# 模拟退火应用举例

口 例题 已知背包的装载量为c=8,现有n=5个物品,它们的重量和价值分别是(2, 3, 5, 1, 4)和(2, 5, 8, 3, 6)。试使用模拟退火算法求解该背包问题,写出关键的步骤。

□ 求解:假设问题的一个可行解用0和1的序列表示,例如 *i*=(1010)表示选择第1和第3个物品,而不选择第2和第4个物品。用模拟退火算法求解关键过程如图所示:

# 模拟退火应用举例

己知:

物体个数: n=5 背包容量: c=8

重量 w = (2, 3, 5, 1, 4)

价值 v = (2, 5, 8, 3, 6)

第三步:降温,假设温度降为 T=9。如果没有达到结束标准,则 返回第二步继续执行

假设在继续运行的时候,从当前解i=(10110)得到一个新解j=(00111),这时候的函数值为f(j)=8+3+6=17,这是一个全局最优解。可见上面过程中接受了劣解是有好处的。

第二步: 在T温度下局部搜索,直到"平衡", 假设平衡条件为执行了3次内层循环。

(2-1)产生当前解i的一个邻域解j(如何构造邻域根据具体的问题而定,这里假设为随机改变某一位的0/1值或者交换某两位的0/1值),假设j=(11100)

要注意产生的新解的合法性,要舍弃那些总重量超过背包装载量的非法解

(2-2) f(j) = 2+5+8=15 > 13=f(i),所以接受新解j i=j; f(i)=f(j)=15; 而且s=i; 要注意求解的是最大值,因此适应值越大越优

(2-3) 返回(2-1)继续执行。

(a) 假设第二轮得到的新解j=(11010),由于f(j) = 2+5+3=10 < 15=f(i),所以需要计算接受概率P(T)=exp((f(j)-f(i))/T) = exp(-0.5) = 0.607,假设random(0,1)>P(T),则不接受新解

(b) 假设第三轮得到的新解j=(10110),由于f(j) = 2+8+3=13 < 15=f(i),所以需要计算接受概率P(T)=exp((f(j)-f(i))/T) = exp(-0.3) = 0.741,假设random(0,1)<P(T),则接受新解按照一定的概率接受劣解,也是跳出局部最优的一种手段

(2-4) 这时候,*T*温度下的"平衡"已达到(即已经完成了3次的邻域产生),结束内层循环

- ☐ The Traveling Salesman Problem (TSP) is one of the most widely studied combinatorial optimization problems.
- Its statement is deceptively simple: A salesperson seeks the shortest tour through n cities.

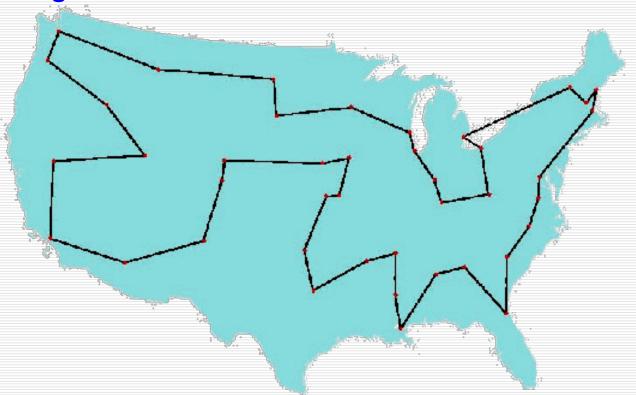


Fig. 1 George Dantzig, Ray Fulkerson, and Selmer Johnson (1954) a description of a method for solving the TSP :49 cities

### Existing Instances

### 49 city problem

Dagtzig, G., D. Fulkerson and S. Johnson: "Solution of a large scale traveling salesman problems", *Operations Research*, vol. 2, pp. 393-410, 1954.

### 120 city problem

☐ Grötschel, M.: "On the symmetric traveling salesman problem: solution of a 120 city problem", *Mathematical Programming Studies*, vol. 12, pp. 61-77, 1980.

### 318 city problem

□ Crowder, H. and M. Padberg: "Solving large scale symmetric traveling salesman problems to optimality", *Management Science*, vol. 22, pp. 15-24, 1995.

### 532 city problem

□ Padberg, M. and G. Rinaldi: "Optimization of 532 city symmetric traveling salesman problem by branch and cut", *Operations Research Letters*, vol. 6, pp. 1-7, 1987.

### 666 city problem

☐ Grötschel, M. and O. Holland: "Solution of large scale symmetric traveling salesman problems", *Mathematical Programming Studies*, vol. 51, pp. 141-202, 1991.

### 2392 city problem

- Padberg, M. and G. Rinaldi: "A branch and cut algorithm for the resolution of large scale symmetric traveling salesman problem", SIAM Review, vol. 33, pp. 60-100, 1991.
- The earlier studies using the genetic algorithm to solve TSP
  - ☐ Grefenstette, J.: Proceedings of the First International Conference on Genetic Algorithms, Lawrence Erlbaum Associates, Hillsdale, NJ, 1985.
- TSP has become a target for the genetic algorithm community.
  - Michalewicz, Z.: Genetic Algorithm + Data structure = Evolution Programs, 2nd ed., Springer-Verlag, New York, 1994.

### Notations

Indices

```
i, j: the index of city, i, j = 1, 2, ..., n
```

### Parameters

n: the total number of cities

 $d_{ij}$ : the distance city i to city j, i.e., the distance of route (i,j); the distance matrix  $(d_{ij})$  is symmetric.

### Decision Variables

 $x_{ij}$ : the 0,1 decision variable; 1, if route (i,j) is selected, and 0, otherwise.

### ■ Mathematical Model of TSP

$$\min \quad z = \sum_{i=1}^{n} \sum_{j=1}^{n} \left( d_{ij} x_{ij} \right)$$

s.t. 
$$\sum_{i=1}^{n} x_{ij} = 1$$
,  $j = 1, 2, 3, \dots, n$ 

$$\sum_{i=1}^{n} x_{ij} = 1, i = 1, 2, 3, \dots, n$$

$$x_{ij} = \begin{cases} 1, & \text{if route } (i,j) \text{ is selected} \\ 0, & \text{otherwise} \end{cases}$$

#### data set for non-directed graph

				Ų i	
i	j	$d_{ij}$	i	j	$d_{ij}$
1	2	8	3	7	7
	3	5		8	12
	4	9		9	12
	5	12	4	5	3
	6	14		6	17
	7	12		7	10
	8	16		8	7
	9	17		9	15
2	3	9	5	6	8
	4	15		7	10
	5	17		8	6
	6	8		9	15
	7	11	6	7	9
	8	18		8	14
	9	14		9	8
3	4	7	7	8	8
	5	9		9	6
	6	11	8	9	11

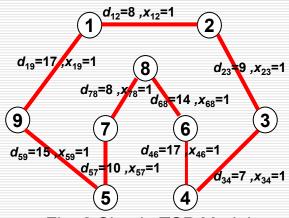
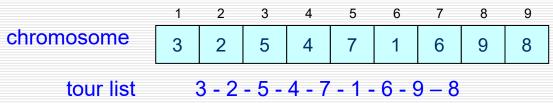


Fig. 2 Simple TSP Model

### 1 Representation

#### Permutation Representation

This direct representation is perhaps the most natural representation of a TSP, where cities are listed in the order in which they are visited.



This representation is also called a path representation or order representation.

```
procedure: Permutation Encoding
Input: city set, total number of cities N
output: chromosome v
begin

for j=1 to N

v(j) \leftarrow j;
for i=1 to \lceil n/2 \rceil

repeat

j \leftarrow \text{random}[1, N];

l \leftarrow \text{random}[1, N];

until l \neq j

swap(v(j), v(l));
output chromosome v;
end
```

### 1 Representation

- Random Keys Representation
  - This indirect representation encodes a solution with random numbers from (0,1).
  - These values are used as sort keys to decode the solution.

where position *i* in the list represents city *i*.

```
procedure: Random Keys Encoding
Input: city set,
        total number of cities N
output: chromosome v
begin
    for i = 1 to N
        v[i] ← random[0,1];
    output chromosome v;
end
```

```
procedure: Random Keys Decoding
Input: chromosome v,
        total number of cities N

output: tour list L

begin

L \leftarrow \emptyset;

for i = 1 to N

L \leftarrow L \cup i;

sort L by v[i];

output tour list L;

end
```

- During the past decade, several crossover operators have been proposed for permutation representation, such as partial-mapped crossover (PMX), order crossover (OX), cycle crossover (CX), position-based crossover, order-based crossover, heuristic crossover, and so on.
- □ These operators can be classified into two classes:

### Canonical approach

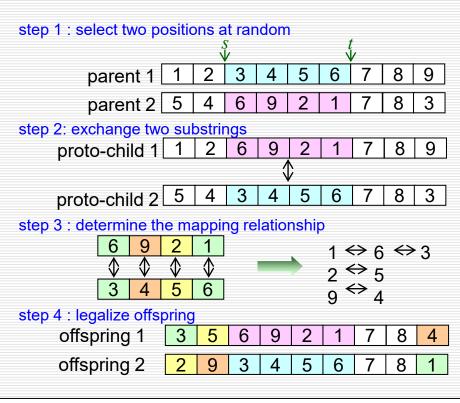
□ The canonical approach can be viewed as an extension of two-point or multipoint crossover of binary strings to permutation representation.

### Heuristic approach

□ The application of heuristics in crossover intends to generate an improved offspring.

### 1. Partial-Mapped Crossover (PMX)

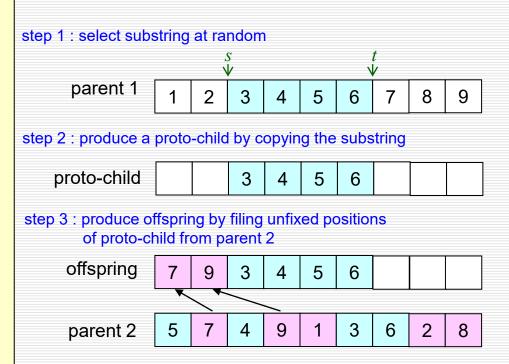
```
procedure: PMX crossover
input: chromosome v_1, v_2,
         length of chromosome l
output: offspring v_1', v_2'
begin
      R \leftarrow \phi:
      // step 1: select two positions
      at random
      s \leftarrow \text{random}[1:l-1];
      t \leftarrow \text{random}[s+1:l];
      // step 2: exchange two substrings
         \leftarrow v_1[1:s-1] // v_2[s:t] // v_1[t+1:l];
       v_1' \leftarrow v_2[1:s-1] // v_1[s:t] // v_2[t+1:l];
      //vstep 3: determine the mapping
                    relationship
      R \leftarrow \text{relation}(v_1[s:t], v_2[s:t]);
      // step 4: legalize offspring
      legalize (,,R);
      output offspring
end
```



 $v_1$ : parent chromosome 1  $v_2$ : parent chromosome 2 l: length of chromosome  $v_1'$ : offspring chromosome 1  $v_2'$ : offspring chromosome 2 l: relationships l: end position of substring l: end position of substring relation(l): searching relationship between l0 and l2 legalize(l0, l0, l0 change genes value of l0, l0 based on relationship l2

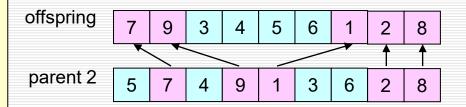
#### 2. OX crossover

```
procedure: Order Crossover (OX)
input :chromosome v_1, v_2,
        length of chromosome l
output: offspring v'
begin
      w \leftarrow 1:
        // step 1: select substring at random
       s \leftarrow \text{random}[1: l-1];
       t \leftarrow \text{random}[s+1: l];
        // step 2: produce a proto-child by
                    copying the substring
       v' \leftarrow v_1[s:t];
        // step 3: produce offspring by filing
                   unfixed positions of proto-
                   child from parent 2
      for i=1 to s-1
            for j=w to l
                fg ←0;
                 for k=s to t
                     if v_2[j] = v_1[k] then
                         fg \leftarrow 1; break;
                 if fg=0 then
                    v'[i] \leftarrow v_2[j];
                    w \leftarrow i + 1; break:
```



 $v_1$ : parent chromosome 1  $v_2$ : parent chromosome 2  $v_3$ : parent chromosome 2  $v_3$ : offspring chromosome  $v_3$ 

```
for i=t+1 to l
            for j=w to l
                  fg ←0;
                  for k=s to t
                       if v_2[j] = v_1[k] then
                            fg \leftarrow 1; break;
                  if fg=0 then
                         v'[i] \leftarrow v_2[j];
                       w \leftarrow j +1; break;
output offspring v';
end;
```



v<sub>1</sub>: parent chromosome 1I: length of chromosomew: working data

 $\boldsymbol{s}$ : start position of substring

v<sub>2</sub>: parent chromosome 2

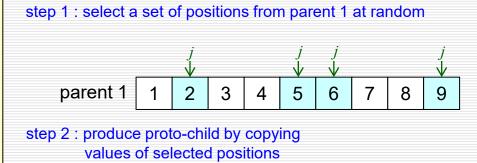
 $v^{\prime}$  : offspring chromosome

*fg* : flag

t: end position of substring

### 3. Position-based Crossover (PBX)

```
procedure: Position-based Crossover
input: chromosome v_1, v_2,
         length of chromosome l
output: offspring v'
begin
      T \leftarrow \emptyset, S \leftarrow \emptyset, w \leftarrow 1:
       // step 1: select a set of positions
                   from parent 1 at random
      N \leftarrow \text{random}[1:l];
        // step 2: produce proto-child by
                    copying values of
                    selected positions
      for i=1 to N
            j \leftarrow \text{random}[1:l];
            v'[j] \leftarrow v_1[j];
           T \leftarrow T \cup j;
           S \leftarrow S \cup v_1[j];
```



proto-child

 $v_1$ : parent chromosome 1

```
I: length of chromosome v': offspring chromosome N: total number of selected positions T=\{t[j]\}, j=1,2,...,N: selected positions set S=\{s[m]\}, m=1,2,...,N: genes value set of selected positions fg_1: flag 1 fg_2: flag 2 w: working data
```

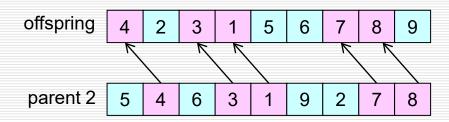
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 $v_2$ : parent chromosome 2

```
// step 3: produce offspring by filing unfixed
              positions of proto-child from parent 2
         for i=1 to l
               fg_1 \leftarrow 0;
               for i = 1 to N
                    if i=t[j] then fg_1 \leftarrow 1;
               if fg_1 = 1 then continue;
               for k=w to l
                   fg_2 \leftarrow 0;
                   for m=1 to N
                       if v_2[k]=s[m] then
                        fg_2 \leftarrow 1; break;
                   if fg_2 = 0 then
                     v'[i] \leftarrow v_2[k];
                      w \leftarrow k + 1: break:
  output offspring v';
end
```

step 3 : produce offspring by filing unfixed positions of proto-child from parent 2



 $v_1$ : parent chromosome 1  $v_2$ : parent chromosome 2  $v_3$ : offspring chromosome

N: total number of selected positions

 $T=\{t[j]\}$ , j=1,2,...,N: selected positions set

 $S = \{s[m]\}, m=1,2,..., N : genes value set of selected positions$ 

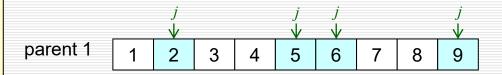
 $fg_1$ : flag 1  $fg_2$ : flag 2

w: working data

### 4. Order-Based Crossover (OBX)

```
procedure : Order-Based Crossover
input: chromosome v_1, v_2,
         length of chromosome 1
output: offspring v'
begin
      S \leftarrow \emptyset, T \leftarrow \emptyset, w \leftarrow 1;
       // step 1: select a set of positions
                   from parent 1 at random
      N \leftarrow \text{random}[1:l];
      for i=1 to N
             j \leftarrow \text{random}[1:l];
             S \leftarrow S \cup v_1[j];
```

step 1 : select a set of positions from parent 1 at random



 $v_1$ : parent chromosome 1  $v_2$ : parent chromosome 2  $v_2$ : offspring chromosome

N: total number of selected positions

 $T=\{t[j]\}$ , j=1,2,...,N: positions set of assigned genes from  $v_2$  to v'

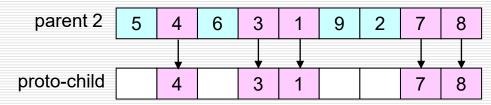
 $S = \{s[i]\}, i=1,2,..., N : genes value set of selected positions$ 

 $fg_1$ : flag 1  $fg_2$ : flag 2

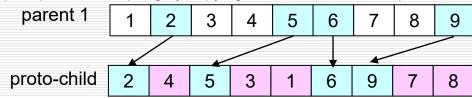
w: working data

```
// step 2: produce proto-child by copying
              non-selected value from parent 2
       for i=1 to l
             fg_1 \leftarrow 0;
             for j=1 to N
                if v_2[i] = s[j] then
                      fg_1 \leftarrow 1; break;
             if fg_1=0 then
                 v'[i] \leftarrow v_2[i],
                  T \leftarrow T \cup i:
// step 3: produce offspring by copying selected
              values from parent 1
       for i=1 to l
             fg_2 \leftarrow 0;
             for j=1 to N
                if i = t[j] then fg_2 \leftarrow 1;
             if fg_2=1 then continue;
             v'[i] \leftarrow s[w];
             w \leftarrow w+1;
       output offspring v';
end
```

step 2: produce proto-child by copying non-selected value from parent 2



step 3: produce offspring by copying selected values from parent 1



 $v_1$ : parent chromosome 1  $v_2$ : parent chromosome 2 l: length of chromosome  $v_2$ : offspring chromosome

N: total number of selected positions

 $T=\{t[j]\}$ , j=1,2,...,N: positions set of assigned genes from  $v_2$  to v'

 $S = \{s[i]\}, i=1,2,..., N : genes value set of selected positions$ 

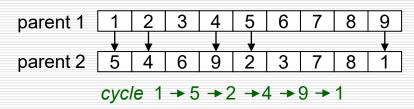
 $fg_1$ : flag 1  $fg_2$ : flag 2

w: working data

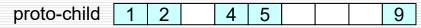
### 5. Cycle Crossover (CX)

```
procedure: CX crossover
input: chromosome v_1, v_2,
         length of chromosome l
output: offspring v'
begin
       S \leftarrow \emptyset, T \leftarrow \emptyset, w \leftarrow 1:
        // step 1: find the cycle between parents
       C \leftarrow \text{cy}(v_1, v_2);
        // step 2: produce proto-child by copying
                    gene values in cycle from parent 1
       for i=1 to l
           for j=1 to N-1
                if v_1[i] = c[j] then
                    v'[i] \leftarrow v_1[i];
                    T \leftarrow T \cup i:
                    S \leftarrow S \cup v_1[i];
```

step 1: find the cycle between parents

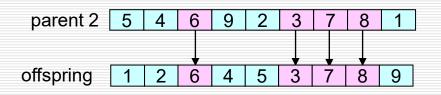


step 2 : produce proto-child by copying gene values in cycle from parent 1



```
// step 3: produce offspring by filling
            unfixed position from parent 2
        for i=1 to l
            fg_1 \leftarrow 0;
            for n=1 to |T|
                  if i=t[n] then fg_1 \leftarrow 1;
             if fg_1 = 1 then continue;
             for j=w to l
                  fg_2 \leftarrow 0;
                  for k=1 to |S|
                       if v_2[j]=s[k] then
                           fg_2 \leftarrow 1; break;
                  if fg_2 = 0 then
                       v'[i] \leftarrow v_2[j];
                       w \leftarrow i + 1; break;
       output offspring ;
end
```

step 3: produce offspring by filling unfixed position from parent 2



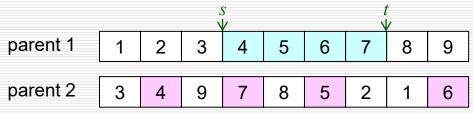
```
v_1: parent chromosome 1 v_2: parent chromosome 2 I: length of chromosome v': offspring chromosome N: total number of values in cycle T=\{t[n]\}, n=1,2,\ldots,N-1: positions set of S in proto-child S=\{s[k]\}, k=1,2,\ldots,N-1: proto-child genes value set in cycle C=\{c[j]\}, j=1,2,\ldots,N-1: value set of cycle fg_1: flag 1 fg_2: flag 2 w: working data cycle (v_1,v_2): searching cycle between v_1 and v_2
```

#### 6. Subtour Exchange Crossover

```
procedure: Subtour Exchange Crossover
        input: chromosome v_1, v_2,
                  length of chromosome l
        output: offspring v_1', v_2'
        begin
                S \leftarrow \emptyset. T \leftarrow \emptyset:
                // step 1: select subtours in parents
                s \leftarrow \text{random}[1:l-1];
                t \leftarrow \text{random}[s+1:l];
                for i=1 to l
                    for j=s to t
                         if v_2[i] = v_1[j] then
                                S \leftarrow S \cup v_2[i];
                         else
                               v_2'[i] \leftarrow v_2[i],
                                T \leftarrow T \cup i:
```

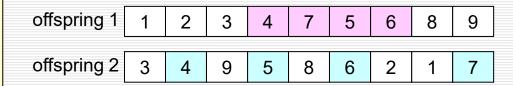
step 1 : select subtours in parents

fg: flag



```
// step 2: exchange subtours
       v_1' \leftarrow v_1[1:s-1] // S // v_1[t+1:l];
     k \leftarrow s;
     for i=1 to l
          fg \leftarrow 0;
          for j=1 to |T|
                if i=t[j] then fg \leftarrow 1;break;
         if fg=1 then continue;
         v_2[i] \leftarrow v_1[k];
         k \leftarrow k+1:
     output offspring v'_1, v'_2;
end
```

#### step 2 : exchange subtours



```
v_1: parent chromosome 1 v_2: parent chromosome 2 v_1: length of chromosome v_2: offspring chromosome 1 v_2: offspring chromosome 2
```

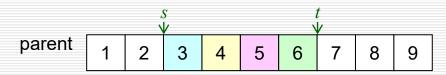
N: total number of values in subtour  $S = \{s[i]\}, i=1,2,..., N$ : value set of subtour  $T = \{t[j]\}, j=1,2,..., N$ : positions set of S

s: start position of substring in  $v_1$  t: end position of substring  $v_1$  t: fg: flag

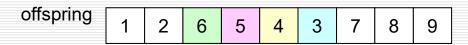
#### 1. Inversion Mutation

```
procedure: Inversion Mutation
input: chromosome v_1, v_2,
        length of chromosome 1
output: offspring v'
begin
       // step 1: select subtour at random
       s \leftarrow \text{random}[1:l-1];
       t \leftarrow \text{random}[s+1:l];
       // step 2: produce offspring by
                  copying inverse string of
                  substring
       S \leftarrow \text{invert}(v[s:t]);
       v' \leftarrow v[1:s-1] // S // v[t+1:l];
      output offspring v';
end
```

step 1: select subtour at random



step 2 : produce offspring by copying inverse string of substring

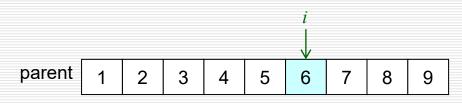


```
v: parent chromosome l: length of chromosome v': offspring chromosome s: start position of substring t: end position of substring s: inverse string of substring invert(string): inversely changing order of string
```

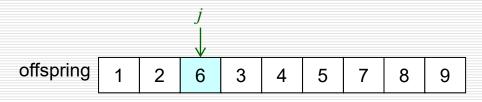
#### 2. Insertion Mutation

```
procedure: Insertion Mutation
input: chromosome v_1, v_2,
        length of chromosome l
output: offspring v'
begin
       // step 1 : select a position in
                   parent 1 at random
       i \leftarrow \text{random}[1:l];
      // step 2: insert selected value in
                 randomly selected
                 position parent 2
       j \leftarrow \text{random}[1:l-1];
       W \leftarrow v[1:i-1] // v[i+1:l];
       v' \leftarrow W[1:j-1] // v[i] // W[j:l-1];
      output offspring v';
end
```

step 1: select a position in parent 1 at random



step 2: insert selected value in randomly selected position of parent 2

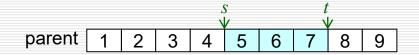


```
v: parent chromosome
v': offspring chromosome
j: selected position in parent 2
l: length of chromosome
j: selected position in parent 1
W: working data set
```

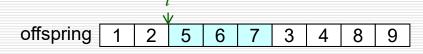
### 3. Displacement Mutation

```
procedure: Displacement Mutation
input: chromosome v_1, v_2,
         length of chromosome l
output: offspring v'
begin
     // step 1: select subtour
     s \leftarrow \text{random}[1:l-1];
     t \leftarrow \text{random}[s+1:l];
     // step 2: insert subtour in a
                random position
     n \leftarrow t-(s-1);
      i \leftarrow \text{random}[1:l-n];
      W \leftarrow v [1:s-1] // v [t+1:l];
      v' \leftarrow W[1:i-1] // v[s:t] // W[i:l-n];
      output offspring v';
end
```

#### step 1 : select subtour



#### step 2: insert subtour in a random position



```
v: parent chromosome
v': offspring chromosome
t: end position of substring
i: insert position
W: working data set
l: length of chromosome
s: start position of substring
n: length of subtour
i: length of chromosome
s: start position of substring
n: length of chromosome
s: start position of substring
n: length of chromosome
s: start position of substring
n: length of chromosome
s: start position of substring
n: length of chromosome
s: start position of substring
n: length of chromosome
```

### 4. Swap Mutation

```
procedure: Swap Mutation
input: chromosome v_1, v_2,
        length of chromosome 1
output: offspring v'
begin
     // step 1: select two position at random
     i \leftarrow \text{random}[1:l-1];
     j \leftarrow \text{random}[i+1:l];
     // step 2: produce offspring by swapping
               selected positions
     v' \leftarrow v[1: i-1] // v[j] // v[i+1: j-1] // v[i] // v[j+1:
      l];
     output offspring
end
```

step 1: select two position at random

parent 1 2 3 4 5 6 7 8 9

step 2 : produce offspring by swapping selected positions offspring 1 2 6 4 5 3 7 8 9

v: parent chromosome

*j*: selected position

v': offspring chromosome

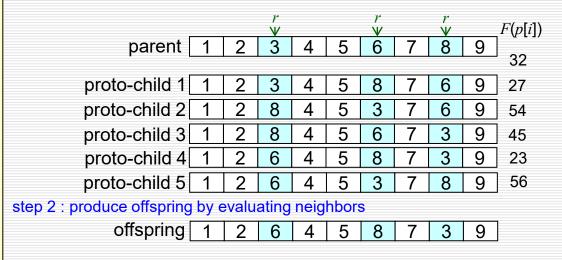
*I* : length of chromosome

*i* : selected position

#### 5. Heuristic Mutation

```
procedure: Heuristic Mutation
input: chromosome v_1, v_2,
         length of chromosome 1
output: offspring v'
begin
     P← Ø:
     // step 1: select positions and
                  produce neighbors
     for i=1 to m {
        r \leftarrow \text{random}[1:l];
       P \leftarrow P \cup \mathsf{nb}(v[r]);
     // step 2: produce offspring by
                evaluating neighbors
     w \leftarrow F(p[1]);
     for i=2 to |P|
         if w > F(p[i]) then
               w \leftarrow F(p[i]), n \leftarrow i;
      v' \leftarrow p[n];
      output offspring v';
end:
```

step 1: select positions and produce neighbors



```
      v: parent chromosome
      I: length of chromosome

      v': offspring chromosome
      m: total number of selected positions

      r: selected position
      N: total number of neighbor chromosomes

      w:working data
      n: position of chromosome with best fitness value in P

      P(p[i]) i=1.2
      N: poighbor chromosome set
```

 $P\{p[i]\}, i=1,2,...,N$ : neighbor chromosome set

nb(v[r]): searching neighbors of rth gene

F(p[i]): fitness value of p[i]

# 4 Overall Algorithm

### □ GA procedure for Traveling Salesperson Problem

```
procedure: GA for Traveling Salesperson Problem (TSP)
Input: TSP data set, GA parameters
output: best tour route
begin
     t ←0;
     initialize P(t) by permutation encoding or random keys encoding;
     fitness eval(P) by permutation decoding or random keys decoding;
     while (not termination condition) do
            crossover P(t) to yield C(t) by partial-mapped crossover;
            mutation P(t) to yield C(t) by swap mutation;
           fitness eval(C) by permutation decoding or random keys decoding;
           select P(t+1) from P(t) and C(t);
            t \leftarrow t+1:
     end
     output best tour route;
end
```