# **Evolutionary Computing**



#### Chapter 4: Representation, Mutation, and Recombination

- Role of representation and variation operators.
- Most common representation of genomes:
  - Binary;
  - Integer;
  - Real-Valued or Floating-Point;
  - Permutation;
  - Tree.

# Scheme of an EA: General scheme of EAs



Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

# Role of representation and variation operators

- First stage of building an EA and most difficult one: choose *right* representation for the problem
- Variation operators: mutation and crossover
- Type of variation operators needed depends on chosen representation

#### • TSP problem

- What are possible representations?



# Binary Representation: Mutation

- Alter each gene independently with a probability p<sub>m</sub>
- p<sub>m</sub> is called the mutation rate
  - Typically between 1/pop\_size and 1/ chromosome\_length



child	0	1	0	0	1	0	1	1	0	0	0	1	0	1	1	0	0	1	
-------	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	--

• Mutation can cause variable effect (use gray coding)

# Binary Representation: 1-point crossover

- Choose a random point on the two parents
- Split parents at this crossover point
- Create children by exchanging tails
- P<sub>c</sub> typically in range (0.6, 0.9)



# Binary Representation: Alternative Crossover Operators

- Why do we need other crossover(s)?
- Performance with 1-point crossover depends on the order that variables occur in the representation
  - More likely to keep together genes that are near each other
  - Can never keep together genes from opposite ends of string
  - This is known as Positional Bias
  - Can be exploited if we know about the structure of our problem, but this is not usually the case

# Binary Representation: n-point crossover

- Choose n random crossover points
- Split along those points
- Glue parts, alternating between parents
- Generalisation of 1-point (still some positional bias)



# Binary Representation: Uniform crossover

- Assign 'heads' to one parent, 'tails' to the other
- Flip a coin for each gene of the first child
- Make an inverse copy of the gene for the second child
- Inheritance is independent of position



## Binary Representation: Crossover OR mutation? (1/3)

- Decade long debate: which one is better / necessary / main-background
- Answer (at least, rather wide agreement):
  - it depends on the problem, but
  - in general, it is good to have both
  - both have another role
  - mutation-only-EA is possible, xover-only-EA would not work

Binary Representation: Crossover OR mutation? (2/3)

**Exploration:** Discovering promising areas in the search space, i.e. gaining information on the problem

**Exploitation:** Optimising within a promising area, i.e. using information

There is co-operation AND competition between them

• Crossover is explorative, it makes a *big* jump to an area somewhere "in between" two (parent) areas

• Mutation is exploitative, it creates random *small* diversions, thereby staying near (in the area of ) the parent

# Binary Representation: Crossover OR mutation? (3/3)

- Only crossover can combine information from two parents
- Only mutation can introduce new information (alleles)
- Crossover does not change the allele frequencies of the population (thought experiment: 50% 0's on first bit in the population, ?% after performing n crossovers)
- To hit the optimum you often need a 'lucky' mutation

#### Integer Representation

- Nowadays it is generally accepted that it is better to encode numerical variables directly (integers, floating point variables)
- Some problems naturally have integer variables, e.g. image processing parameters
- Others take categorical values from a fixed set e.g. {blue, green, yellow, pink}
- N-point / uniform crossover operators work
- Extend bit-flipping mutation to make
  - "creep" i.e. more likely to move to similar value
    - Adding a small (positive or negative) value to each gene with probability p
  - Random resetting (esp. categorical variables)
    - With probability  $p_m$  a new value is chosen at random
- Same recombination as for binary representation

#### Real-Valued or Floating-Point Representation

- Many problems occur as real valued problems, e.g. continuous parameter optimisation  $f: \mathcal{R}^n \rightarrow \mathcal{R}$
- Illustration: Ackley's function (often used in EC)

$$f(\mathbf{x}) = -20 \cdot \exp\left(-0.2\sqrt{\frac{1}{n}} \cdot \sum_{i=1}^{n} \mathbf{x}_{i}^{2}\right)$$
$$-\exp\left(\frac{1}{n}\sum_{i=1}^{n} \cos(2\pi \mathbf{x}_{i})\right) + 20 + \mathbf{e}$$

Real-Valued or Floating-Point Representation: Mapping real values on bit strings

 $z \in [x,y] \subseteq \mathscr{R} \text{represented by } \{a_1, \dots, a_L\} \in \{0,1\}^L$ 

- $[x,y] \rightarrow \{0,1\}^{L}$  must be invertible (one phenotype per genotype)
- $\Gamma: \{0,1\}^{L} \rightarrow [x,y]$  defines the representation

$$\Gamma(a_1,...,a_L) = x + \frac{y - x}{2^L - 1} \cdot (\sum_{j=0}^{L-1} a_{L-j} \cdot 2^j) \in [x, y]$$

- Only 2<sup>L</sup> values out of infinite are represented
- L determines possible maximum precision of solution
- High precision → long chromosomes (slow evolution)

Real-Valued or Floating-Point Representation: Uniform Mutation

• General scheme of floating point mutations

$$\overline{x} = \langle x_1, ..., x_l \rangle \longrightarrow \overline{x'} = \langle x'_1, ..., x'_l \rangle$$

$$x_i, x_i' \in \left[ LB_i, UB_i \right]$$

- Uniform Mutation
  - $x'_i$  drawn randomly (uniform) from  $[LB_i, UB_i]$
- Analogous to bit-flipping (binary) or random resetting (integers)

#### Real-Valued or Floating-Point Representation: Nonuniform Mutation

- Non-uniform mutations:
  - Many methods proposed, such as time-varying range of change etc.
  - Most schemes are probabilistic but usually only make a small change to value
  - Most common method is to add random deviate to each variable separately, taken from N(0,  $\sigma$ ) Gaussian distribution and then curtail to range

 $x'_i = x_i + N(0,\sigma)$ 

- Standard deviation  $\sigma$ , *mutation step size*, controls amount of change (2/3 of drawings will lie in range (-  $\sigma$  to +  $\sigma$ ))

Real-Valued or Floating-Point Representation: Self-Adaptive Mutation (1/2)

- Step-sizes are included in the genome and undergo variation and selection themselves:  $\langle x_1,...,x_n, \sigma \rangle$
- Mutation step size is not set by user but coevolves with solution
- Different mutation strategies may be appropriate in different stages of the evolutionary search process.

Real-Valued or Floating-Point Representation: Self-Adaptive Mutation (2/2)

- Mutate  $\sigma$  first
- Net mutation effect:  $\langle x, \sigma \rangle \rightarrow \langle x', \sigma' \rangle$
- Order is important:
  - first  $\sigma \rightarrow \sigma'$  (see later how)
  - then  $x \rightarrow x' = x + N(0,\sigma')$
- Rationale: new  $\langle \ x' \ , \sigma' \ \rangle$  is evaluated twice
  - Primary: x' is good if f(x') is good
  - Secondary:  $\sigma$ ' is good if the x' it created is good
- Reversing mutation order this would not work

Real-Valued or Floating-Point Representation: Uncorrelated mutation with one  $\sigma$  (1/2)

• Chromosomes:  $\langle x_1, ..., x_n, \sigma \rangle$ 

$$-\sigma' = \sigma \cdot \exp(\tau \cdot \mathsf{N}(0,1))$$

- $x'_i = x_i + \sigma' \cdot N_i(0,1)$
- Typically the "learning rate"  $\tau \propto$  1/  $n^{\frac{1}{2}}$
- And we have a boundary rule  $\sigma' < \varepsilon_0 \Rightarrow \sigma' = \varepsilon_0$



#### Circle: mutants having the same chance to be created

Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

Real-Valued or Floating-Point Representation: Uncorrelated mutation with n  $\sigma$ 's (1/2)

- Chromosomes:  $\langle x_1, ..., x_n, \sigma_1, ..., \sigma_n \rangle$ 
  - $\sigma'_{i} = \sigma_{i} \cdot \exp(\tau' \cdot N(0,1) + \tau \cdot N_{i}(0,1))$
  - $x'_{i} = x_{i} + \sigma'_{i} \cdot N_{i} (0,1)$
- Two learning rate parameters:
  - $-\tau$ ' overall learning rate
  - $-\tau$  coordinate wise learning rate
- $\tau' \propto 1/(2 n)^{\frac{1}{2}}$  and  $\tau \propto 1/(2 n^{\frac{1}{2}})^{\frac{1}{2}}$
- Boundary rule:  $\sigma_i' < \epsilon_0 \Rightarrow \sigma_i' = \epsilon_0$

Real-Valued or Floating-Point Representation: Uncorrelated mutation with n  $\sigma$ 's (2/2)

Mutants with equal likelihood



Ellipse: mutants having the same chance to be created

Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

Real-Valued or Floating-Point Representation: Correlated mutations (1/3)

- Chromosomes:  $\langle x_1, ..., x_n, \sigma_1, ..., \sigma_n, \alpha_1, ..., \alpha_k \rangle$ where k = n • (n-1)/2
- Covariance matrix C is defined as:

$$- c_{ii} = \sigma_i^2$$

- $-c_{ij} = 0$  if i and j are not correlated
- $c_{ij} = \frac{1}{2} \cdot (\sigma_i^2 \sigma_j^2) \cdot tan(2 \alpha_{ij})$  if i and j are correlated
- Note the numbering / indices of the  $\alpha\mbox{`s}$

Real-Valued or Floating-Point Representation: Correlated mutations (2/3)

The mutation mechanism is then:

- $\sigma'_i = \sigma_i \cdot \exp(\tau' \cdot N(0,1) + \tau \cdot N_i(0,1))$
- $\alpha'_{j} = \alpha_{j} + \beta \cdot N(0,1)$
- x' = x + N(0,C')
  - $\textbf{\textit{x}}$  stands for the vector  $\langle \ \textbf{x}_1, \ldots, \textbf{x}_n \ \rangle$
  - C' is the covariance matrix C after mutation of the  $\alpha$  values
- $\tau \propto 1/(2 n)^{\frac{1}{2}}$  and  $\tau \propto 1/(2 n^{\frac{1}{2}})^{\frac{1}{2}}$  and  $\beta \approx 5^{\circ}$
- $\sigma_i' < \epsilon_0 \Rightarrow \sigma_i' = \epsilon_0$  and
- $|\alpha'_{j}| > \pi \Rightarrow \alpha'_{j} = \alpha'_{j} 2 \pi \operatorname{sign}(\alpha'_{j})$
- NB Covariance Matrix Adaptation Evolution Strategy (CMA-ES) is probably the best EA for numerical optimisation, cf. CEC-2005 competition

#### Real-Valued or Floating-Point Representation: Correlated mutations (3/3)

Mutants with equal likelihood



#### Ellipse: mutants having the same chance to be created

Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

#### Real-Valued or Floating-Point Representation: Crossover operators

- Discrete:
  - each allele value in offspring z comes from one of its parents (x,y) with equal probability:  $z_i = x_i$  or  $y_i$
  - Could use n-point or uniform
- Intermediate
  - exploits idea of creating children "between" parents (hence a.k.a. *arithmetic* recombination)
  - $-z_i = \alpha x_i + (1 \alpha) y_i$  where  $\alpha : 0 \le \alpha \le 1$ .
  - The parameter  $\alpha$  can be:
    - constant: uniform arithmetical crossover
    - variable (e.g. depend on the age of the population)
    - picked at random every time

Real-Valued or Floating-Point Representation: Single arithmetic crossover

- Parents:  $\langle x_1, \dots, x_n \rangle$  and  $\langle y_1, \dots, y_n \rangle$
- Pick a single gene (k) at random,
- child<sub>1</sub> is:

$$\langle x_1, \dots, x_k, \boldsymbol{\alpha} \cdot \boldsymbol{y}_k + (1 - \boldsymbol{\alpha}) \cdot \boldsymbol{x}_k, \dots, \boldsymbol{x}_n \rangle$$

• Reverse for other child. e.g. with  $\alpha = 0.5$ 



Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

Real-Valued or Floating-Point Representation: Simple arithmetic crossover

- Parents:  $\langle x_1, ..., x_n \rangle$  and  $\langle y_1, ..., y_n \rangle$
- Pick a random gene (k) after this point mix values
- child<sub>1</sub> is:

$$\langle x_1, \dots, x_k, \alpha \cdot y_{k+1} + (1-\alpha) \cdot x_{k+1}, \dots, \alpha \cdot y_n + (1-\alpha) \cdot x_n \rangle$$

• reverse for other child. e.g. with  $\alpha = 0.5$ 



Real-Valued or Floating-Point Representation: Whole arithmetic crossover

- Most commonly used
- Parents:  $\langle x_1, \dots, x_n \; \rangle \; and \; \langle y_1, \dots, y_n \rangle$
- Child<sub>1</sub> is:  $a \cdot \overline{x} + (1-a) \cdot \overline{y}$
- reverse for other child. e.g. with  $\alpha = 0.5$

0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9

0.2 0.2 0.3 0.3 0.4 0.4 0.5 0.5 0.6

0.3 0.2 0.3 0.2 0.3 0.2 0.3 0.2 0.3

0.2 0.2 0.3 0.3 0.4 0.4 0.5 0.5 0.6

Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

#### Real-Valued or Floating-Point Representation: Blend Crossover

- Parents:  $\langle x_1, ..., x_n \rangle$  and  $\langle y_1, ..., y_n \rangle$
- Assume  $x_i < y_i$
- $d_i = y_i x_i$
- Random sample  $z_i = [x_i \alpha d_i, x_i + \alpha d_i]$
- Original authors had best results with  $\alpha = 0.5$

#### Real-Valued or Floating-Point Representation: Overview different possible offspring



- Single arithmetic:
- $\{S_1, S_2, S_3, S_4\}$
- Simple arithmetic / whole arithmetic:
- inner box (w = alpha 0.5)
- Blend crossover:
- outer box

#### Real-Valued or Floating-Point Representation: Multi-parent recombination

- Recall that we are not constricted by the practicalities of nature
- Noting that mutation uses n = 1 parent, and "traditional" crossover n = 2, the extension to n > 2 is natural to examine
- Been around since 1960s, still rare but studies indicate useful

Real-Valued or Floating-Point Representation: Multi-parent recombination, type 1

- Idea: segment and recombine parents
- Example: diagonal crossover for *n* parents:
  - Choose *n-1* crossover points (same in each parent)
  - Compose n children from the segments of the parents in along a "diagonal", wrapping around



Multiple children

• This operator generalises 1-point crossover

Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

Real-Valued or Floating-Point Representation: Multi-parent recombination, type 2

- Idea: arithmetical combination of (real valued) alleles
- Example: arithmetic crossover for *n* parents:
  - *i*-th allele in child is the average of the parents' *i*-th alleles
- Creates center of mass as child
- Odd in genetic algorithms, long known and used in evolution strategies

#### **Permutation Representations**

- Ordering/sequencing problems form a special type
- Task is (or can be solved by) arranging some objects in a certain order
  - Example: production scheduling: important thing is which elements are scheduled before others (order)
  - Example: Travelling Salesman Problem (TSP) : important thing is which elements occur next to each other (<u>adjacency</u>)
- These problems are generally expressed as a permutation:
  - if there are *n* variables then the representation is as a list of *n* integers, each of which occurs exactly once

# Permutation Representation: TSP example

- Problem:
  - Given n cities
  - Find a complete tour with minimal length
- Encoding:
  - Label the cities 1, 2, ... , *n*
  - One complete tour is one permutation (e.g. for n =4 [1,2,3,4], [3,4,2,1] are OK)
- Search space is BIG: for 30 cities there are 30! ≈ 10<sup>32</sup> possible tours



# Permutation Representations: Mutation

- Normal mutation operators lead to inadmissible solutions
  - e.g. bit-wise mutation: let gene *i* have value *j*
  - changing to some other value k would mean that k occurred twice and j no longer occurred
- Therefore must change at least two values
- Mutation parameter now reflects the probability that some operator is applied once to the whole string, rather than individually in each position

#### Permutation Representations: Swap mutation

• Pick two alleles at random and swap their positions



1 5 3 4 2 6 7 8 9

Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

#### Permutation Representations: Insert Mutation

- Pick two allele values at random
- Move the second to follow the first, shifting the rest along to accommodate
- Note that this preserves most of the order and the adjacency information

1 2 3 4 5 6 7 8 9



#### Permutation Representations: Scramble mutation

- Pick a subset of genes at random
- Randomly rearrange the alleles in those positions

#### 1 2 3 4 5 6 7 8 9 **1** 3 5 4 2 6 7 8 9

#### Permutation Representations: Inversion mutation

- Pick two alleles at random and then invert the substring between them.
- Preserves most adjacency information (only breaks two links) but disruptive of order information

Permutation Representations: Crossover operators

 "Normal" crossover operators will often lead to inadmissible solutions



 Many specialised operators have been devised which focus on combining order or adjacency information from the two parents

# Permutation Representations: Order 1 crossover (1/2)

- Idea is to preserve relative order that elements occur
- Informal procedure:
  - 1. Choose an arbitrary part from the first parent
  - 2. Copy this part to the first child
  - 3. Copy the numbers that are not in the first part, to the first child:
    - starting right from cut point of the copied part,
    - using the **order** of the second parent
    - and wrapping around at the end
  - 4. Analogous for the second child, with parent roles reversed



Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

# Permutation Representations: Partially Mapped Crossover (PMX) (1/2)

Informal procedure for parents P1 and P2:

- 1. Choose random segment and copy it from P1
- 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 *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 *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 offspring can be filled from P2.

#### Second child is created analogously

#### Permutation Representations: Partially Mapped Crossover (PMX) (2/2)



Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

# Permutation Representations: Cycle crossover (1/2)

#### Basic idea:

Each allele comes from one parent *together with its position*. Informal procedure:

- 1. Make a cycle of alleles from P1 in the following way.
  - (a) Start with the first allele of P1.
  - (b) Look at the allele at the same position in P2.
  - (c) Go to the position with the same allele in P1.
  - (d) Add this allele to the cycle.
  - (e) Repeat step b through d until you arrive at the first allele of P1.
- 2. Put the alleles of the cycle in the first child on the positions they have in the first parent.
- 3. Take next cycle from second parent

#### Permutation Representations: Cycle crossover (2/2)

• Step 1: identify cycles



Step 2: copy alternate cycles into offspring
 1 2 3 4 5 6 7 8 9
 1 3 7 4 2 6 5 8



Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014

#### Permutation Representations: Edge Recombination (1/3)

- Works by constructing a table listing which edges are present in the two parents, if an edge is common to both, mark with a +
- e.g. [1 2 3 4 5 6 7 8 9] and [9 3 7 8 2 6 5 1 4]

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	$1,\!4,\!6+$		

### Permutation Representations: Edge Recombination (2/3)

Informal procedure: once edge table is constructed

- 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 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 Representations: Edge Recombination (3/3)

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
<b>5</b>	1,4,6+		

Choices	Element	Reason	Partial
	selected		$\operatorname{result}$
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	$[1\ 5\ 6\ 2\ 8\ 7\ 3\ 9]$
4	4	Last element	[156287394]

#### Tree Representation (1/6)

- Trees are a universal form, e.g. consider
- Arithmetic formula:  $2 \cdot \pi + \left( (x+3) \frac{y}{5+1} \right)$
- Logical formula:  $(x \land true) \rightarrow ((x \lor y) \lor (z \leftrightarrow (x \land y)))$
- Program:

   i = 1;
   while (i < 20)</li>
   i = i + 1
   i



Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014





Adapted from A.E. Eiben and J.E. Smith, Introduction to Evolutionary Computing 2014



#### Tree Representation (6/6)

- Symbolic expressions can be defined by
  - Terminal set T
  - Function set F (with the arities of function symbols)
- Adopting the following general recursive definition:
  - Every  $t \in T$  is a correct expression
  - $f(e_1, ..., e_n)$  is a correct expression if f ∈ F, arity(f)=n and  $e_1, ..., e_n$  are correct expressions
  - There are no other forms of correct expressions
- In general, expressions in GP are not typed (closure property: any f ∈ F can take any g ∈ F as argument)

#### Tree Representation: Mutation (1/2)

 Most common mutation: replace randomly chosen subtree by randomly generated tree



# Tree Representation: Mutation (2/2)

- Mutation has two parameters:
  - Probability  $p_m$  to choose mutation
  - Probability to chose an internal point as the root of the subtree to be replaced
- Remarkably p<sub>m</sub> is advised to be 0 (Koza'92) or very small, like 0.05 (Banzhaf et al. '98)
- The size of the child can exceed the size of the parent

# Tree Representation: Recombination (1/2)

- Most common recombination: exchange two randomly chosen subtrees among the parents
- Recombination has two parameters:
  - Probability  $p_c$  to choose recombination
  - Probability to chose an internal point within each parent as crossover point
- The size of offspring can exceed that of the parents

#### Tree Representation: Recombination (2/2)

