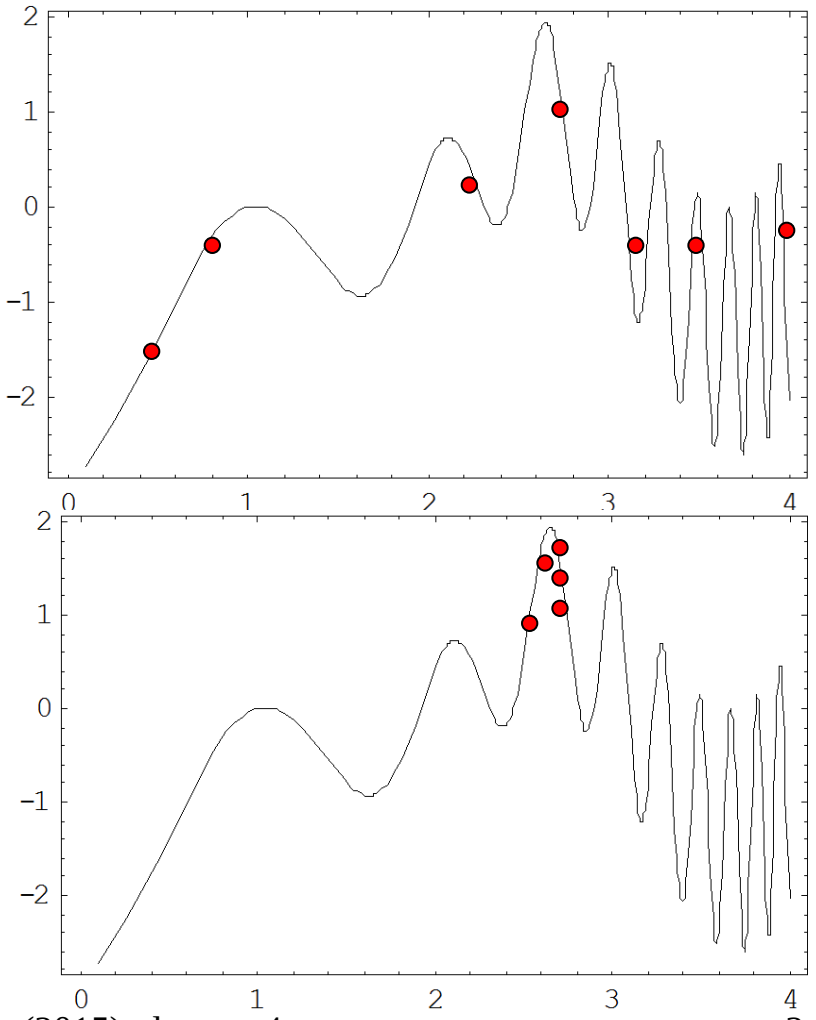
Population based metaheuristics

- Particularities
- Classes of population based metaheuristics
- General structure
- Main components
- Evolutionary algorithms:
  - Encoding
  - Selection
  - Reproduction: crossover and mutation

Population based metaheuristics

Problem solving =

- Search for the solution using a population of candidate solutions
- The search is guided by a function which „measures” the closeness to the solution

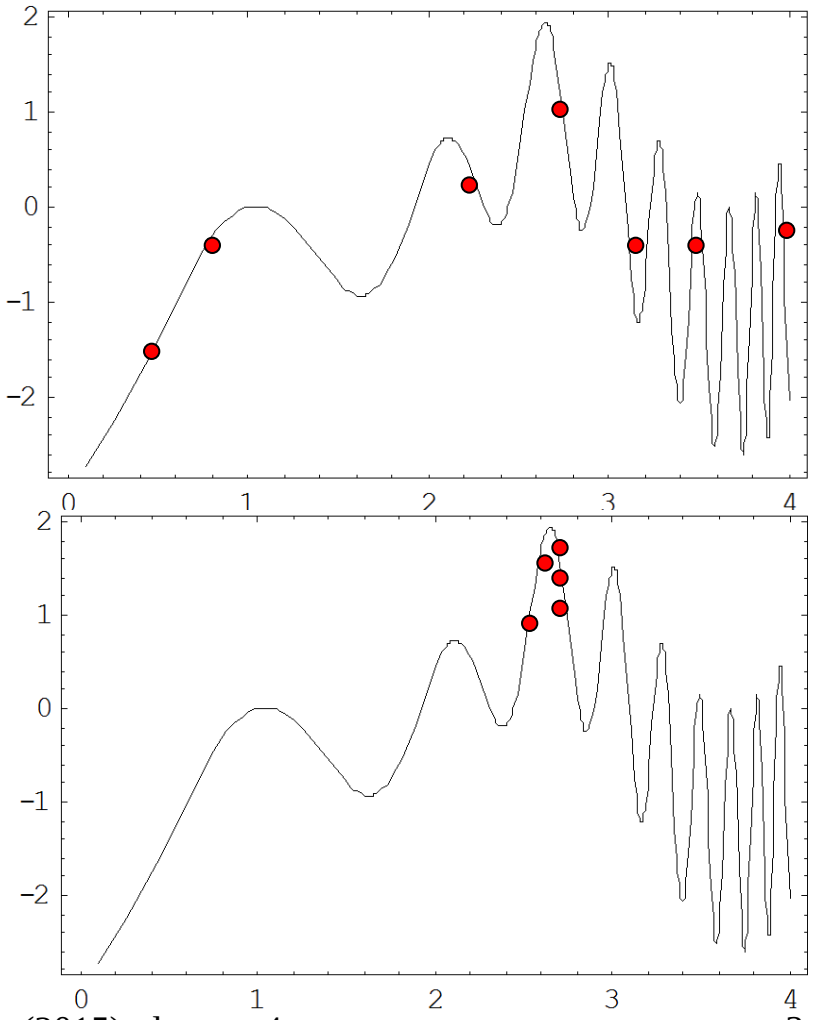


Population based metaheuristics

There are two main search mechanisms:

- exploration = the search space is explored by the population elements which collect information about the problem (it involves cooperation between the population elements)
- exploitation = the information collected during exploration is exploited and the potential solution(s) is/are refined (it involves competition between the population elements)

Remark: There are many metaheuristics based on this paradigm



Population based metaheuristics

- Evolutionary algorithms
  - Genetic Algorithms
  - Evolution Strategies
  - Evolutionary Programming
  - Genetic Programming
- Swarm intelligence algorithms
  - Particle Swarm Optimization
  - Ant Colony Optimization
  - Artificial Bee Colony
  - ... a large set of bio-inspired metaheuristics
- Other population based algorithms
  - Differential Evolution
  - Estimation of Distribution Algorithms

General structure

Population initialization (random or based on some specific heuristics)

Population evaluation (computation of the objective function value(s))

REPEAT

    Construct a new population of candidate solutions

    Evaluate the candidate solutions

    Select the elements of a new population

UNTIL <stopping condition>

Remark:

- The generation of new candidate solutions depend on the algorithm type
- At each cycle (generation) an entire new population is constructed and it competes with the previous population for „survival” (this is a so-called generational or synchronous updating strategy)

General structure

Variant: the candidate solutions are analyzed and potentially assimilated into population just after their generation (steady state or asinchronous updating strategy)

Population initialization: $(s_1, s_2, \ldots, s_m)$

Population evaluation (computation of the objective function value(s))

REPEAT

FOR i =1:m

construct a new candidate solution (s'_i)

evaluate the new candidate solution

decide if the new candidate solution is accepted into the population

UNTIL <stopping condition>

Remark: a new candidate solution is usually accepted if it is better than the poorest element of the current population

Evolutionary computing

Evolutionary computing = design and application of techniques inspired by natural evolution

Inspiration: evolution of species =

- The species evolve by the development of new characteristics during reproduction caused by crossover and random mutations
- In the evolutionary process the fittest individuals survive (those which are well adapted to the environment)

Analogy: evolution - optimization

Evolutionary process	Problem solving
Natural environment	Information about the problem
Individual (chromosome)	Configuration (candidate solution)
Population of individuals	Population of candidates
Fitness (degree of adaptation to the environment)	Measure of the solution quality
Selection	Exploitation mechanism
Reproduction (crossover and mutation)	Exploration mechanism

Evolutionary computing: basic notions

Chromosome = set of genes corresponding to an individual (potential solution for the problem)

(1,0,0,1)

Population = finite set of individuals (chromosomes, candidate solutions)

{(0,0,0,0), (0,0,1,1), (1,0,0,1),(1,0,1,0)}

Genotype = the pool of all genes of an individual or population

Phenotype = the set of all features represented by a genotype

{0,3,9,10}

Evolutionary computing: basic notions

Fitness = measure of the quality of an individual (with respect to the problem to be solved)

Generation = stage in the evolutionary process of a population (iteration in the search process)

Reproduction = generation of new individuals (offsprings) starting from the current population (parents) by

- crossover
- mutation

Ex: ONEMAX problem

= find the binary string which maxinmizes the number of ones

(1,0,0,1) → 2

Crossover:

(1,0,0,1) → (1,0,1,1)

(0,0,1,1) → (0,0,0,1)

Mutation:

(1,0,1,1) → (1,1,1,1)

Evolutionary computing: applications

Scheduling: vehicle routing problems, timetabling, routing in telecommunication networks

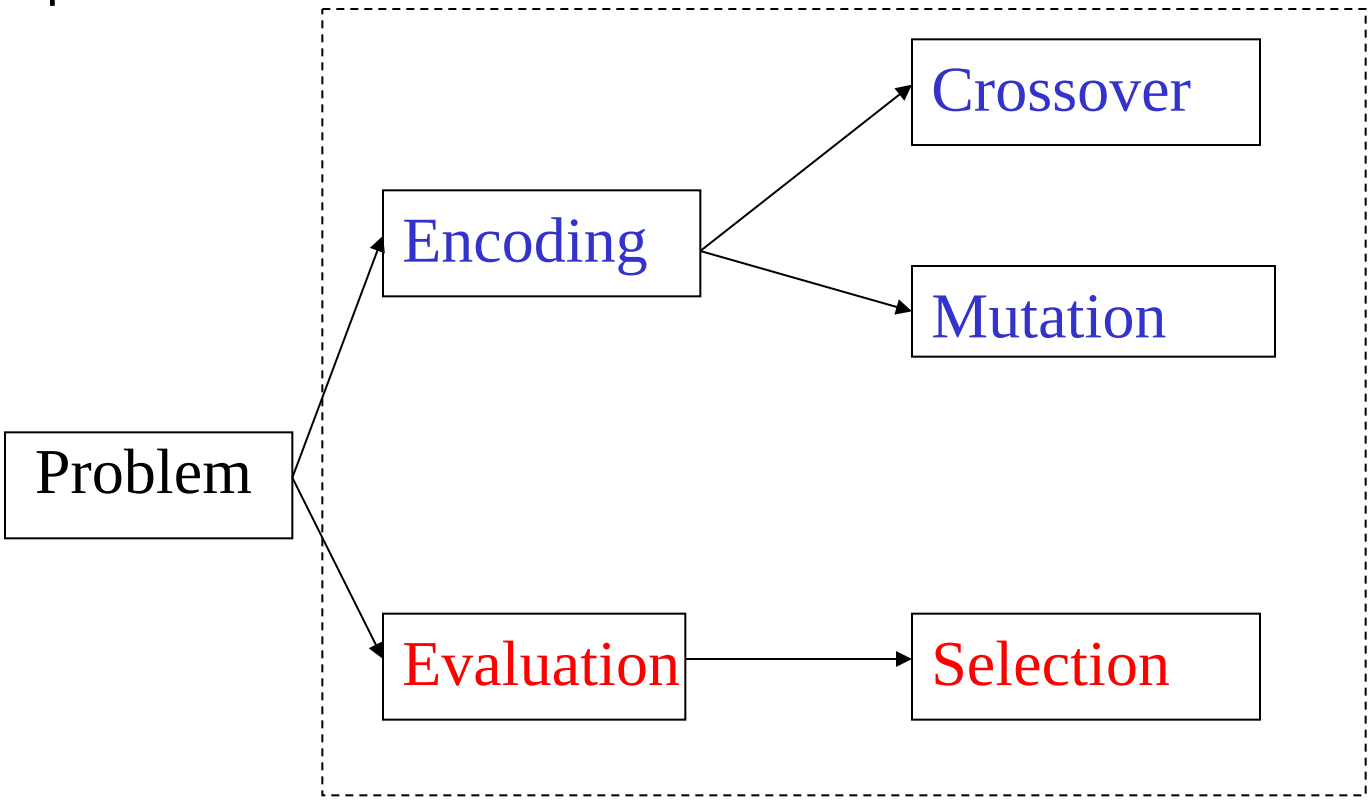
Design: digital circuits, filters, neural networks

Modelling: predictive models in economy, finances, medicine etc.

Data mining: design of classification systems in engineering, biology, medicine etc.

Designing an Evolutionary Algorithm

Components:



Structure of an EA

Population initialization
Population evaluation
REPEAT
    Parents selection
    Crossover
    Mutation
    Offspring evaluation
    Survivors selection
UNTIL <stopping condition>

Directions in Evolutionary Computing

Genetic Algorithms (Holland, 1962-1967):

Encoding: binary

Crossover: main operator

Mutation: secondary operator

Applications: combinatorial optimization

Genetic Programming (Koza, 1990):

Encoding: tree-like structures

Crossover: main operator

Mutation: secondary operator

Applications: programs evolution

Evolution Strategies (Rechenberg,Schwefel 1965):

Encoding: real

Mutation: main operator

Recombination: secondary operator

Applications: continuous optimization

Evolutionary Programming (L. Fogel, D. Fogel, 1960-1970):

Encoding: real / state digrams

Mutation: the only operator

Applications: continuous optimization

Encoding

Is a key element when a genetic algorithm is designed

The encoding method is related to the problem to be solved

Variants:

- Binary encoding (the classical variant for GA)
- Real encoding (appropriate for continuous optimization)
- Specific encoding (e.g. permutation, tree, graph etc)

Binary encoding

Chromosome = binary sequence

Search space: $\{0,1\}^n$, n is given by the problem size

Examples:

1. ONEMAX: find the binary sequence $(x_1,\ldots,x_n)$ which maximizes the function $f(x_1,\ldots,x_n)=x_1+\ldots+x_n$
2. Knapsack: there is a set of n objects of weights $(w_1,\ldots,w_n)$ and values $(v_1,\ldots,v_n)$ and a knapsack of capacity C; find a subset of objects which can be included in the knapsack without overpassing its capacity and such that the total value of selected objects is maximal

   Encoding: $(s_1,\ldots,s_n)$

   s_i=0 object i is not selected

   s_i=1 object i is selected

Binary encoding

3. Optimization of a function defined on a continuous domain.

$f:[a_1,b_1]x...x[a_n,b_n] \rightarrow R$

$X=(x_1,\ldots,x_n) \rightarrow V=(v_1,\ldots,v_n) \rightarrow U=(u_1,\ldots u_n)$
$\rightarrow Y=(y_1,\ldots,y_r, y_{r+1},\ldots y_{2r},\ldots ,y_{nr)}$

$v_i=(x_i-a_i)/(b_i-a_i)$ (v_i belongs to [0,1])

$u_i=[v_i*(2^r-1)]$ (u_i is a natural number from $\{0,\ldots 2^r-1\}$ => it can be represented in base 2 on r positions)

$(y_{r(i-1)+1},\ldots y_{ri})$ = binary representation of u_i

Binary encoding

Remark. The binary encoding has the disadvantage that close values can correspons to binary sequences with a large Hamming distance (ex. $7=(0111)_2$, $8=(1000)_2$)

Solution: use of the Gray code (successive values have binary sequences which are different in only one position)

$(b_1,\ldots,b_r) \rightarrow (g_1,\ldots,g_r)$

$g_1=b_1$

$g_i=(b_{i-1} + b_i) \bmod 2$

Binary encoding

Gray code:

$(b_1,\ldots,b_r) \rightarrow (g_1,\ldots,g_r)$

$g_1=b_1$

$g_i=(b_{i-1} + b_i) \bmod 2$

Decoding:

$b_j=(g_1+\ldots+g_j) \bmod 2$

Nr.	Binary	Gray
0	000	000
1	001	001
2	010	011
3	011	010
4	100	110
5	101	111
6	110	101
7	111	100

Particular encoding

It is specific to the problem to be solved

Example: permutation-like encoding

$(s_1,s_2,\ldots,s_n)$, s_i in {1,…,n}, $s_i <> s_j$ for all i<>j

Problem: TSP

s_i = index of the town visited at step i

Remarks. It ensures the fact that the constraints are satisfied.

Evaluation of the population elements

Fitness

- measures the quality of an individual
- as the value of the fitness is larger the probability of the element to survive is larger

Problem: unconstrained optimization

The fitness function is proportional with the objective function (for a maximization problem) and inverse proportional with the objective function (for a minimization problem)

Problem: constrained optimization

The fitness function depends both on the objective function and on the constraints

Evaluation of the population elements

Constraints: included in the objective function by using the penalty method

$$\max_{x \in D} f(x)$$

$$g_i(x) = 0, \; i = \overline{1, k_1}$$

$$h_i(x) \geq 0, \; i = \overline{1, k_2}$$

$$F(x) = f(x) - a\sum_{i=1}^{k_1} g_i^2(x) - b\sum_{i=1}^{k_2} \varphi(h_i(x)), \quad a > 0, b > 0$$

$$\varphi(u) = \begin{cases} 0, & u \geq 0 \\ -u, & u < 0 \end{cases}$$

(no penalty if the constraint is satisfied)

(the penalty is larger if the constraint is not satisfied)

Evaluation of the population elements

Example: knapsack problem

$$\max_s \sum_{i=1}^{n} v_i s_i$$

$$C - \sum_{i=1}^{n} w_i s_i \geq 0$$

Fitness function

$$F(s) = \begin{cases} \sum_{i=1}^{n} v_i s_i, & \text{daca } \sum_{i=1}^{n} w_i s_i \leq C \\ a\sum_{i=1}^{n} v_i s_i - b\left(\sum_{i=1}^{n} w_i s_i - C \right), & \text{daca } \sum_{i=1}^{n} w_i s_i > C \end{cases}$$

$$a, b > 0, a + b = 1$$

Rmk: the weights a and b control the relative importance of the two componente: objective function and constraints

Selection

Aim:

- decide which of the elements from the current populations will be used to construct offspring (parents selection)
- decide which of the elements from the offspring population will belong to the next generation (survivors selection)

Basic idea:

- the elements with a high fitness have a higher chance to be selected

Selection mechanisms:

- proportional selection
- rank based selection
- tournament selection
- truncation selection

Proportional selection

Current population: $P=(x^1,\ldots,x^m)$

Fitness values:

$(F_1,\ldots,F_m)$

Selection probabilities:

$p_i=F_i/(F_1+\ldots+F_m)$

Rmk. If F_i are not strictly larger than 0 than they can be changed as follows:

$F'_i=F_i-\min(F_i)+eps$

Steps:

a) Compute the selection probabilities

b) Generate random values according to the distribution

1	2	…	m
p_1	p_2	…	p_m

Implementation:

(i) “Roulette Wheel”

(ii) “Stochastic Universal Sampling” (SUS)

Proportional Selection

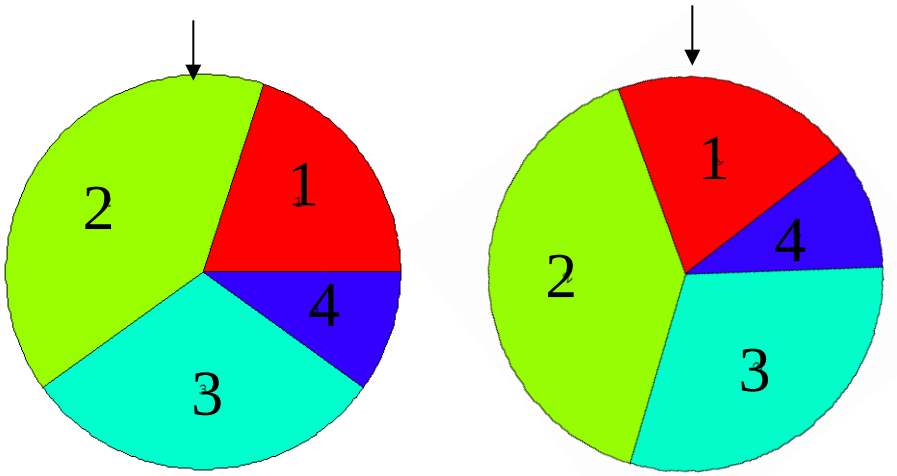
Roulette Wheel

- Let us consider a roullete divided in m sectors having areas proportional to the selection probabilities.

- Spin off the roulette and the index of the sector in front of the indicator gives the element to be selected from the population

Example:

1	2	3	4
0.2	0.4	0.3	0.1



Proportional selection

Implementation:

```
Ruleta (p[1..m])
        i=1
        s=p[1]
        u=random(0,1)
        while s<u do
             i=i+1
             s=s+p[i]
       endwhile
       return i
```

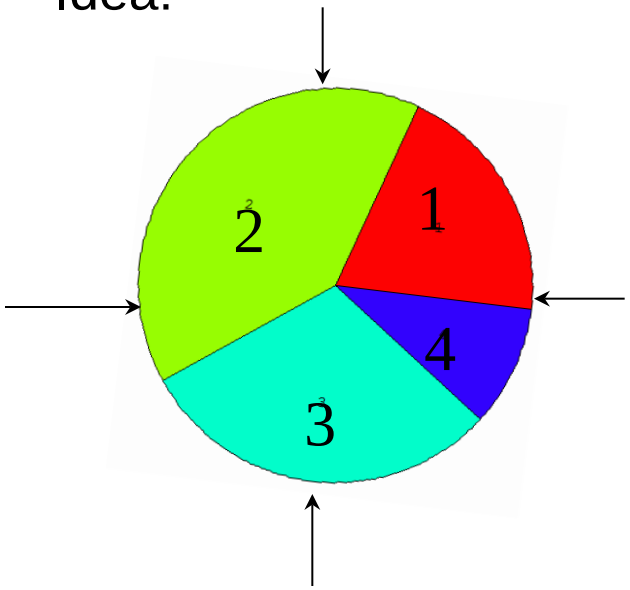
Rmk.

1. This algorithm corresponds to the simulation of a random variable starting from its distribution
2. One run gives the index of one element
3. To simultaneously generate the indices of several elements, the SUS (Stochastic Universal Sampling) variant can be used

Proportional selection

Stochastic Universal Sampling

Idea:



Rmk: k represents the number of elements which should be selected

c[1..m] will contain the number of copies of each element

Algorithm:

```
SUS(p[1..m],k)
   u=random(0,1/k)
   s=0
   for i=1,m  do
        c[i]=0
        s=s+p[i]
        while u<s do
             c[i]=c[i]+1
             u=u+1/k
        endwhile
   endfor
   Return c[1..m]
```

Proportional selection

Disadvantages:

1. If the objective function does not have positive values the fitness values should be transformed

2. If the difference between the fitness value of the best element and that of other elements is large then it is possible to fill the populations with copies of the best element (this would stop the evolutionary process)

Rank based selection

Particularities:

the selection probabilities are computed based on the rank of elements in an increasingly sorted list by fitness (in the case o a maximization problem)

Steps:

1. increasingly sort the fitness values
2. each distinct value in the list will have a rank (the smallest fitness value corresponds to rank 1)
3. divide the population in classes of elements having the same rank (e.g. k classes)
4. compute the selection probabilities: $P_i = i/(1+2+\ldots+k)$
5. select classes using the roulette wheel or SUS methods; randomly select an element from each class.

Tournament selection

Idea:

an element is selected based on the result of a comparison with other elements in the population

The following steps should be followed to select an element:

1. Randomly select k elements from the population
2. From the k selected elements choose the best one

Remark.

1. Typical case: k=2

Truncated selection

Idea:

from the joined population of parents and offspring the k best elements are selected

Remark.

1. This is the only completely deterministic selection
2. It is mainly used for evolution strategies

Properties of selection

Elitism:

- A selection method has the property of elitism if the best element in population is always selected as survivor (it always remains in the population for the next generations)
- Truncation selection is the only method satisfying always this property
- In order to ensure the elitism the best element of the current population can be explicitly inserted in the new population (e.g. by replacing the worst element)

Properties of selection

Selection pressure:

- It measures the likelihood that the best element in the population will take over the population
- A strong selection pressure generates a high exploitation and reduces the exploration of the search space (it could lead to local optima or stagnation)
- In the case of probabilistic selection (e.g. proportional selection, tournament selection) the selection pressure can be measured by using the “takeover time” = number of generations needed to fill the entire population with copies of the best element if only selection would be applied

Crossover

Aim: combine two or several elements in the population in order to obtain one or several offsprings

Remark: in genetic algorithms there are usually two parents generating two children

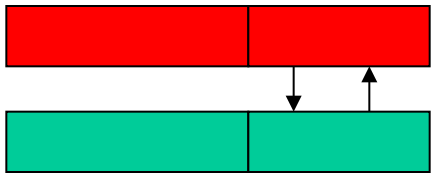
Variants:

- one cut-point
- uniform
- convex
- tailored for a given problem

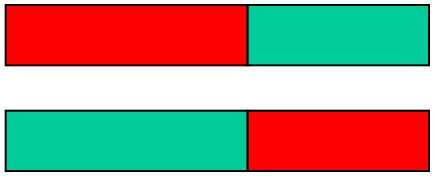
Cut-points crossover

One cut point

Parents

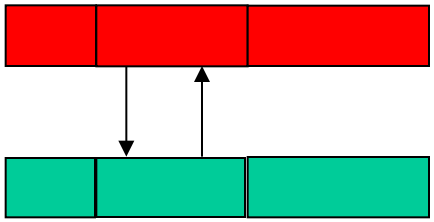


Children

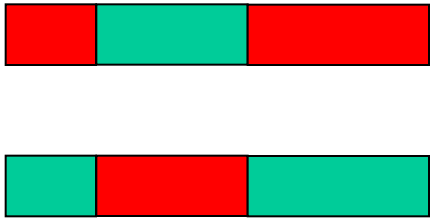


Two cut points

Parents



Children



Cut-points crossover

Remarks:

1. For each pair of selected parents the crossover is applied with a given probability (0.2<=Pc<=0.9)

2. The cut points are randomly selected

3. Numerical experiments suggest that two cut-points crossover leads to better results than one cut-point crossover

Uniform crossover

Particularity : the genes of offspring are randomly selected from the genes of parents

Notations: $x = (x_1, \ldots x_n)$, $y = (y_1, \ldots, y_n)$ – parents

$x' = (x'_1, \ldots x'_n)$, $y' = (y'_1, \ldots, y'_n)$ – offspring

$$x_i' = \begin{cases} x_i, & \text{with probability p} \\ y_i, & \text{with probability } 1-\text{p} \end{cases}$$

$$y_i' = \begin{cases} y_i, & \text{if } x_i' = x_i \\ x_i, & \text{if } x_i' = y_i \end{cases}$$

Convex crossover

Specific: is used for vectors of real values

Notations: $x = (x_1, \ldots x_n)$, $y = (y_1, \ldots, y_n)$ – parents

$x' = (x'_1, \ldots x'_n)$, $y' = (y'_1, \ldots, y'_n)$ – offsprings

$$x'_i = a x_i + (1-a) y_i$$

$$y'_i = a y_i + (1-a) x_i$$

Remark.

- It can be extended in the case of an arbitrary number of parents - only one offspring is generated

- The coefficient a can be randomly selected from (0,1)
- More general variants:
  - A can be chosen from the interval (-p,p+1)
  - A different random value can be chosen for each component

$$x'_i = a_i x_i + (1-a_i) y_i$$

$$y'_i = b_i y_i + (1-b_i) x_i$$

Crossover for permutation – like elements

Aim: include heuristic schemes which are particular

Example: TSP (a tour is given by the order of visiting the towns)

Parents: A B C D E F G Cutpoint: 3
A B E G D C F

Offspring: A B C E G D F
A B E C D F G

Mutation

Aim: it allows to introduce new genes in the gene pool (which are not in the current genotype)

Remark: the mutation depends on the encoding variant

Binary encoding: the mutation consists of complementing some randomly selected genes

Real encoding: random perturbation

Specific encoding: perturbation based on particular heuristics

Variants:

1. Local (at chromosome level)
2. Global (at gene pool level)

Mutation

Chromosome level

Steps:

1. Select chromosomes to be mutated (using a small mutation probability)

2. For each selected chromosome select a random gene which is mutated

Remark:

The mutation probability is correlated with the population size (e.g. $P_m=1/m$)

Mutation

Pool gene level

Assumptions: all chromosomes are concatenated, thus they form a long binary sequence

Mutation: All genes are visited and for each one is decided (based on a mutation probability) if it is mutated or not

Remark:

1. This variant allows to change several genes of the same chromosome

Control parameters

The behavior of evolutionary algorithms is influenced by the parameters which control the structure of the population and the evolutionary mechanisms

Control parameters:

- Population size
- Parameters involved in the stopping condition: maximal number of generations, maximal number of objective function evaluations, maximal number of stagnation steps etc
- Parameters involved in selection:
  - Sample size in the case of tournament selection
- Parameters involved in crossover:
  - Crossover probability
- Parameters involved in mutation:
  - Mutation probability
  - Parameters which correspond to the probability distributions used in random perturbation