Temperature is not High Enough, Algorithm Gets Stuck

T	Move	Solution	f	Δf	New Neighbor Solution
100	1	00011	2287	112	10011
90	3	10111	1227	1172	10011
81	5	10010	2692	<0	10010
72.9	2	11010	516	2176	10010
65.6	4	10000	**3236**	<0	10000
59	3	10100	2100	1136	10000

Move Acceptance

- The system can escape from local optima due to the probabilistic acceptance of a non-improving neighbor.
- At high temperature, the probability of accepting worse moves is high (Why?).
- If $T = +\infty$, all moves are accepted, which corresponds to a random walk in the feasible region.
- If $T = 0$, no worse moves are accepted and the search is equivalent to local search.

Equilibrium State

- To reach an equilibrium state at each temperature, a number ($N_{nonimprov}$) of non-improving iterations must be performed.
- This number must be set according to the size of the problem instance and particularly proportional to the neighborhood size $|N(s)|$.
- This number may be set by the following two ways:
  - **Static**: this number is determined before the search starts.
  - **Adaptive**: This number will be adjusted during the search process.

Cooling

- The temperature is decreased gradually such that
  $T_i > 0, \forall i$ and $\lim_{i \to +\infty} T_i = 0$.
- If the temperature is decreased slowly, better solutions are obtained but with more computation time.
- The temperature T can be updated in different ways:
  - **Linear**: $T = T - \beta$, where β is a specific constant value. Hence, we have $T_i = T_0 - i \times \beta$.
  - **Geometric**: $T = \alpha T$, where $\alpha \in [0, 1]$. It is the most popular cooling function. Experience has shown that α should be between 0.5 and 0.99.
  - **Adaptive**: In an adaptive cooling schedule, the decreasing rate is dynamic and depends on some information obtained during the search.

Stopping Condition

- Reaching a final temperature T_F which is the most popular stopping criteria. This temperature must be low (e.g., $T_{\min} = 0.01$).
- Achieving a predetermined number of iterations without improving the best found solution.

Thank you!