

- Evolutionary algorithms: Origins
- Evolutionary algorithms: Components
- Evolutionary algorithms: Applications





Heuristic Search and Evolutionary Algorithms

Lecture 6: Evolutionary Algorithms – Representation, Mutation and Recombination

Chao Qian (钱超)

Associate Professor, Nanjing University, China

Email: qianc@nju.edu.cn Homepage: http://www.lamda.nju.edu.cn/qianc/

Representation and variation operators

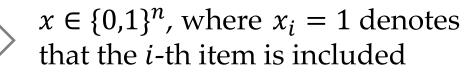
- The first stage of applying evolutionary algorithms is to decide a right representation for the problem
 - Binary representation
 - Integer representation
 - Real-valued representation
 - Permutation representation
 - Tree representation
- Variation operators depend on the chosen representation
 - Mutation
 - Recombination

Binary representation

• Genotype space: $\{0,1\}^n$

Knapsack problem with *n* items





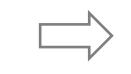
$$\arg \max_{x \in \{0,1,\dots,15\}} x^2$$

 $x \in \{0,1\}^4$, and the corresponding integer is $\sum_{i=1}^4 x_i 2^{4-i}$

Binary representation

• Genotype space: $\{0,1\}^n$

$$\arg \max_{x \in \{0,1,\dots,15\}} x^2$$



Standard binary coding 7 is represented by 0111 8 is represented by 1000 9 is represented by 1001

$x \in \{0,1\}^4$, and the corresponding integer is $\sum_{i=1}^4 x_i 2^{4-i}$

The Hamming distance between consecutive integers can be very large

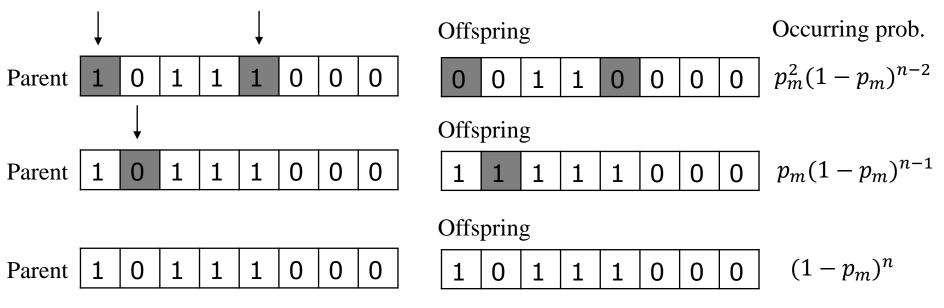
Gray coding

0	0000	4	0110	8	1100	12	1010
1	0001	5	0111	9	1101	13	1011
2	0011	6	0101	10	1111	14	1001
3	0010	7	0100	11	1110	15	1000

The Hamming distance between consecutive integers is always 1

Binary representation: Mutation

• Bit-wise mutation: flip each bit independently with prob. p_m



The common setting of p_m is 1/n, where *n* is the length of the binary string

• One-bit mutation: flip a randomly chosen bit

For the above mutation behaviors, the occurring prob. are 0, 1/n and 0

Binary representation: Mutation

• Bit-wise mutation: flip each bit independently with prob. p_m

The number of flipped bits is a random variable, denoted by *X*

$$\mathbf{P}(X=k) = \binom{n}{k} p_m^k (1-p_m)^{n-k}$$

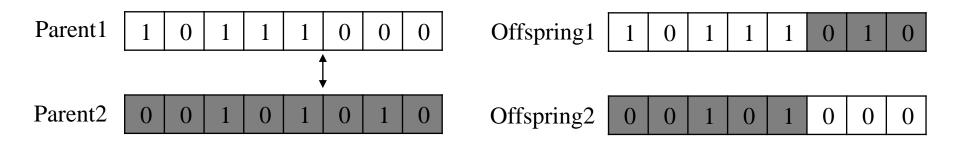
X satisfies the binomial distribution $B(n, p_m)$

The expected number of flipped bits is $E[X] = np_m$, which is 1 for $p_m = 1/n$

• One-bit mutation: flip a randomly chosen bit The number of flipped bits is 1

Binary representation: Recombination

- One-point crossover
 - ≻ Choose a random number $r \in \{1, 2, ..., n 1\}$
 - Split both parents at this point
 - Create two offspring by exchanging the tails

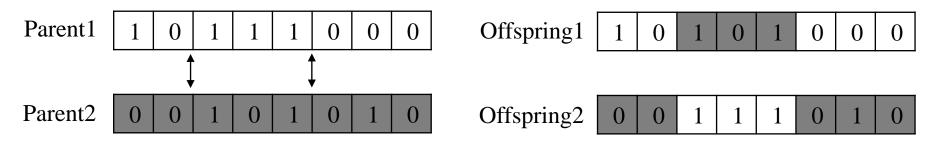


The occurring probability is 1/(n-1)

Binary representation: Recombination

- *m*-point crossover
 - > Choose *m* crossover points from $\{1, 2, ..., n 1\}$
 - Split both parents along these points
 - Create two offspring by taking alternative segments

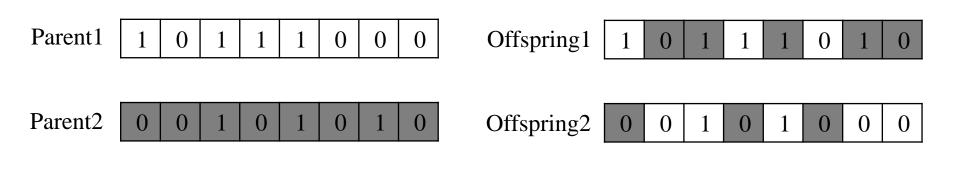
2-point crossover



The occurring probability is 2/((n-1)(n-2))

Binary representation: Recombination

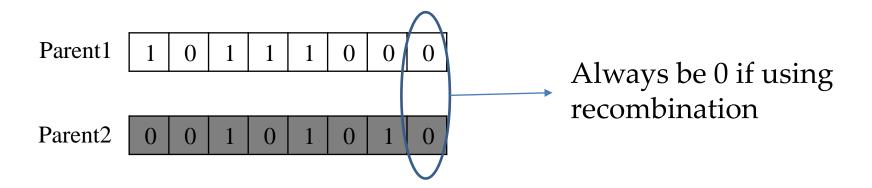
- Uniform crossover
 - For the first offspring, each gene is inherited from the first parent with probability *p* independently; otherwise from the second parent
 - The second offspring is created using the inverse mapping
 The common setting of p is 1/2



The occurring probability is $p^3(1-p)^{n-3}$

Binary representation: Mutation and recombination

• Only mutation can introduce new information



- Only recombination can combine information from two parents
 - One-point and *m*-point crossover: more likely to keep together genes that are near each other
 - Uniform crossover: no positional bias

- Genotype space: N^{*n*}, where N denotes the integer
- Mutation: mutate each gene independently with probability *p_m*

 - Creep mutation: add a small value, which is sampled from a distribution
 Ordinal

attributes

• **Recombination:** same as for binary representation

Real-valued representation: Mutation

- Genotype space: \mathbb{R}^n , where \mathbb{R} denotes the real-number
- Mutation

$$\mathbf{x} = (x_1, \dots, x_n) \rightarrow \mathbf{x}' = (x_1', \dots, x_n')$$
, where $x_i, x_i' \in [lb_i, ub_i]$

Uniform mutation: for each x_i, with prob. p_m, change it to a value drawn uniformly randomly from [lb_i, ub_i]

$$x'_{i} = \begin{cases} x_{i} & \text{with prob. } 1 - p_{m} \\ U(lb_{i}, ub_{i}) & \text{otherwise} \end{cases}$$

Nonuniform mutation: for each x_i , add a value drawn randomly from a Gaussian distribution $N(0, \sigma^2)$

 σ : mutation step size

$$x'_i = x_i + \delta$$
, where $\delta \sim N(0, \sigma^2)$

Real-valued representation: Nonuniform mutation

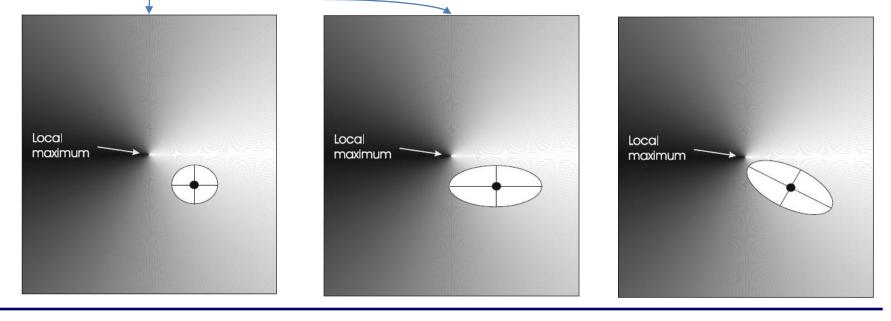
• Uncorrelated mutation with one step size σ :

$$x_i' = x_i + \sigma \cdot N_i(0,1)$$

• Uncorrelated mutation with *n* step sizes:

$$C x_i' = x_i + \sigma_i \cdot N_i(0,1)$$





Real-valued representation: Nonuniform mutation

• Correlated mutation:

$$\delta \sim N(\mathbf{0}, \mathbf{I}) \xrightarrow{\text{scaling}} \mathbf{S}\delta = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \delta \xrightarrow{\text{rotation}} \mathbf{R}S\delta = \begin{bmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{bmatrix} \mathbf{S}\delta$$

bivariate standard normal distribution
$$(\mathbf{Cov}(\delta') = \mathbf{R}S \operatorname{Cov}(\delta) (\mathbf{R}S)^{\mathrm{T}} = \begin{bmatrix} a^{2}\cos^{2}(\alpha) + b^{2}\sin^{2}(\alpha) & (a^{2} - b^{2})\sin(2\alpha)/2 \\ (a^{2} - b^{2})\sin(2\alpha)/2 & a^{2}\sin^{2}(\alpha) + b^{2}\cos^{2}(\alpha) \end{bmatrix}$$
$$\begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix}$$
$$\tan(2\alpha) = 2c_{12}/(c_{11} - c_{22})$$

Generalization:
$$c_{ii} = \sigma_i^2$$
, $c_{ij,i\neq j} = (\sigma_i^2 - \sigma_j^2) \tan(2\alpha_{ij})/2$

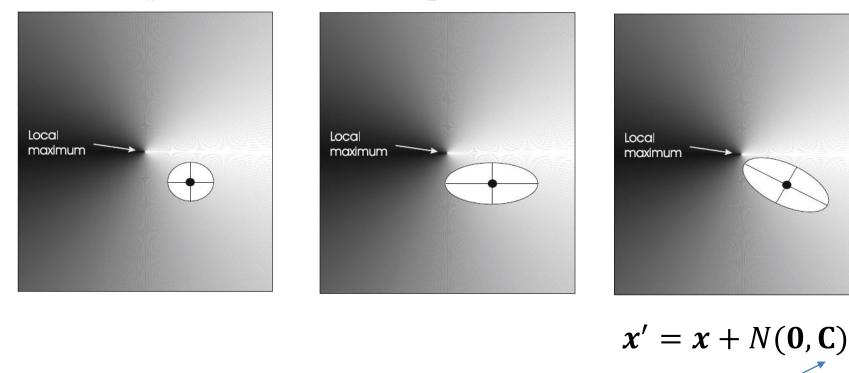
rotation angle for the *i*-th and *j*-th dimension

Real-valued representation: Nonuniform mutation

Uncorrelated mutation with one step size σ

Uncorrelated mutation with *n* step sizes

Correlated mutation



$$c_{ii} = \sigma_i^2$$
, $c_{ij,i\neq j} = (\sigma_i^2 - \sigma_j^2) \tan(2\alpha_{ij})/2$

- Self-adaptive mutation: Mutation step size σ is not set by user but coevolves with solution
- For example, the genotype is now $(x_1, ..., x_n, \sigma)$ Self-adaptation $\sigma \rightarrow \sigma'$ $x'_i = x_i + \sigma' \cdot N_i(0, 1)$
 - The fitness of x' can be used to measure the goodness of both the offspring x' and the mutation step size σ'
 - Why? Under different circumstances, different step sizes will behave differently

• Uncorrelated mutation with one step size σ :

$$(x_{1}, \dots, x_{n}, \sigma) \rightarrow (x'_{1}, \dots, x'_{n}, \sigma')$$
Self-adaptation $\sigma' = \sigma \cdot e^{\tau \cdot N(0,1)}$

$$x'_{i} = x_{i} + \sigma' \cdot N_{i}(0,1)$$

$$Typically \tau \propto 1/\sqrt{n}$$

$$\sigma' < \epsilon_{0} \Rightarrow \sigma' = \epsilon_{0}$$

- Satisfy these requirements:
 - Smaller modifications occur more often than larger ones
 - Greater than 0
 - The median is 1
 - Neural on average: equal prob. of drawing a value and its reciprocal

• Uncorrelated mutation with *n* step sizes:

$$(x_{1}, \dots, x_{n}, \sigma_{1}, \dots, \sigma_{n}) \rightarrow (x'_{1}, \dots, x'_{n}, \sigma'_{1}, \dots, \sigma'_{n})$$
Self-adaptation $\sigma'_{i} = \sigma_{i} \cdot e^{\tau' \cdot N(0,1) + \tau \cdot N_{i}(0,1)}$

$$\begin{cases} \tau' \propto \frac{1}{\sqrt{2n}}, \tau \propto \frac{1}{\sqrt{2\sqrt{n}}} \\ \sigma'_{i} < \epsilon_{0} \Rightarrow \sigma'_{i} = \epsilon_{0} \end{cases}$$

e^{τ'·N(0,1)}: overall change; *e^{τ·N_i(0,1)}*: coordinate-wise change
 The distribution is still lognormal, satisfying those requirements

• Correlated mutation:

$$\mathbf{x}' = \mathbf{x} + N(\mathbf{0}, \mathbf{C}')$$

$$\sigma_i' < \epsilon_0 \Rightarrow \sigma_i' = \epsilon_0$$

$$|\alpha_j'| > \pi \Rightarrow \alpha_j' =$$

$$\alpha_j' - 2\pi \cdot sign(\alpha_j')$$

Real-valued representation: Recombination

- **Discrete recombination:** Same as for binary representation, e.g., *m*-point crossover and uniform crossover
- Arithmetic recombination: Create offspring "between" parents

$$z_i = (1 - \alpha)x_i + \alpha y_i$$
, where $\alpha \in [0, 1]$

• Blend recombination: Create offspring in a larger region $z_i = (1 - \gamma)x_i + \gamma y_i$, where $\gamma = (1 + 2\alpha)u - \alpha$, $u \in [0,1]$ Real-valued representation: Arithmetic recombination

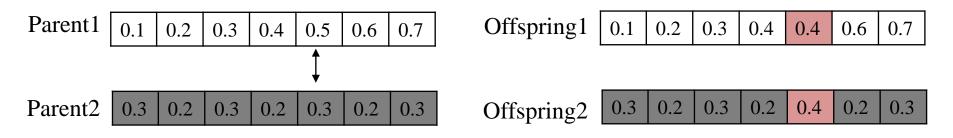
• Single arithmetic recombination:

$$(x_1, \dots, x_n) \qquad (y_1, \dots, y_n)$$

Select a random k
$$(x_1, \dots, x_{k-1}, \alpha y_k + (1 - \alpha) x_k, x_{k+1}, \dots, x_n)$$

$$(y_1, \dots, y_{k-1}, \alpha x_k + (1 - \alpha) y_k, y_{k+1}, \dots, y_n)$$

Example with $\alpha = 0.5$



Real-valued representation: Arithmetic recombination

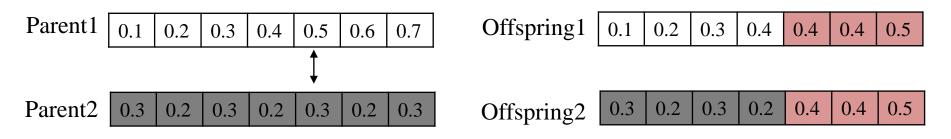
• Simple arithmetic recombination:

$$(x_1, \dots, x_n) \qquad (y_1, \dots, y_n)$$

Select a random k
$$(x_1, \dots, x_{k-1}, \alpha y_k + (1 - \alpha) x_k, \dots, \alpha y_n + (1 - \alpha) x_n)$$

$$(y_1, \dots, y_{k-1}, \alpha x_k + (1 - \alpha) y_k, \dots, \alpha x_n + (1 - \alpha) y_n)$$

Example with $\alpha = 0.5$



Real-valued representation: Arithmetic recombination

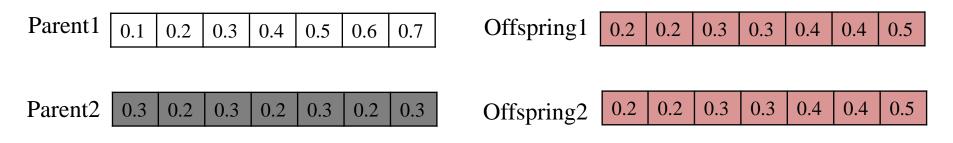
• Whole arithmetic recombination:

$$(x_{1}, ..., x_{n}) \qquad (y_{1}, ..., y_{n})$$

$$(\alpha y_{1} + (1 - \alpha)x_{1}, ..., \alpha y_{n} + (1 - \alpha)x_{n})$$

$$(\alpha x_{1} + (1 - \alpha)y_{1}, ..., \alpha x_{n} + (1 - \alpha)y_{n})$$

Example with $\alpha = 0.5$



Real-valued representation: Blend recombination

• Blend recombination: Create offspring in a larger region

$$z_{i} = (1 - \gamma)x_{i} + \gamma y_{i}, \text{ where } \gamma = (1 + 2\alpha)u - \alpha, u \in [0,1]$$

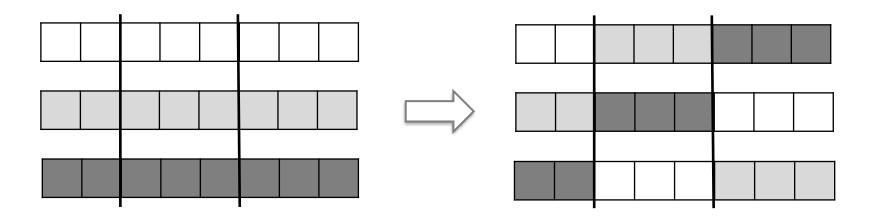
$$Q_{i} = x_{i} + (y_{i} - x_{i})(1 + 2\alpha)u - \alpha(y_{i} - x_{i})$$

$$Q_{i}$$

$$u \sim U(0,1) \Rightarrow z_{i} \sim U(x_{i} - \alpha d_{i}, y_{i} + \alpha d_{i})$$
How about $z_{i} = (1 - \gamma)y_{i} + \gamma x_{i}$?

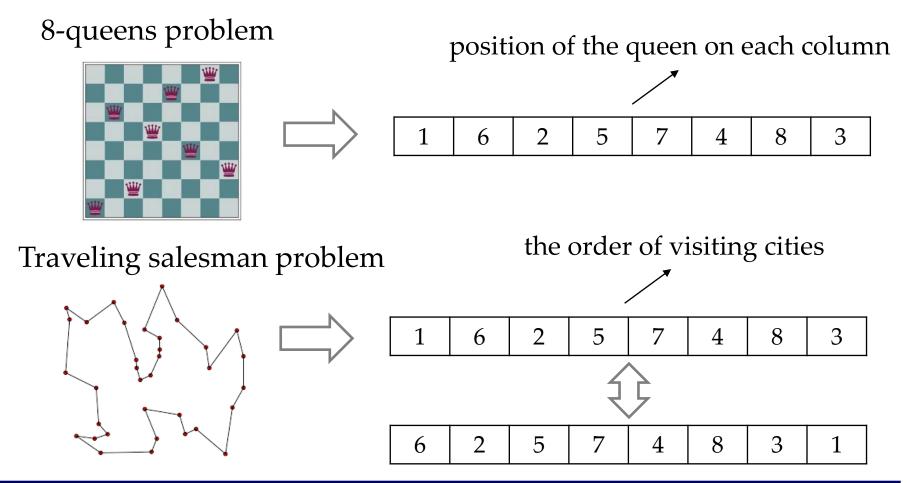
Multi-parent recombination

- For example, diagonal crossover for *m* parents:
 - > Choose m 1 crossover points randomly
 - Compose *m* offspring from the segments of the parents in along a "diagonal", wrapping around



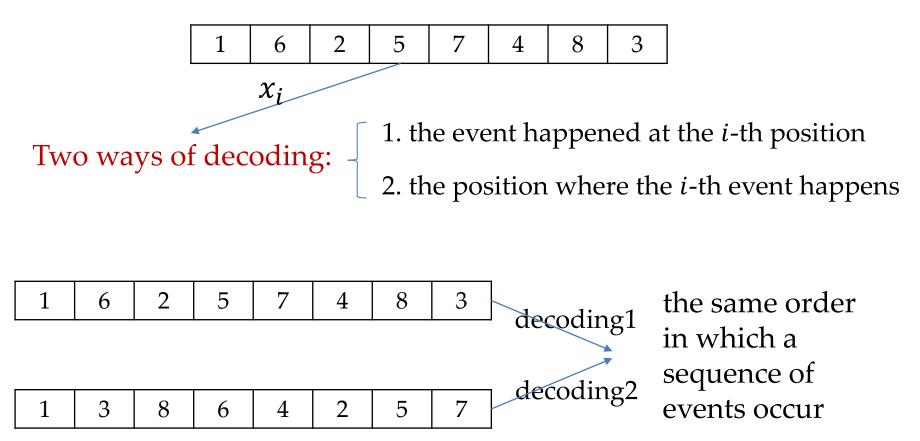
Permutation representation

• Genotype space: a permutation of a fixed set of values



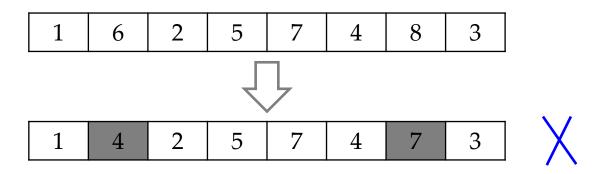
Permutation representation

• Genotype space: a permutation of a fixed set of values



Permutation representation: Mutation

• Mutation operators for binary, integer and real-valued representation will lead to inadmissible solutions

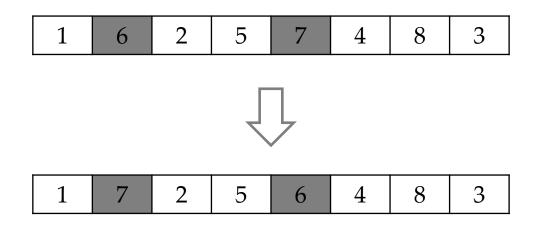


- Common mutation for permutation representation
 - Swap mutation
 - Insert mutation
 - Scramble mutation
 - Inversion mutation

The mutation probability now reflects the probability of applying mutation, rather than altering a single gene

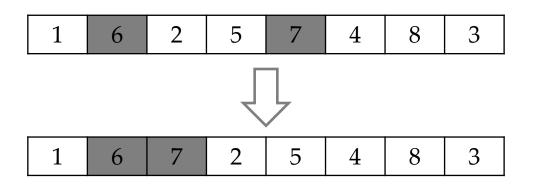
Permutation representation: Swap mutation

- Swap mutation:
 - Select two positions randomly
 - Swap their values



Permutation representation: Insert mutation

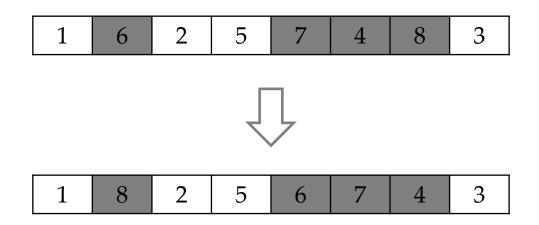
- Insert mutation:
 - Select two positions randomly
 - Move the second next to the first
 - Shift the rest along to accommodate



Preserve most of the order and the adjacency information

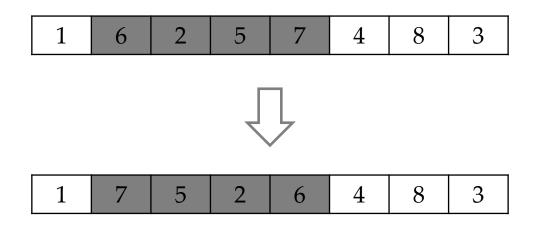
Permutation representation: Scramble mutation

- Scramble mutation:
 - Select a subset of positions randomly
 - Rearrange their values randomly



Permutation representation: Inversion mutation

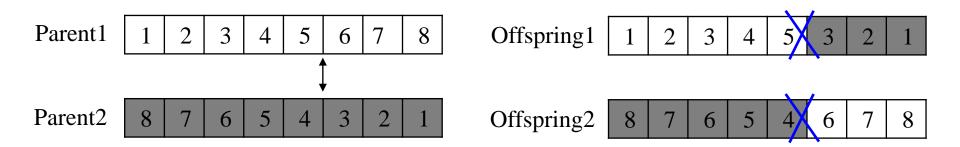
- Inversion mutation:
 - Select two positions randomly
 - Invert the values between them



Preserve most adjacency information (only breaks two links), but disruptive of order information

Permutation representation: Recombination

• Recombination operators for binary, integer and real-valued representation will lead to inadmissible solutions



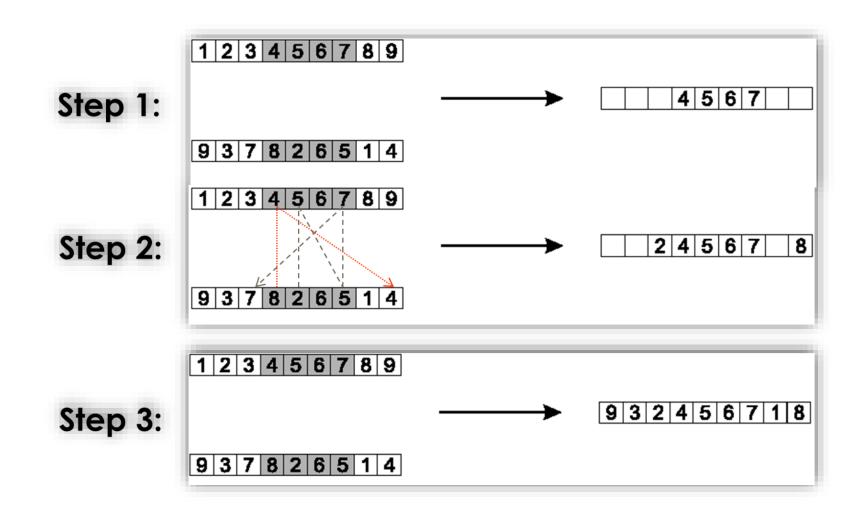
- Common recombination for permutation representation
 - Partially mapped crossover
 - Edge crossover
 - Order crossover
 - Cycle crossover

combine order or

 adjacency information from the two parents Permutation representation: Partially mapped crossover

- Partially mapped crossover:
 - 1. Choose two crossover points randomly, and copy the segment between them from parent P1 into the first offspring
 - 2. Starting from the first crossover point, look for elements in that segment of P2 that have not been copied
 - 3. For each of these *i*, look in the offspring to see what element *j* has been copied in its place from P1
 - 4. Place *i* into the position occupied by *j* in P2, since we know that we will not be putting *j* there (as is already in offspring)
 - 5. If the place occupied by *j* in P2 has already been filled in the offspring by *k*, put *i* in the position occupied by *k* in P2
 - 6. Having dealt with the elements from the crossover segment, the rest of the first offspring can be filled from P2
 - 7. Create the second offspring analogously with parental roles reversed

Permutation representation: Partially mapped crossover



Permutation representation: Edge crossover

• First step, construct a table listing which edges are present in the two parents; if an edge is common, mark with a +

Permutation representation: Edge crossover

- Edge crossover: After constructing the edge table,
 - 1. Pick an initial element, entry, at random and put it in the offspring
 - 2. Set the variable current element = entry
 - 3. Remove all references to current element from the table
 - 4. Examine the list for current element:
 - ➢ If there is a common edge, pick that to be next element
 - Otherwise, pick the entry in the list which itself has the shortest list
 - ➢ Ties are split at random
 - 5. In the case of reaching an empty list: a new element is chosen at random

Permutation representation: Edge crossover

Element	Edges	Element	Edges
1	$2,\!5,\!4,\!9$	6	2,5+,7
2	$1,\!3,\!6,\!8$	7	3,6,8+
3	$2,\!4,\!7,\!9$	8	2,7+,9
4	$1,\!3,\!5,\!9$	9	1,3,4,8
5	1,4,6+		

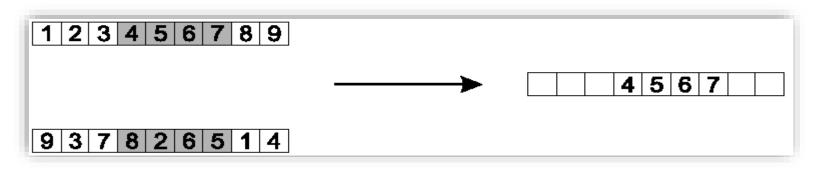
Choices	Element	Reason	Partial
	selected		result
All	1	Random	[1]
2,5,4,9	5	Shortest list	[1 5]
4,6	6	Common edge	[1 5 6]
2,7	2	Random choice (both have two items in list)	[1 5 6 2]
3,8	8	Shortest list	$[1 \ 5 \ 6 \ 2 \ 8]$
7,9	7	Common edge	[156287]
3	3	Only item in list	[1 5 6 2 8 7 3]
4,9	9	Random choice	[15628739]
4	4	Last element	[156287394]

Permutation representation: Order crossover

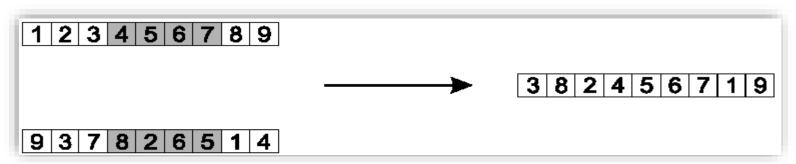
- Order crossover:
 - 1. Choose two crossover points randomly
 - 2. Copy the segment between them from the first parent to the first offspring
 - 3. Copy the numbers that are not in the segment, to the first offspring:
 - starting right from the second crossover point
 - using the order of the second parent
 - > and wrapping around at the end
 - 4. Create the second offspring in an analogous manner, with the parent roles inversed

Permutation representation: Order crossover

1. Copy a randomly selected segment from the first parent



2. Copy the remaining numbers into the offspring in the order that they appear in the second parent



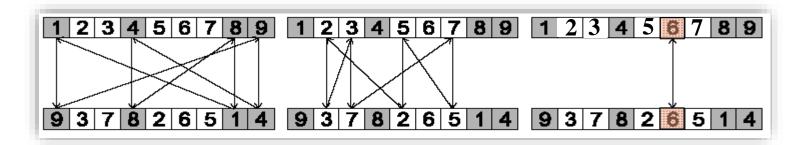
Permutation representation: Cycle crossover

• Cycle crossover:

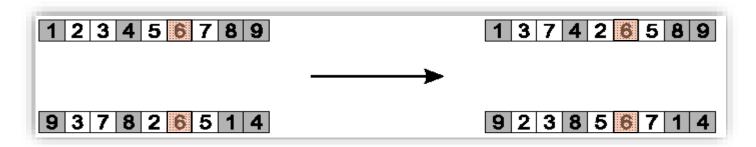
- 1. Divide the alleles into cycles
 - Start with the first unused position and allele of P1
 - Look at the allele in the same position in P2
 - ➢ Go to the position with the same allele in P1
 - Add this allele to the cycle
 - Repeat steps 2-4 until arriving at the first allele of P1
- 2. Create the offspring by selecting alternate cycles from each parent

Permutation representation: Cycle crossover

1. Identify cycles



2. Copy alternate cycles into offspring

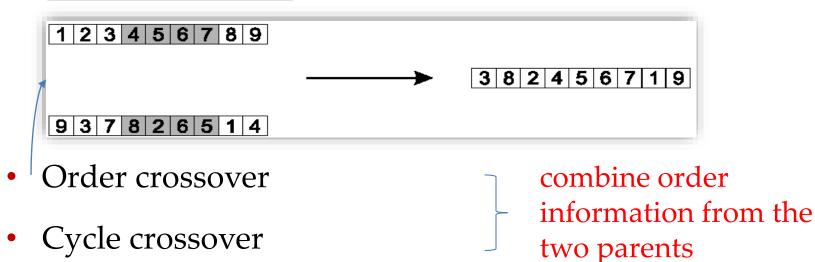


Permutation representation: Recombination

- Partially mapped crossover
- Edge crossover

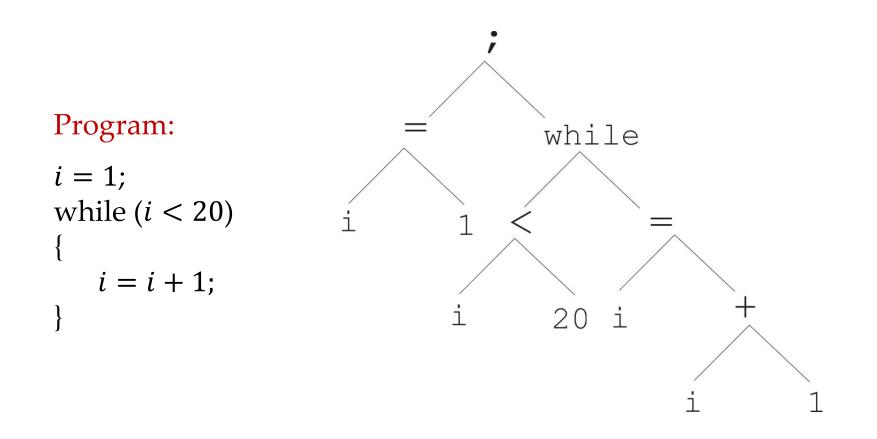
	Element	Edges	Element	Edges
	1	2,5,4,9	6	2,5+,7
1	2	1,3,6,8	7	3,6,8+
	3	2,4,7,9	8	2,7+, 9
	4	$1,\!3,\!5,\!9$	9	$1,\!3,\!4,\!8$
	5	1,4,6+		

combine adjacency information from the two parents



Tree representation

• Genotype space: a tree

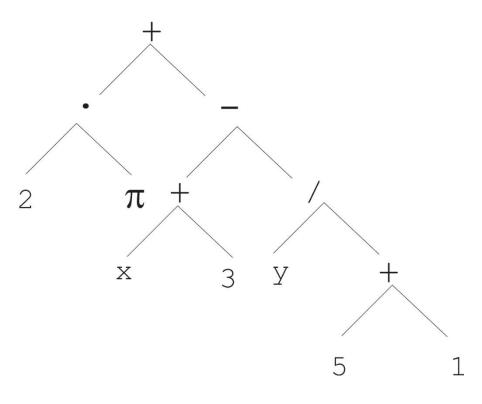


Tree representation

• Genotype space: a tree

Arithmetic formula:

$$2 \cdot \pi + \left((x+3) - \frac{y}{5+1} \right)$$



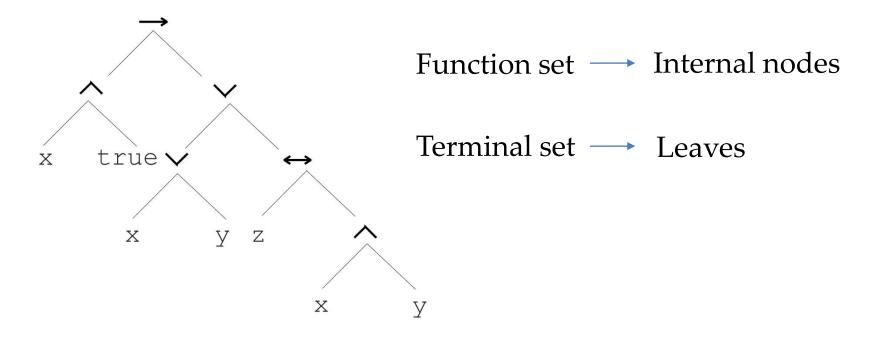
Tree representation

• Genotype space: a tree

Logical formula:

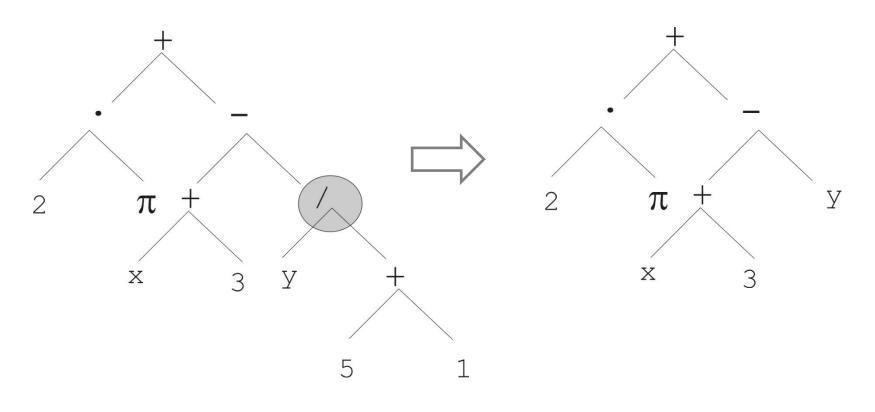
Variable structure

 $(x \land true) \rightarrow ((x \lor y) \lor (z \leftrightarrow (x \land y)))$



Tree representation: Mutation

• Mutation: replace randomly chosen subtree by randomly generated tree



Tree representation: Recombination

 Recombination: exchange two randomly chosen subtrees among the parents

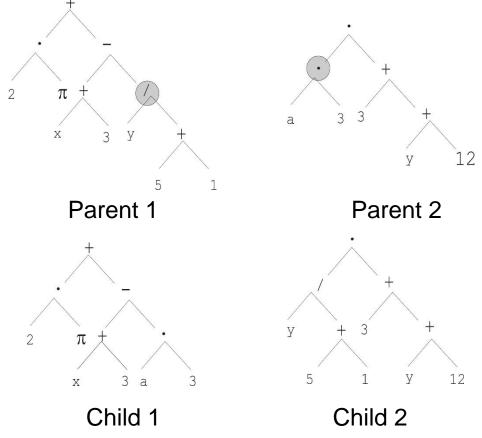
Assume uniform selection within each parent for exchanging

1

9

13

The probability:



- Decade long debate: which one is better
 - Evolutionary programming: originally without recombination
 - Genetic programming: originally without mutation
- Recombination is explorative, which can make a big jump to an area somewhere "in between" two (parent) areas
- Mutation is exploitative, which creates random small diversions, thereby staying near (in the area of) the parent
- Now, it is good to have both in general

Summary

- Binary representation
- Integer representation
- Real-valued representation
- Permutation representation
- Tree representation

RepresentationMutationRecombination

• A. E. Eiben and J. E. Smith. Introduction to Evolutionary Computing. Chapter 4.