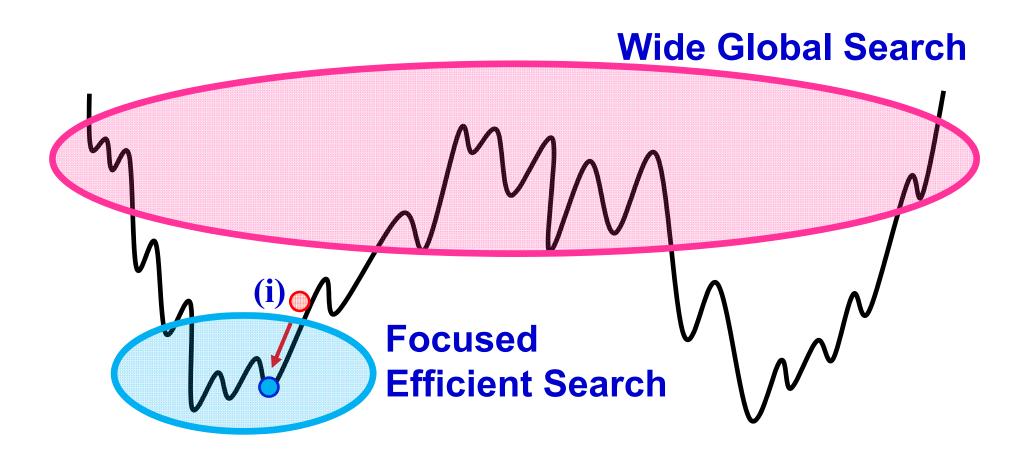
Optimization Methods

- 1. Introduction.
- 2. Greedy algorithms for combinatorial optimization.
- 3. LS and neighborhood structures for combinatorial optimization.
- 4. Variable neighborhood search, neighborhood descent, SA, TS, EC.
- 5. Branch and bound algorithms, and subset selection algorithms.
- **6.** Linear programming problem formulations and applications.
- 7. Linear programming algorithms.
- 8. Integer linear programming algorithms.
- **9.** Unconstrained nonlinear optimization and gradient descent.
- 10. Newton's methods and Levenberg-Marquardt modification.
- 11. Quasi-Newton methods and conjugate direction methods.
- **12.** Nonlinear optimization with equality constraints.
- **13.** Nonlinear optimization with inequality constraints.
- **14.** Problem formulation and concepts in multi-objective optimization.
- 15. Search for single final solution in multi-objective optimization.
- **16:** Search for multiple solutions in multi-objective optimization.

Optimization Algorithm Design:

Find a good balance between the wide global search and the focused efficient search (the good balance depends on the problem size and the available computation time)

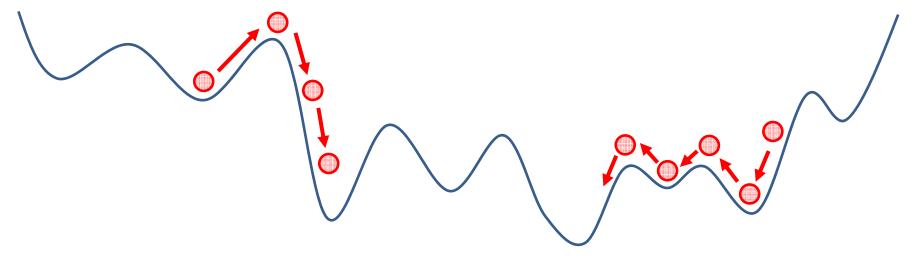


Move to a Better Solution

- Local Search (LS)
- Iterated Local Search (ILS)
- Variable Neighborhood Search (VNS)

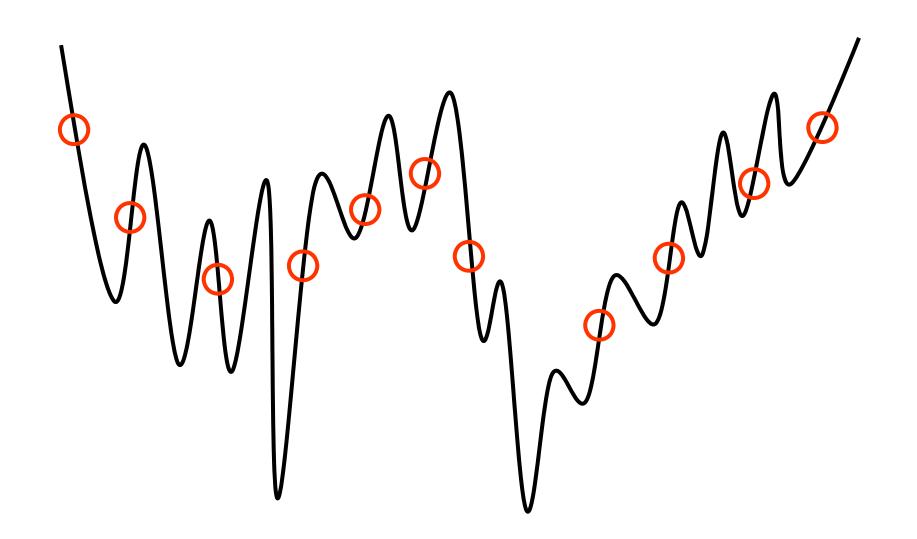
Allow the Move to a Worse Solution

- Simulated Annealing (SA)
- Tabu Search (TS)



Point-based algorithms: Almost all algorithms LS (Local Search), Iterated LS, Variable Neighborhood Search, SA, TS

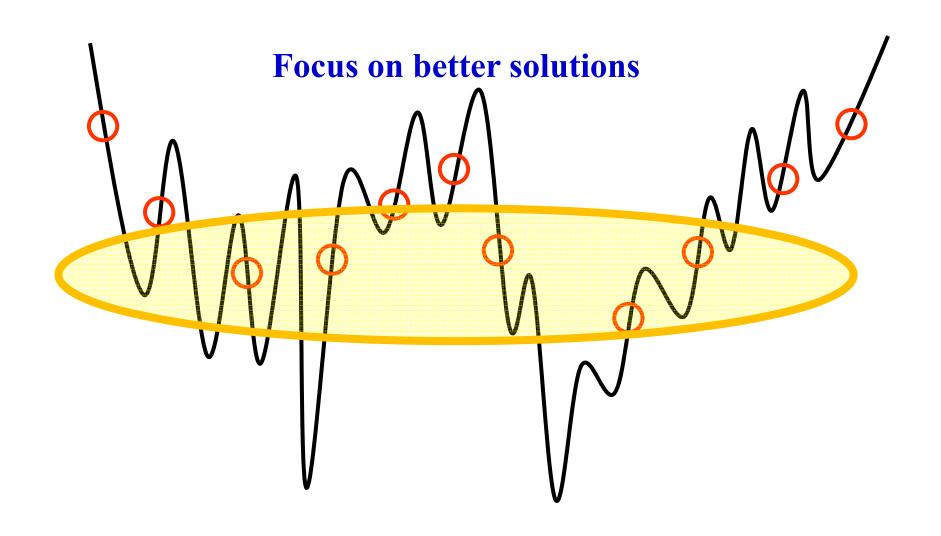
Genetic Algorithms: Population-based search (multi-point search)



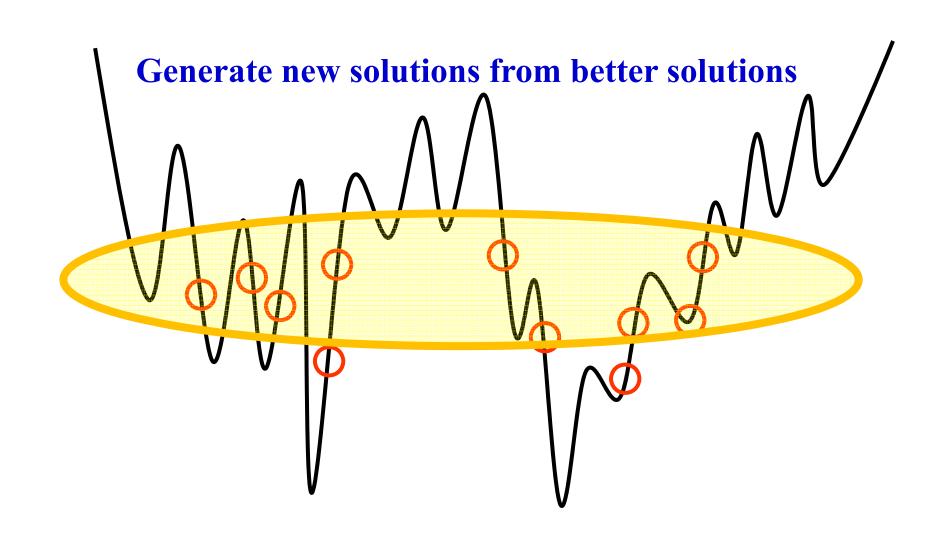
- Population-based search algorithms
- Multi-point search algorithms



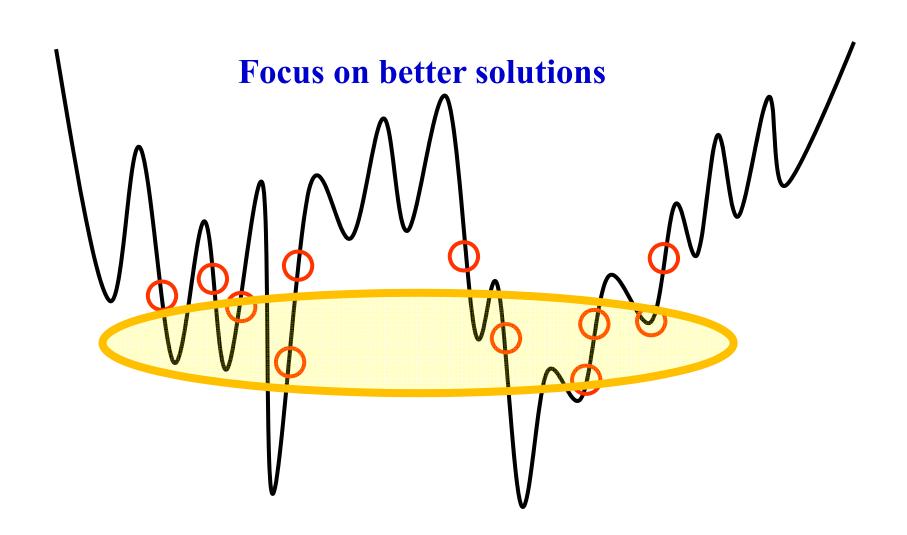
- Population-based search algorithms
- Multi-point search algorithms



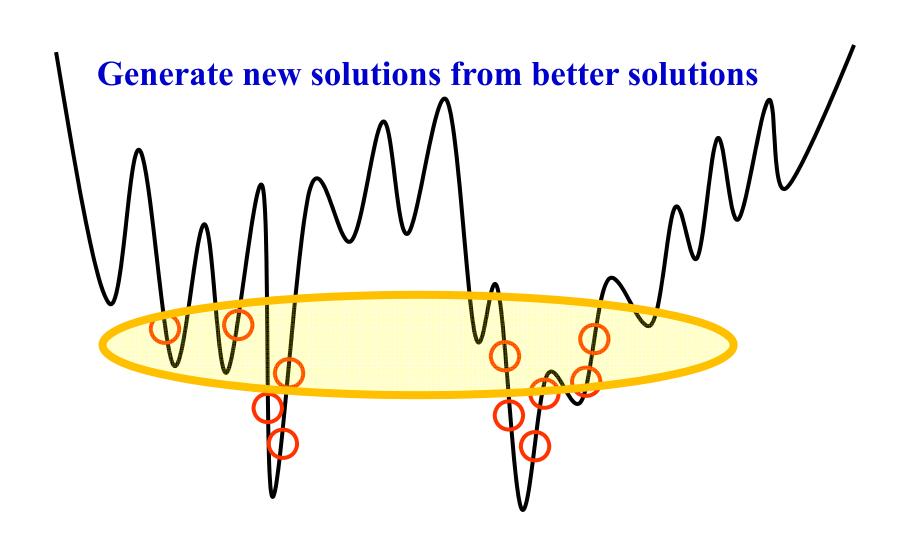
- Population-based search algorithms
- Multi-point search algorithms



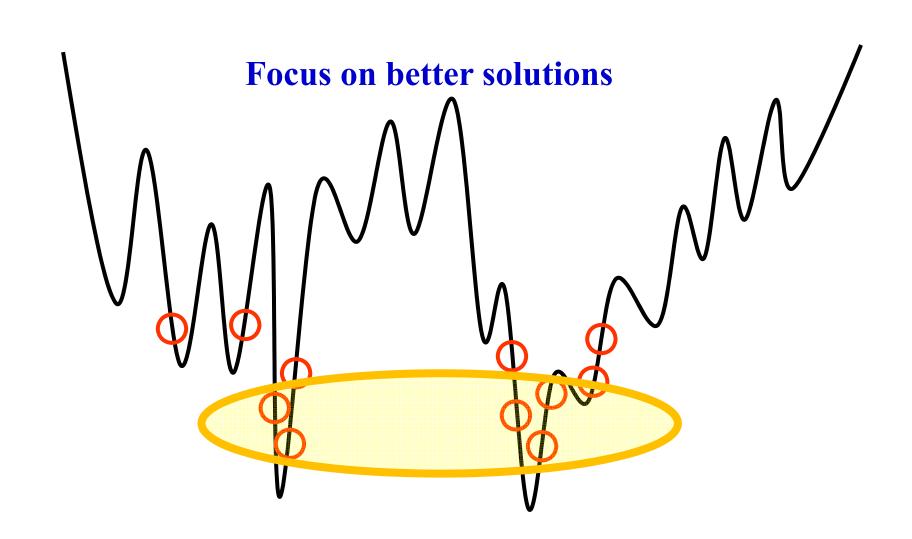
- Population-based search algorithms
- Multi-point search algorithms



- Population-based search algorithms
- Multi-point search algorithms

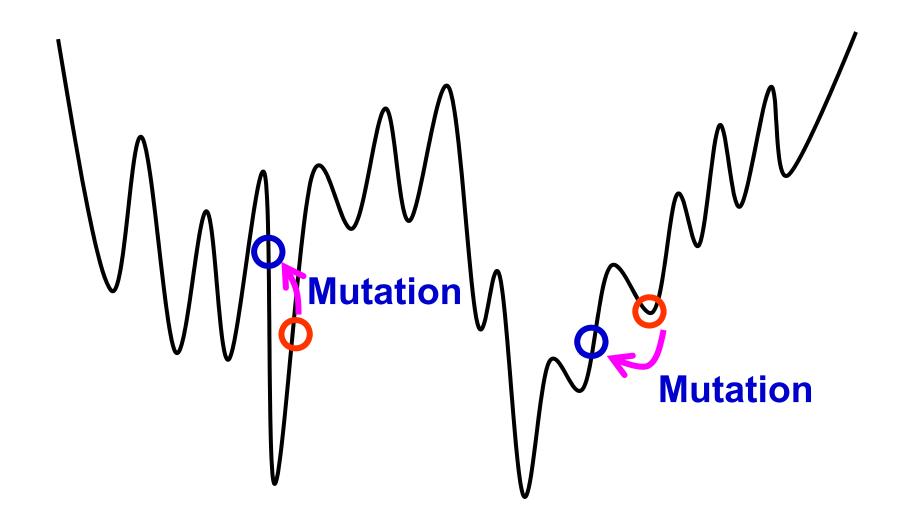


- Population-based search algorithms
- Multi-point search algorithms



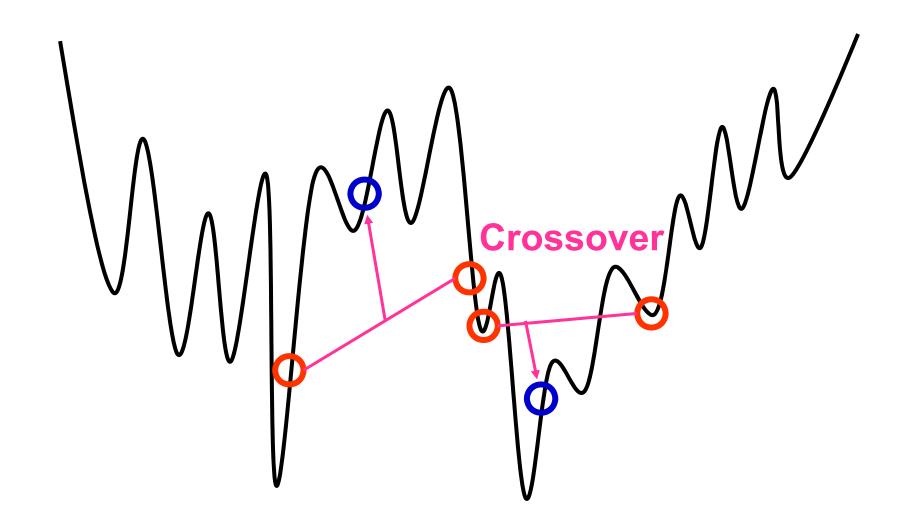
Two Operators for New Solution Generation

- (1) Mutation (Random choice of a neighbor)
- (2) Crossover (Recombination of two parents)

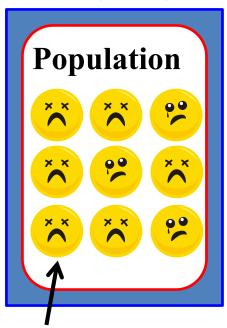


Two Operators for New Solution Generation

- (1) Mutation (Random choice of a neighbor)
- (2) Crossover (Recombination of two parents)



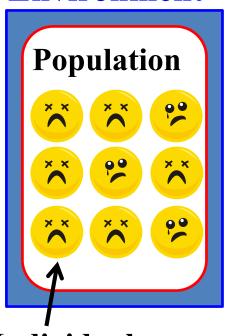
Environment



Individual

- (1) A population of individuals is randomly generated.
- (2) Each individual is evaluated in the environment.

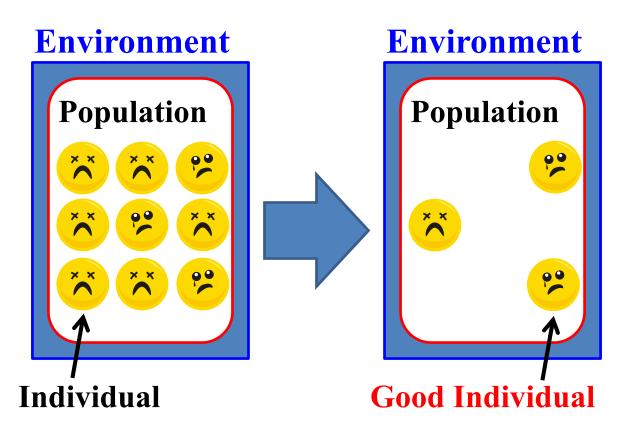
Environment



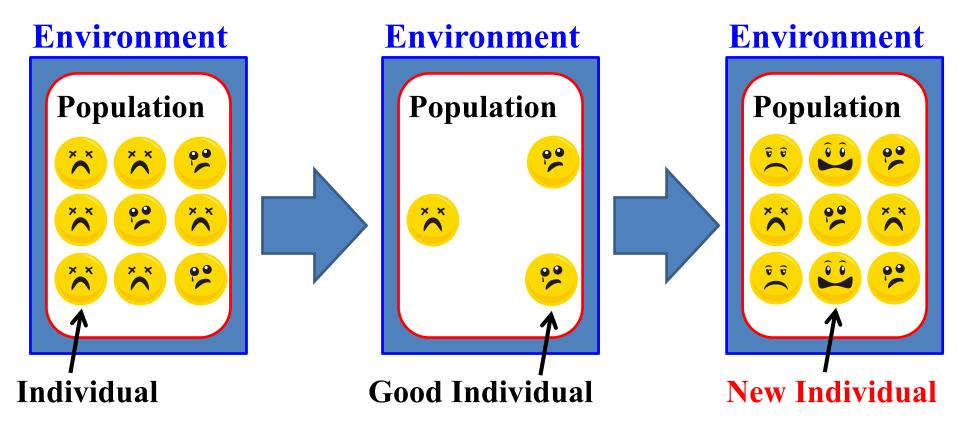
The search ability of evolutionary computation can be significantly improved by using good initial solutions (whereas this is not emphasized).

Individual

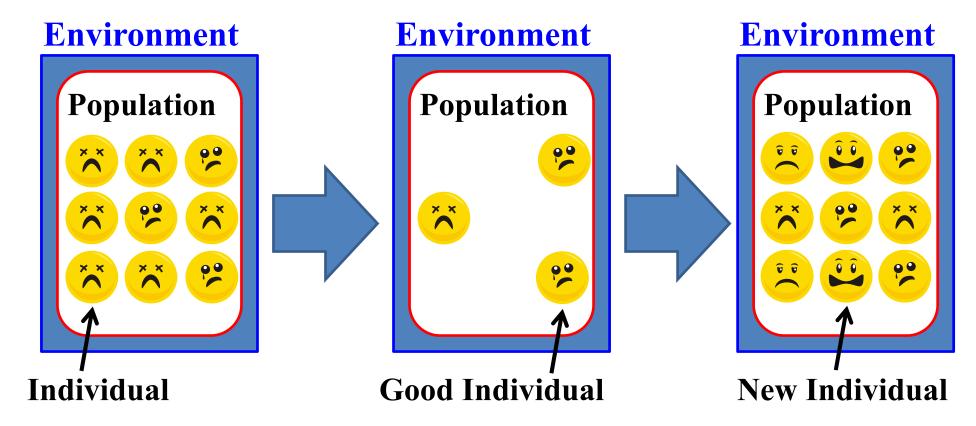
- (1) A population of individuals is <u>randomly</u> generated.
- (2) Each individual is evaluated in the environment.



- (1) A population of individuals is randomly generated.
- (2) Each individual is evaluated in the environment.
- (3) Good individuals survive probabilistically.

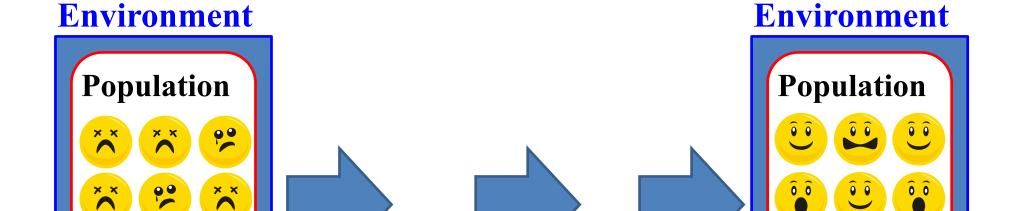


- (1) A population of individuals is randomly generated.
- (2) Each individual is evaluated in the environment.
- (3) Good individuals survive probabilistically.
- (4) New individuals are generated from the good individuals.



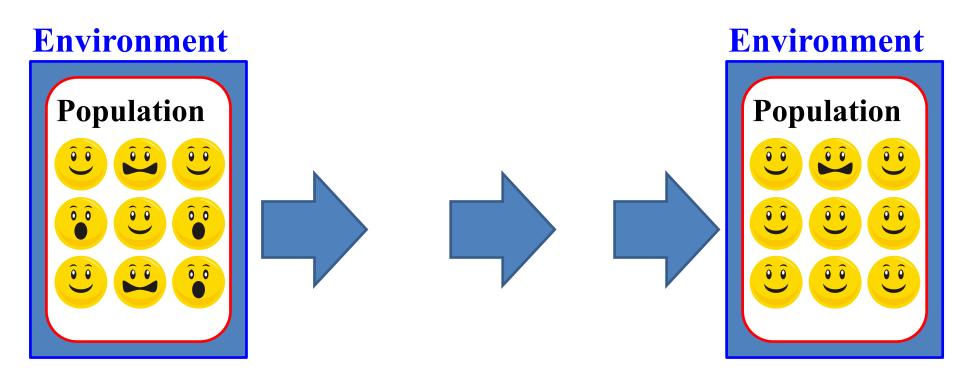
These steps (2)-(4) are iterated many times.

- (2) Each individual is evaluated in the environment.
- (3) Good individuals survive probabilistically.
- (4) New individuals are generated from the good individuals.



These steps (2)-(4) are iterated many times.

- (2) Each individual is evaluated in the environment.
- (3) Good individuals survive.
- (4) New individuals are generated from the good individuals.



These steps (2)-(4) are iterated many times.

- (2) Each individual is evaluated in the environment.
- (3) Good individuals survive.
- (4) New individuals are generated from the good individuals.

After many generations, we may have good solutions.

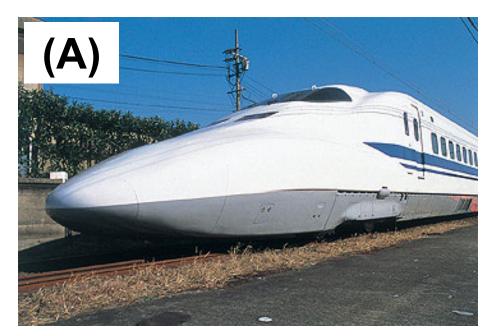
Application of Evolutionary Computation Design of High Speed Train

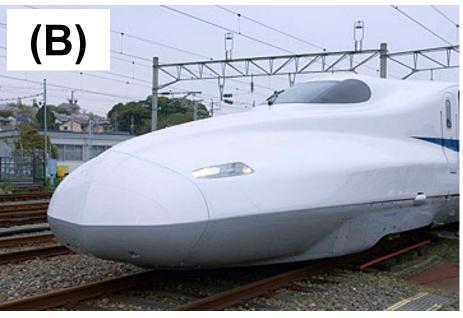
N700系フォトギャラリー



□ 印刷 閉じる

Two Types of High Speed Trains





(A) Old Design by Human Experts.

Old design looks better.

(B) New Design by Genetic Algorithms.

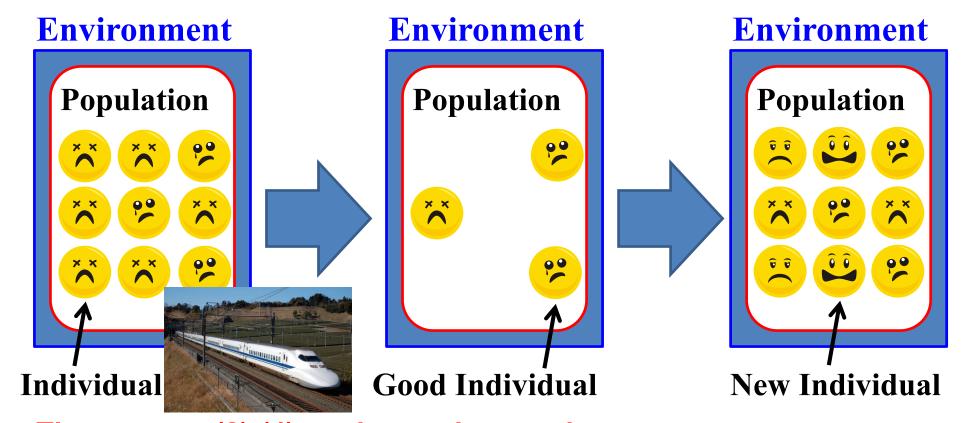
New design looks strange.

High Speed Trains in Japan

N700系フォトギャラリー



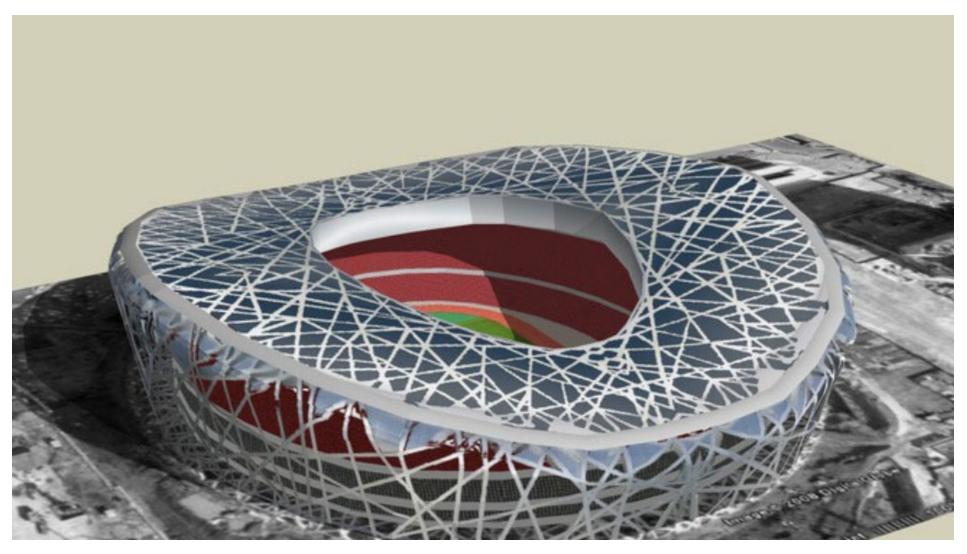
Old design by human experts looks nice!



These steps (2)-(4) are iterated many times.

- (2) Each individual is evaluated in the environment.
- (3) Good individuals survive probabilistically.
- (4) New individuals are generated from the good individuals.

Applications of Evolutionary Computation Construction Planning



http://sketchup3dconstruction.com/skp/warehouse/stadiums/beijing-national-stadium.html

Applications of Evolutionary Computation Construction Planning

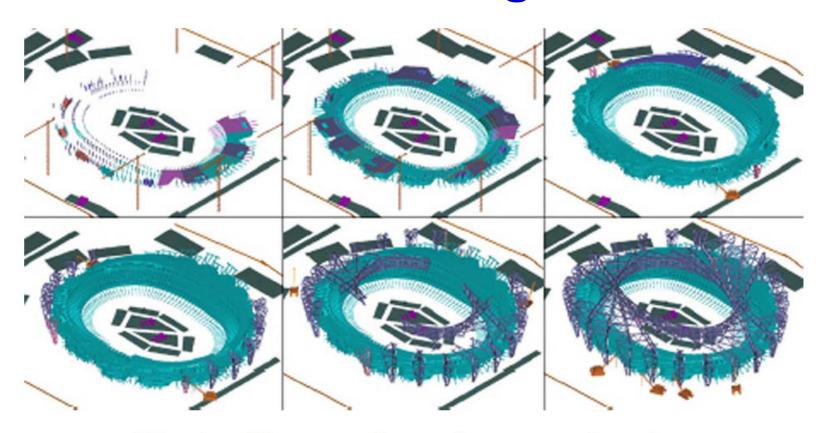


Fig. 4 4D screenshots of construction plan

J.ZHANG, Y. ZHANG, Z. HU, and M.LU: Construction Management Utilizing 4D CAD and Operations Simulation Methodologies, *TSINGHUA SCIENCE AND TECHNOLOGY*, Vol. 13, No. S1, pp. 241-247. Oct 2008.

Design of Rule-Based Systems

Environment

Population

```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

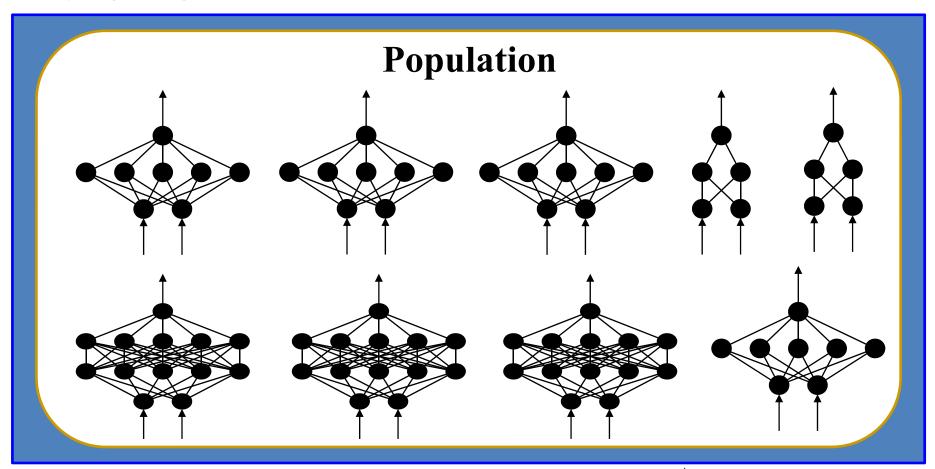
```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

```
If ... Then ...
If ... Then ...
If ... Then ...
If ... Then ...
```

Design of Neural Networks

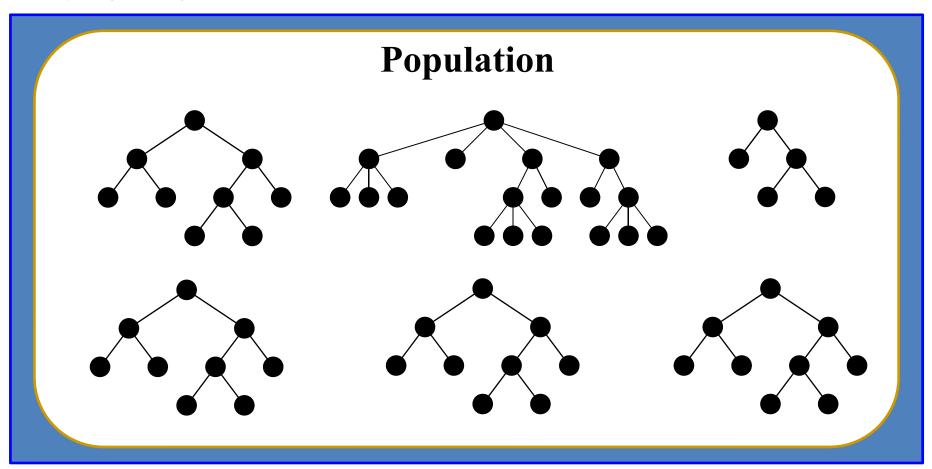
Environment



Individual = Neural Network ()

Design of Decision Trees

Environment



Individual = Decision Tree ()

How to Represent Each Solution for Computer Simulation of Evolution



Any string can be used depending on the problem at hand



Knapsack Problem:

Binary String	1	1	1	0	1	0	0	0	0
Permutation	3	4	2	7	1	8	9	6	5
Random Key	0.23	0.29	0.19	0.59	0.13	0.79	0.91	0.53	0.38

Random Key Genetic Algorithm (1994)

- Each solution is encoded as an array of *n* random keys
- A random key is a real number randomly generated in the interval [0, 1).

Knapsack Problem:

Binary String	1	1	1	0	1	0	0	0	0
Permutation	3	4	2	7	1	8	9	6	5
Random Key	0.23	0.29	0.19	0.59	0.13	0.79	0.91	0.53	0.38

Random Key Genetic Algorithm (1994)

- Each solution is encoded as an array of *n* random keys
- A random key is a real number randomly generated in the interval [0, 1).

Example (Ascending Order as in the Above Example)

Random Key Coding: (0.46, 0.91, 0.33, 0.75, 0.51)

Permutation Coding: ? => ? => ? => ? <u>Send your answer</u>

Knapsack Problem:

Binary String	1	1	1	0	1	0	0	0	0
Permutation	3	4	2	7	1	8	9	6	5
Random Key	0.23	0.29	0.19	0.59	0.13	0.79	0.91	0.53	0.38

Random Key Genetic Algorithm (1994)

- Each solution is encoded as an array of *n* random keys
- A random key is a real number randomly generated in the interval [0, 1).

Example (Ascending Order as in the Above Example)

Random Key Coding: (0.46, 0.91, 0.33, 0.75, 0.51)

Permutation Coding: $3 \Rightarrow 1 \Rightarrow 5 \Rightarrow 4 \Rightarrow 2$

Knapsack Problem:

Binary String	1	1	1	0	1	0	0	0	0
Permutation	3	4	2	7	1	8	9	6	5
Random Key	0.23	0.29	0.19	0.59	0.13	0.79	0.91	0.53	0.38

TSP, Flowshop Scheduling:

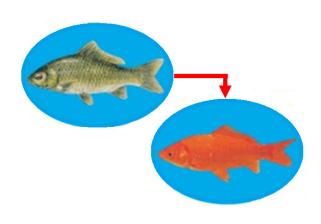
Permutation	3	4	2	7	1	8	9	6	5
Random Key	0.23	0.29	0.19	0.59	0.13	0.79	0.91	0.53	0.38

Function Optimization:

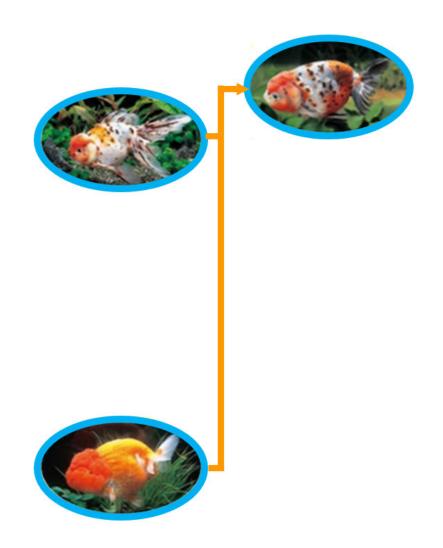
Real number string	25.297	123.45	92.834
Binary String 11101	0000111 010	0 0 0 1 0 0 1 1 0 0 0	001111010000
	x_1	x_2	x_3

How to generate new solutions

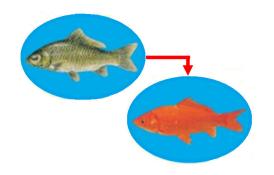
Mutation



Crossover

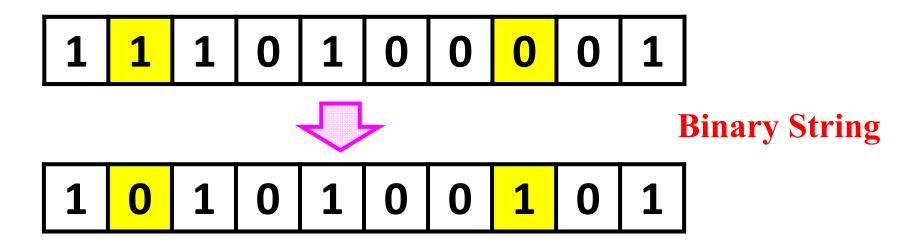


Random change of a part of a string

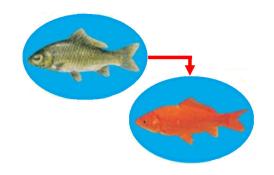


Random change of a part of a string

(Each value has the same mutation probability, e.g., 1/n, 2/n)

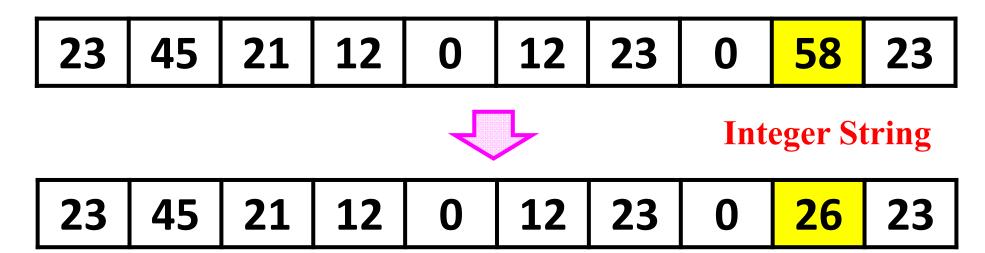


Random change of a part of a string

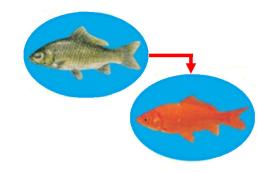


Random change of a part of a string

(Each value has the same mutation probability, e.g., 1/n, 2/n)



Random change of a part of a string



Random change of a part of a string

(Each value has the same mutation probability, e.g., 1/n, 2/n)

23.42	45.20	21.45	12.09	0.00	12.14	23.43	0.00	58.98	23.12

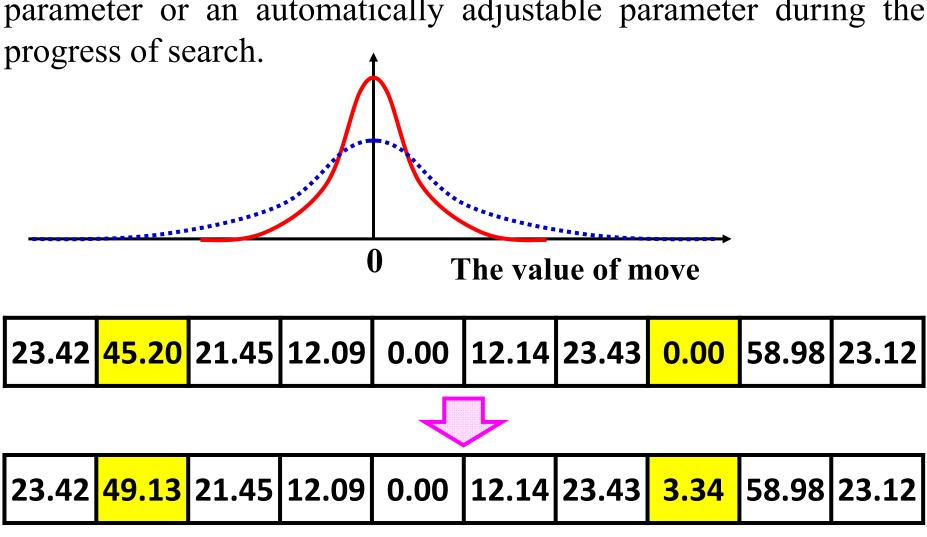


Real Number String

23.42 <mark> 67.13</mark> 21.45 12.09 0.00 12.14 23.43 <mark> 15.34</mark> 58.98 23.12
--

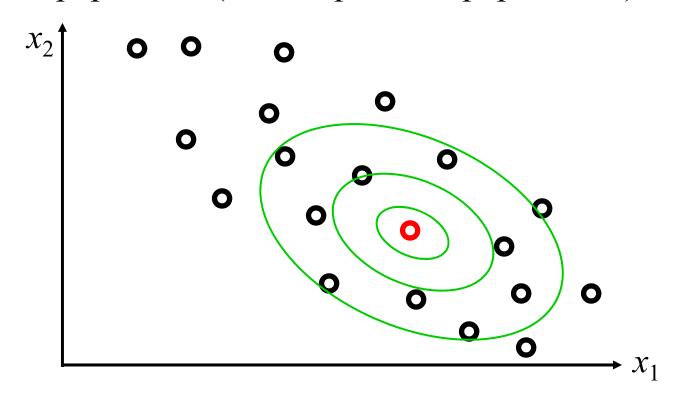
For real number strings, a distribution can be used.

The spread of the distribution is a parameter, which can be a fixed parameter or an automatically adjustable parameter during the



A multi-dimensional distribution can be also used.

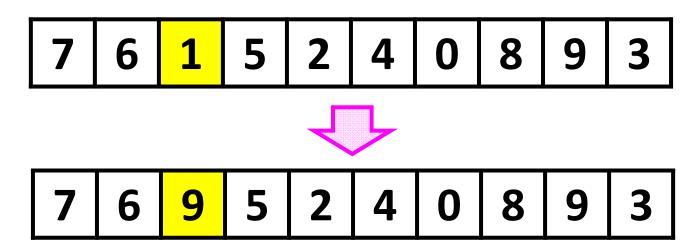
The distribution is usually automatically adjusted by the solutions in the current population (and the previous populations).



- All values of a solution are mutated.
- A mutation probability is assigned to each solution (not each value).

Mutation for Permutation Strings

Random change does not generate a permutation.

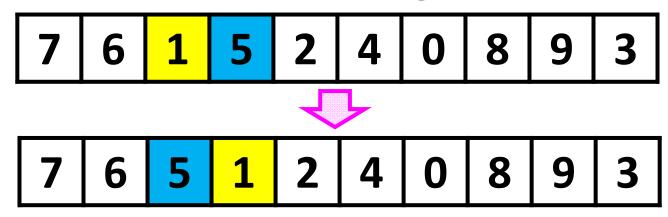


Two "9" and no "1".

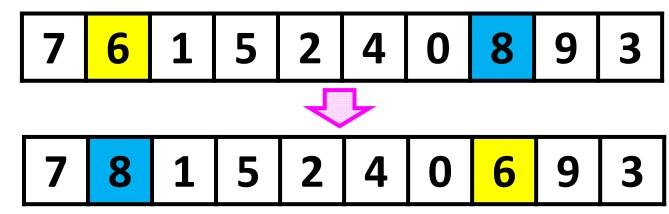
Mutation for Permutation Strings

A neighborhood structure is needed.

Adjacent two-position change

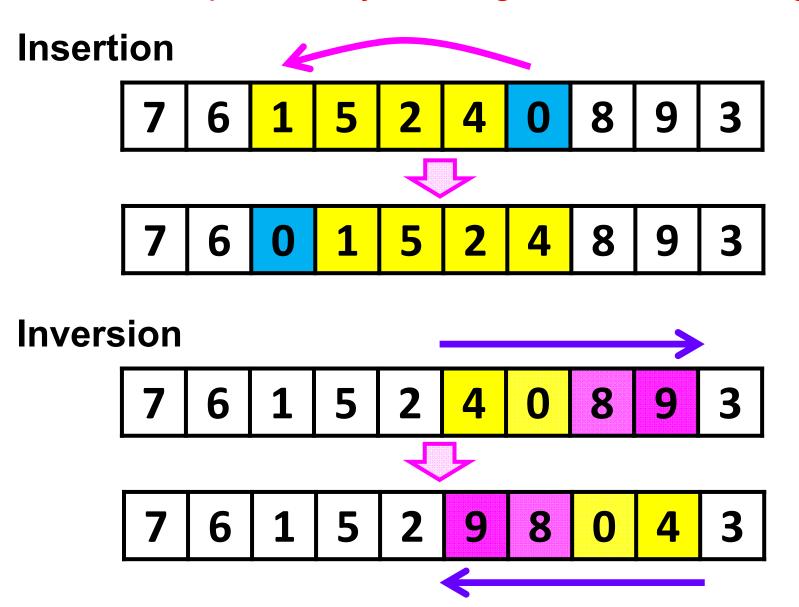


Two-position change

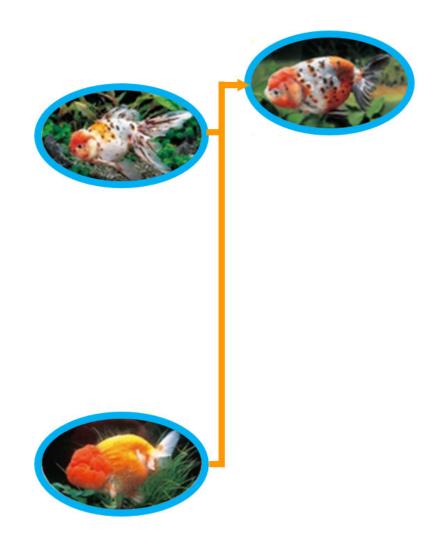


Mutation for Permutation Strings

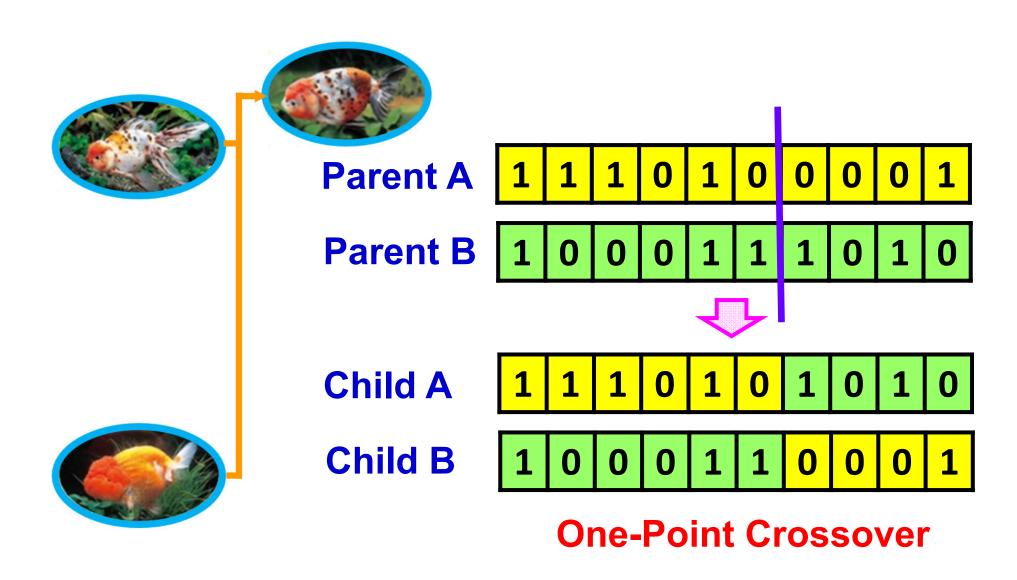
A mutation probability is assigned to each string.



Crossover

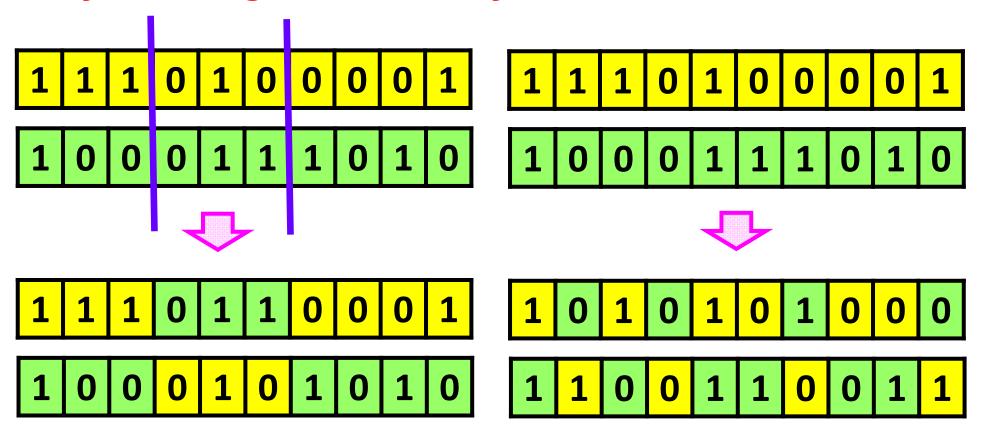


(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)



(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)

Any exchanges are usually OK.

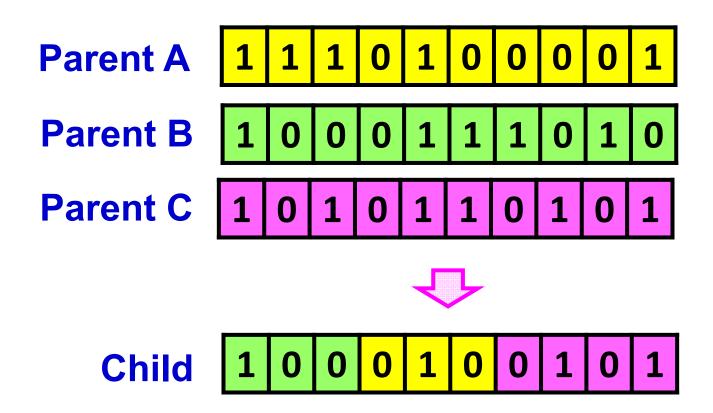


Two-Point Crossover

Uniform Crossover

(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)

Multiple parents can be used.



(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)

Calculation can be used.

0.2 x	1.00	0.00	0.00	1.00	2.00	1.00	1.00	10.00	1.00	1.00	
+											
0.8 x	1.00	1.00	10.00	1.00	10.00	1.00	10.00	10.00	20.00	1.00	
•											

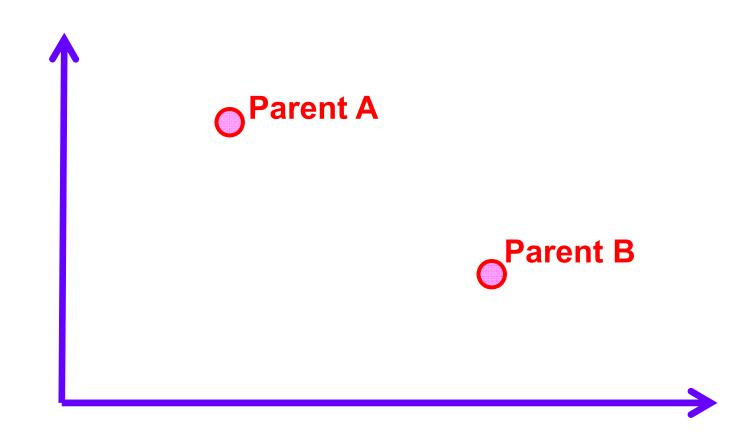
 1.00
 0.80
 8.00
 1.00
 8.40
 1.00
 8.20
 10.00
 16.20
 1.00

(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)

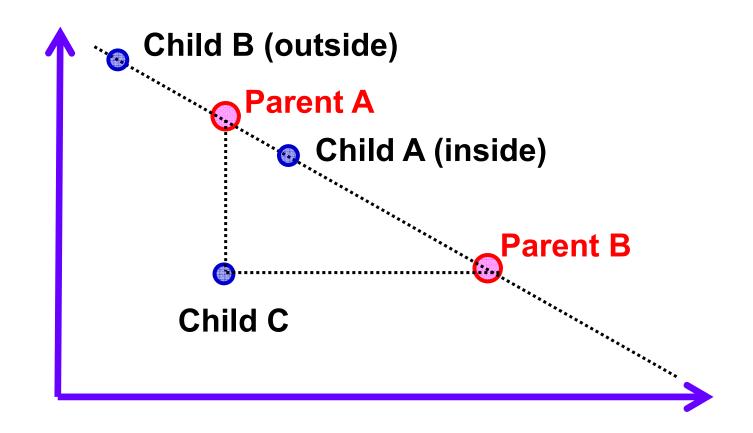
Multiple parents can be also used in calculation:

1.0 x	1.00	0.00	0.00	1.00	2.00	1.00	1.00	10.00	1.00	1.00	
0.6 x	1.00	1.00	10.00	1.00	10.00	1.00	10.00	10.00	20.00	1.00	
_											
0.6 x	3.50	2.00	8.50	2.00	5.00	2.00	4.50	2.00	5.00	2.00	
=											

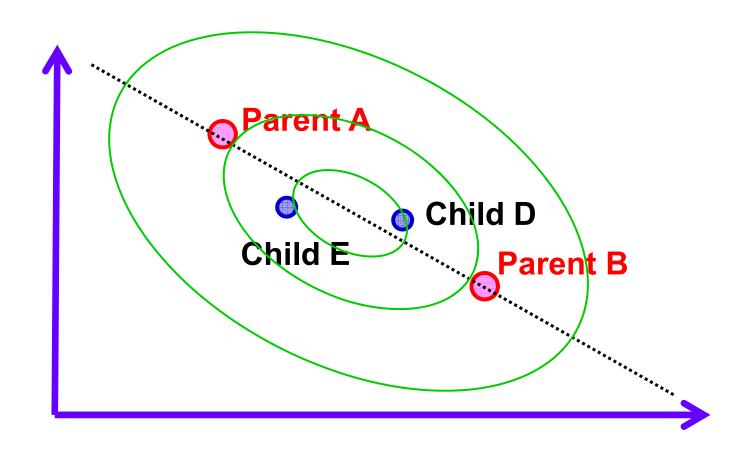
(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)



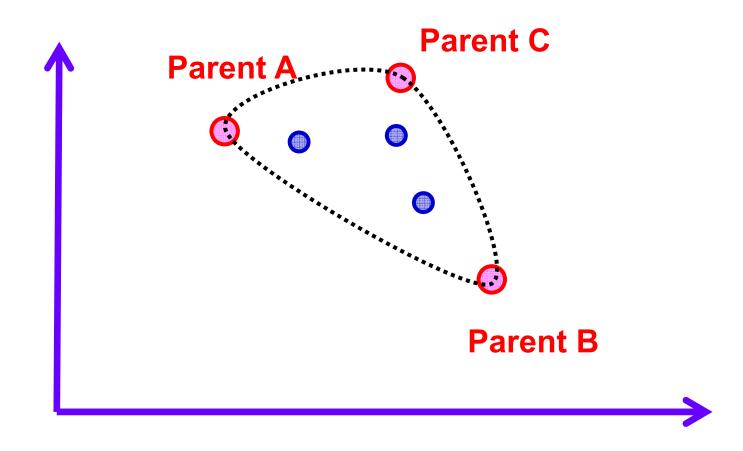
(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)



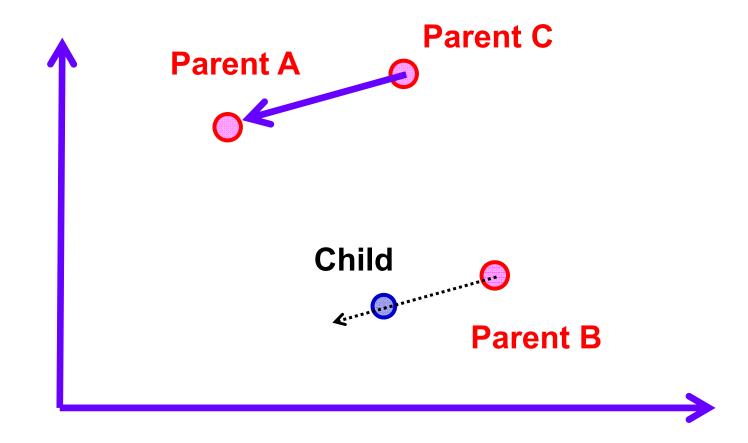
(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)



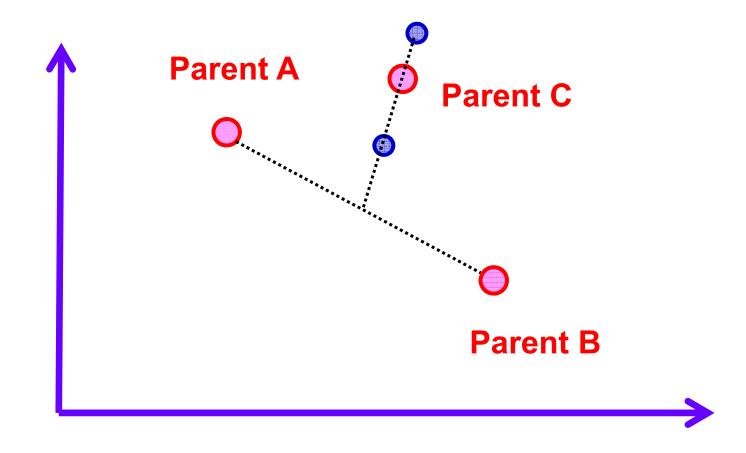
(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)



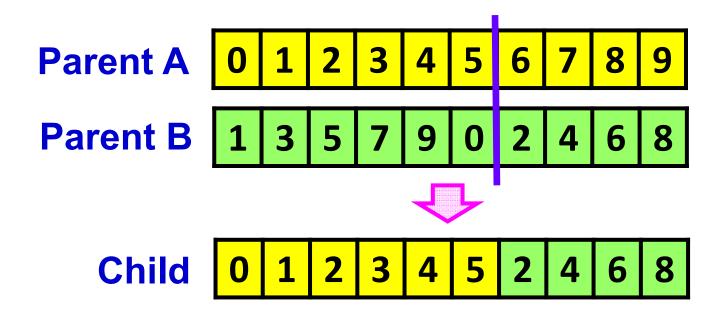
(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)



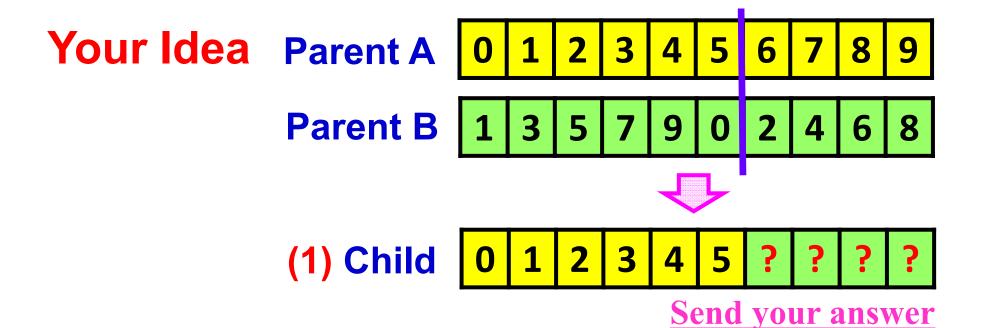
(with a crossover probability, e.g., 0.5, 0.8, 0.9, 1.0)



Simple crossover does not generate a permutation.

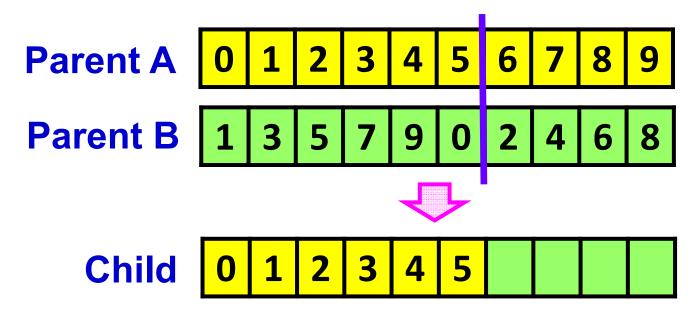


Two "2", two "4", no "7", and no "9".



Special Crossover for Permutation Strings:

One-Point Order Crossover

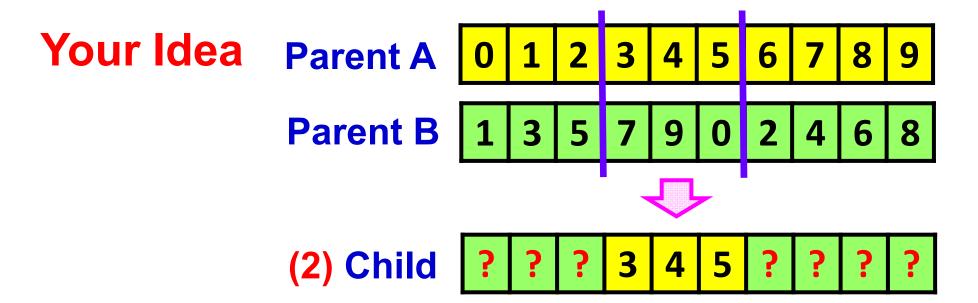


(1) A part of the child directly comes from Parent A.

Special Crossover for Permutation Strings:

One-Point Order Crossover

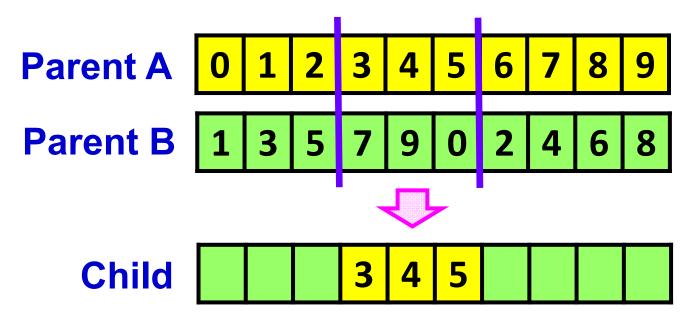
- (1) A part of the child directly comes from Parent A.
- (2) The other part of the child comes from Parent B in the order in Parent B.



Send your answer

Special Crossover for Permutation Strings:

Two-Point Order Crossover



(1) A part of the child directly comes from Parent A.

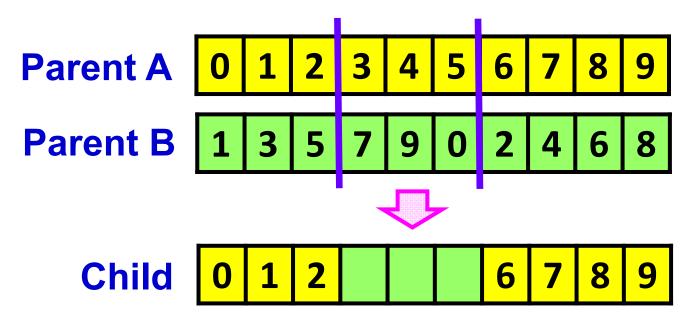
Special Crossover for Permutation Strings:

Two-Point Order Crossover

- (1) A part of the child directly comes from Parent A.
- (2) The other part of the child comes from Parent B in the order in Parent B.

Special Crossover for Permutation Strings:

Two-Point Order Crossover



(1) A part of the child directly comes from Parent A.

Special Crossover for Permutation Strings:

Two-Point Order Crossover

- (1) A part of the child directly comes from Parent A.
- (2) The other part of the child comes from Parent B in the order in Parent B.

How to evaluate each solution

Solution evaluation depends on the problem.

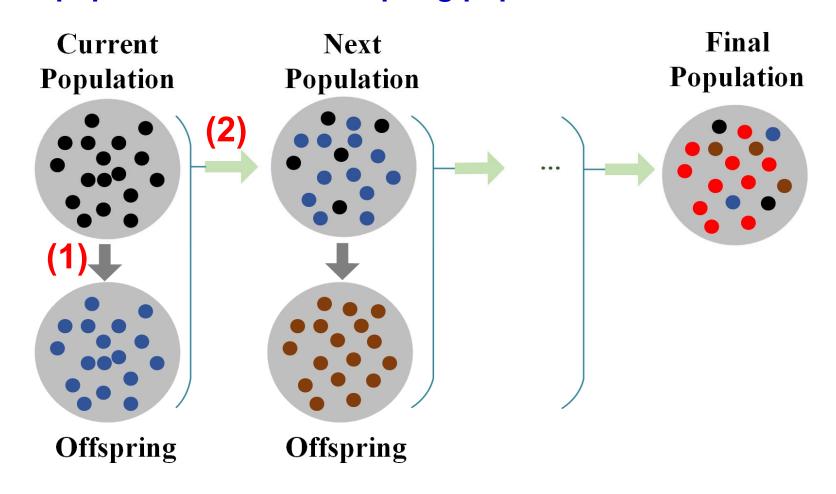
- Profit maximization problem: Profit
- Cost minimization problem: Cost
- Distance minimization problem: Distance
- Error minimization problem: Error

- ...

Selection: How to select good solutions

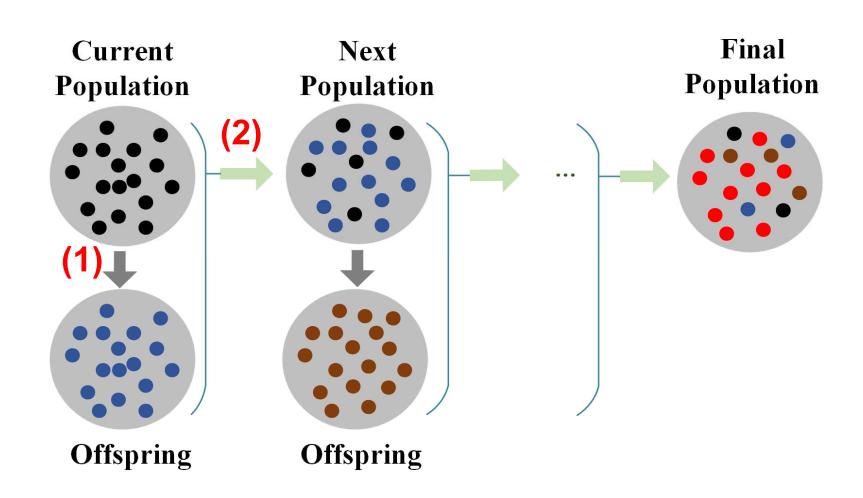
Good solutions are selected through

- (1) selection of parents from current population to generate new solutions
- (2) selection of solutions for the next population from the current population and the offspring population.



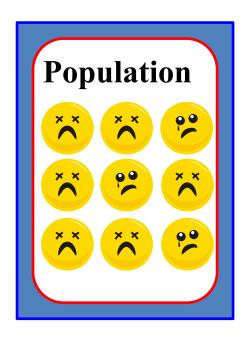
Two Phases of Selection:

- (1) Parent Selection (Mating Selection)
- (2) Generation Update (Environmental Selection)



Basic Idea of Parent Selection:

- Good children will be generated more likely from good parents than poor parents.
- So, let us choose good solutions as parents.

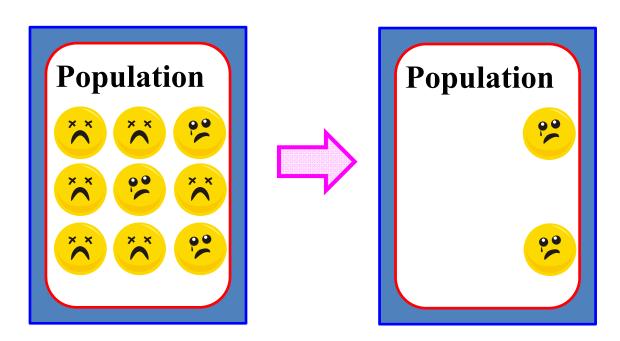


Implementation

The basic idea is simple. However, there are a lot of possible implementations such as

- To choose the best two solutions as parents.

All children are generated from the two solutions.

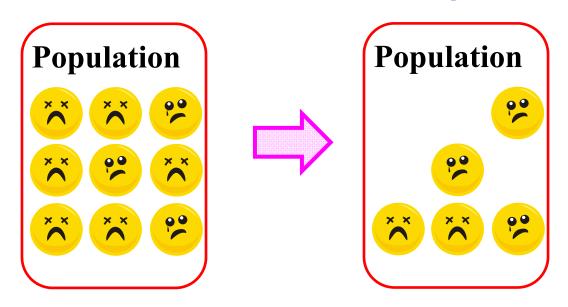


Implementation

The basic idea is simple. However, there are a lot of possible implementations such as

- To choose the best two solutions as parents.

 All children are generated from the two solutions.
- To choose a half solutions as parents.



Implementation

The basic idea is simple. However, there are a lot of possible implementations such as

- To choose the best two solutions as parents.

 All children are generated from the two solutions.
- To choose a half solutions as parents.
- Assign a different selection probability to each solution depending on the fitness value.



Parent Selection (Mating Selection)

Roulette Wheel Selection (Fitness Proportional Selection)

```
Current Solutions: x_1, x_2, ..., x_N (N: Population Size)
```

Their Fitness Values: $fitness(x_1)$, $fitness(x_2)$, ..., $fitness(x_N)$

Their Selection Probabilities: $p(x_1), p(x_2), ..., p(x_N)$

```
p(x_i) = fitness(x_i)/(fitness(x_1) + fitness(x_2) + \dots + fitness(x_N))
```

Parent Selection (Mating Selection)

Roulette Wheel Selection (Fitness Proportional Selection)

Current Solutions: $x_1, x_2, ..., x_N$ (N: Population Size)

Their Fitness Values: $fitness(x_1)$, $fitness(x_2)$, ..., $fitness(x_N)$

Their Selection Probabilities: $p(x_1), p(x_2), ..., p(x_N)$

$$p(x_i) = fitness(x_i)/(fitness(x_1) + fitness(x_2) + \dots + fitness(x_N))$$

Example (N = 10): Exercise

$$fitness(x_1) = fitness(x_2) = fitness(x_3) = fitness(x_4) = fitness(x_5) = fitness(x_6) = 1$$

 $fitness(x_7) = fitness(x_8) = fitness(x_9) = 2$, $fitness(x_{10}) = 8$

$$p(x_1) = p(x_2) = p(x_3) = p(x_4) = p(x_5) = p(x_6) = ?$$

 $p(x_7) = p(x_8) = p(x_9) = ?$
 $p(x_{10}) = p(x_{10}) = ?$

<u>Send your answer</u>

Parent Selection (Mating Selection)

Roulette Wheel Selection (Fitness Proportional Selection)

Current Solutions: $x_1, x_2, ..., x_N$ (N: Population Size)

Their Fitness Values: $fitness(x_1)$, $fitness(x_2)$, ..., $fitness(x_N)$

Their Selection Probabilities: $p(x_1), p(x_2), ..., p(x_N)$

$$p(x_i) = fitness(x_i)/(fitness(x_1) + fitness(x_2) + \dots + fitness(x_N))$$

Example (N = 10): **Exercise**

$$fitness(x_1) = fitness(x_2) = fitness(x_3) = fitness(x_4) = fitness(x_5) = fitness(x_6) = 1$$

 $fitness(x_7) = fitness(x_8) = fitness(x_9) = 2$, $fitness(x_{10}) = 8$
 $p(x_1) = p(x_2) = p(x_3) = p(x_4) = p(x_5) = p(x_6) = 0.05$
 $p(x_7) = p(x_8) = p(x_9) = 0.1$, $p(x_{10}) = 0.4$

Rank Selection

Selection probability is based on the rank of each solution.

Example (N = 10)

```
fitness(x_1) = 12

fitness(x_2) = 23

fitness(x_3) = 43

fitness(x_4) = 99 (Best)

fitness(x_5) = 11

fitness(x_6) = 12

fitness(x_7) = 24

fitness(x_8) = 56

fitness(x_9) = 79 (3rd)

fitness(x_{10}) = 92 (2nd)
```

Example of Selection Probabilities (N = 10)

```
Best: 0.19, 2nd: 0.17, 3rd: 0.15, 4th: 0.13, 5th: 0.11 6th: 0.09, 7th: 0.07, 8th: 0.05, 9th: 0.03, 10th: 0.01
```

Rank Selection

Selection probability is based on the rank of each solution.

Example of Selection Probabilities (N = 10)

```
Best: 0.19, 2nd: 0.17, 3rd: 0.15, 4th: 0.13, 5th: 0.11 6th: 0.09, 7th: 0.07, 8th: 0.05, 9th: 0.03, 10th: 0.01
```

Example of Selection Probabilities (N = 10): Some special cases

Choose the best two solutions:

Best: 0.5, 2nd: 0.5, 3rd: 0, 4th: 0, 5th: 0

6th: 0, 7th: 0, 8th: 0, 9th: 0, 10th: 0

Choose the best half solutions:

Best: 0.2, 2nd: 0.2, 3rd: 0.2, 4th: 0.2, 5th: 0.2

6th: 0, 7th: 0, 8th: 0, 9th: 0, 10th: 0

Rank Selection

Selection probability is based on the rank of each solution.

Example of Selection Probabilities (N = 10)

```
Best: 0.19, 2nd: 0.17, 3rd: 0.15, 4th: 0.13, 5th: 0.11 6th: 0.09, 7th: 0.07, 8th: 0.05, 9th: 0.03, 10th: 0.01
```

Example of Selection Probabilities (N = 10): Some special cases

Choose the best two solutions:

Best: 0.5, 2nd: 0.5, 3rd: 0, 4th: 0, 5th: 0 6th: 0, 7th: 0, 8th: 0, 9th: 0, 10th: 0

Choose the best half solutions:

Best: 0.2, 2nd: 0.2, 3rd: 0.2, 4th: 0.2, 5th: 0.2 6th: 0, 7th: 0, 8th: 0, 9th: 0, 10th: 0

Your Idea: Send your answer

Best: <u>0.?</u>, 2nd: <u>0.?</u>, 3rd: <u>0.?</u>, 4th: <u>0.?</u>, 5th: <u>0.?</u> 6th: <u>0.?</u>, 7th: <u>0.?</u>, 8th: <u>0.?</u>, 9th: <u>0.?</u>, 10th: <u>0.?</u>

Choose the best from randomly selected *K* solutions. (*K*: Tournament Size)

Iterate the following steps:

Step 1: Randomly select *K* solutions from the current population.

Step 2: Select the best solution among the *K* solutions.

- Selection pressure (probabilities) can be adjusted by K.

Large K ==> Only very good solutions can be parents.

Small K ==> Average solutions can have some probabilities

 $K=1 \implies$ Random selection

Choose the best from randomly selected *K* solutions. (*K*: Tournament Size)

Iterate the following steps:

- Step 1: Randomly select *K* solutions from the current population.
- Step 2: Select the best solution among the *K* solutions.
- ==> Selection probability of each solution depends on its rank (and the value of K).
- ==> Tournament selection with a specific value of *K* can be implemented as rank selection by specifying the corresponding selection probability for each rank.

Choose the best from randomly selected *K* solutions. (*K*: Tournament Size)

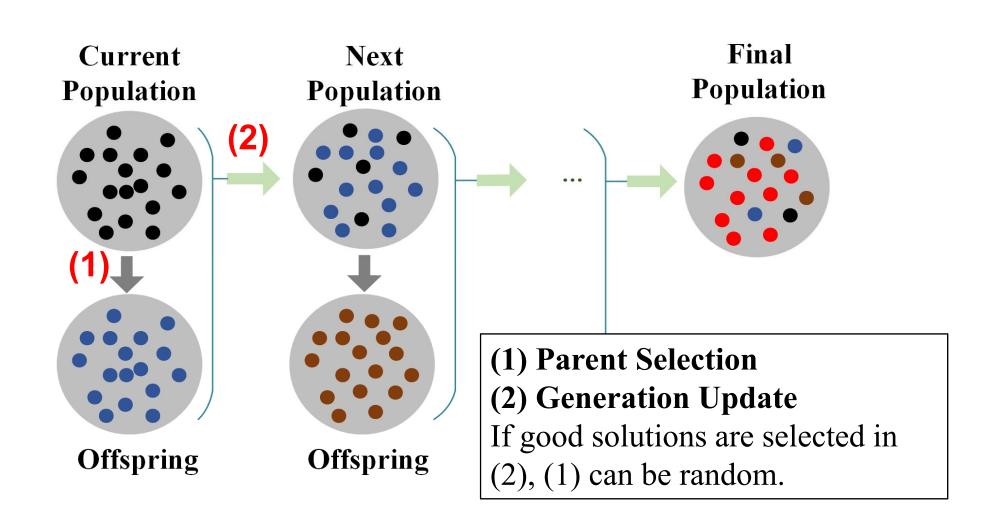
Iterate the following steps:

- Step 1: Randomly select K solutions from the current population (with duplication or without duplication).
- Step 2: Select the best solution among the *K* solutions.
- ==> Selection probability of each solution depends on its rank (and the value of K).

Lab Session Task 1:

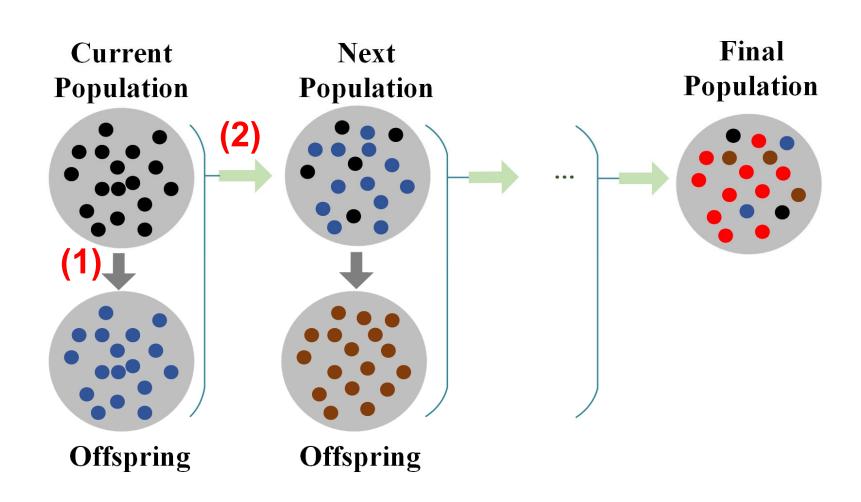
- 1. Calculate the selection probability of the worst solution for the case of N = 10 (population size) and K = 2 (tournament size) "with duplication".
- 2. Calculate the selection probability of the *i*-th worst solution for the case of N = 10 (population size) and K = 2 (tournament size) "with duplication".
- 3. Calculate the selection probability of the *i*-th worst solution for the case of N = 10 (population size) and K = 3 (tournament size) "with duplication".

Special Parent Selection Mechanism: Random Selection Parent can be randomly selected from the current solution.



Two Phases of Selection:

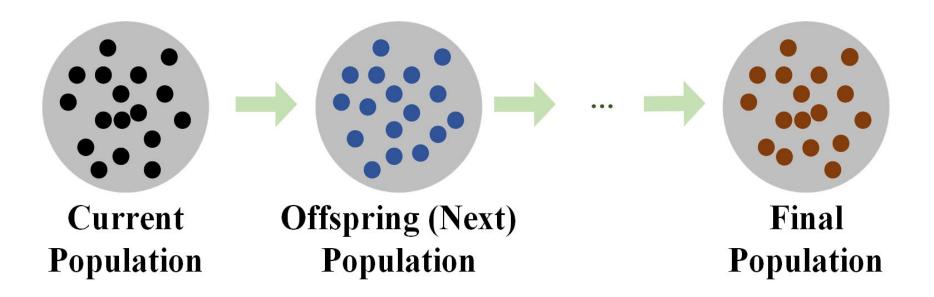
- (1) Parent Selection (Mating Selection)
- (2) Generation Update (Environmental Selection)



Generation Update (Environmental Selection)

Simplest Model: Next Population = Offspring Population

(This model is similar to evolution of many species in nature)



Advantage: Search can easily escape from local solutions.

Disadvantage: Good solutions cannot be efficiently utilized.

Strong selection pressure may be needed for parent selection.

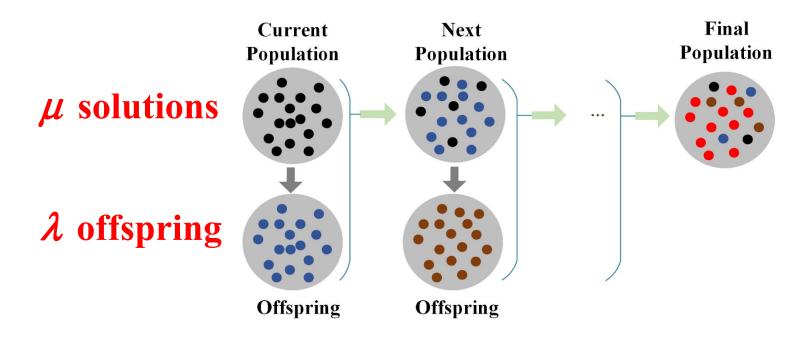
Generation Update in ES (Evolution Strategies)

Plus Strategy: $(\mu + \lambda)$ ES (Fast Convergence) Select the best μ solutions from the $(\mu + \lambda)$ solutions

Comma Strategy: (μ, λ) ES (Escape from Local Solutions) Select the best μ solutions from the λ offspring

 μ : Population size (Main population size)

 λ : The number of offspring (Offspring population size)



Generation Update in ES (Evolution Strategies)

Special Cases

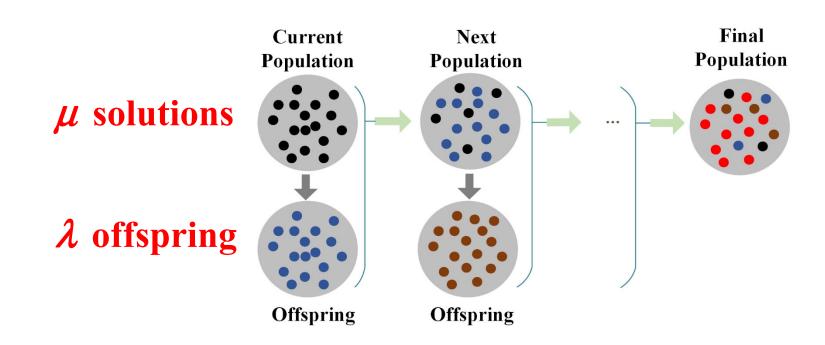
(1, 1)ES: Random search

(1+1)ES: Fast move local search

 $(1 + \lambda)$ ES: Local search

 $(\mu+1)$ ES: Steady state algorithm

 (μ, μ) ES: The simplest model of generation update

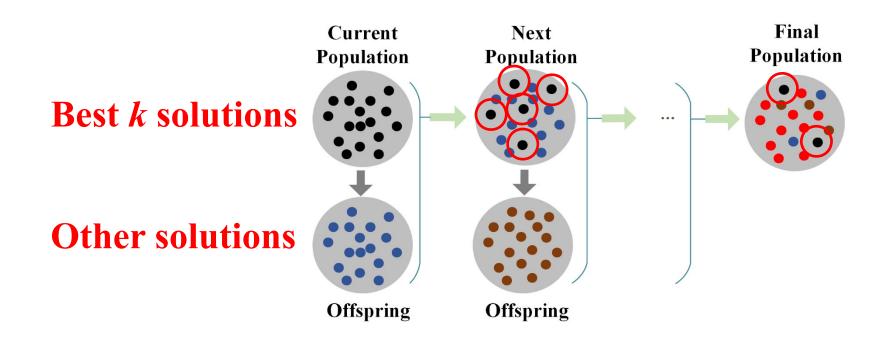


Generation Update in GA (Genetic Algorithms)

Elite Strategy (Elitist Strategy)

Next population with μ solutions:

- k best solutions in the current population (elite)
- (μk) new solutions (offspring)



Choose the best from randomly selected *K* solutions. (*K*: Tournament Size)

Iterate the following steps:

- Step 1: Randomly select K solutions from the current population (with duplication or without duplication).
- Step 2: Select the best solution among the *K* solutions.
- ==> Selection probability of each solution depends on its rank (and the value of K).

Lab Session Task 1:

- 1. Calculate the selection probability of the worst solution for the case of N = 10 (population size) and K = 2 (tournament size) "with duplication".
- 2. Calculate the selection probability of the *i*-th worst solution for the case of N = 10 (population size) and K = 2 (tournament size) "with duplication".
- 3. Calculate the selection probability of the *i*-th worst solution for the case of N = 10 (population size) and K = 3 (tournament size) "with duplication".

Lab Session Task 2:

In evolutionary computation, which do you think the best generation update mechanism among the following mechanisms. Explain your idea with clear reasons.

```
(1, 1)ES: Random search (1+1)ES: Fast move local search (1+\lambda)ES: Local search (\lambda>1 such as \lambda=5, 10, 50, 50, ...) (\mu+1)ES: Steady state algorithm (\mu>1 such as \lambda=5, 10, 50, ...) (\mu, \mu)ES: The simplest model of generation update (\mu>1) (\mu+\mu)ES: The standard model of generation update (\mu>1) (\mu, \lambda)ES: The standard comma strategy (\lambda>\mu>1 such as (\mu, \lambda) = (10, 50), (50, 200), (100, 500), ...)
```