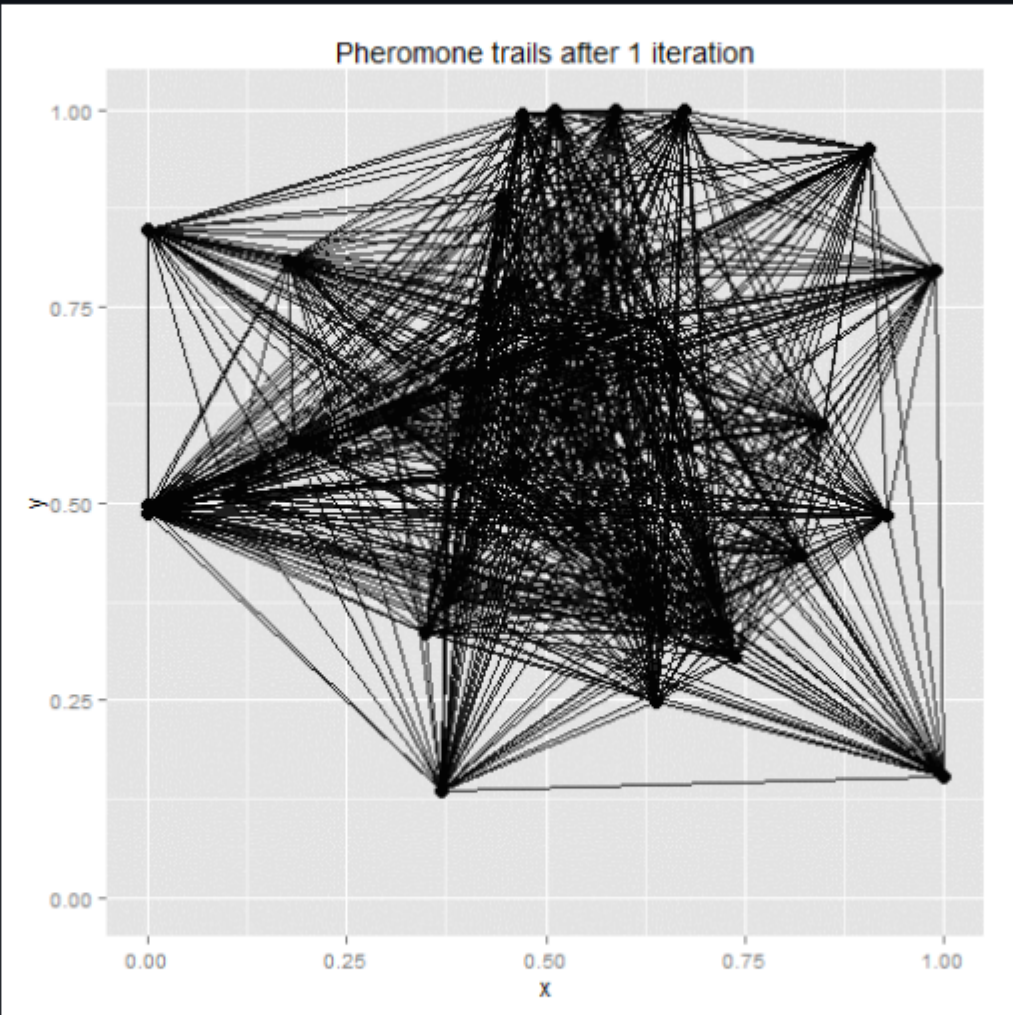


# Metaheuristics

## Ant Colony Optimization



### Description

Bio-inspired metaheuristic. It is inspired on the ants' behavior, where an ant guides the others when they find something good.

### Types of problems

Intended to solve problems related to graphs. i.e. Useful to find paths.

### Representation

For this problem, some terms are defined.

- $C_{ij}$ : Path from the node i to the j
- $\tau_{ij}$ : Pheromones in the path from the node i to the node j
- $\eta_{ij}$ : Heuristic in the path from the node i to node j
- $\rho$ : Evaporation,  $[0, 1]$

### Movement

- Each ant moves around the graph following the criteria:

$$P(C_{ik}) = \frac{\tau_{ik}^{\alpha} * \eta_{ik}^{\beta}}{\sum_{\epsilon \in N_i} \tau_{ij}^{\alpha} * \eta_{ij}^{\beta}}$$

Note. To optimize distance  $\eta_{ik} = \frac{1}{d_{ik}}$  is proposed where  $d_{ik}$  is the length of the component  $C_{ik}$ .

### Update

After all the ants traverse the graph, the pheromones:

Are updated

$$\Delta \tau_{ij}^{\alpha} = \begin{cases} \frac{1}{L_{\alpha}} & Used \\ 0 & Otherwise \end{cases}$$

And evaporate

$$\tau_{ij} = (1 - \rho) * \tau_{ij}$$

### Pseudocode

Ant colony

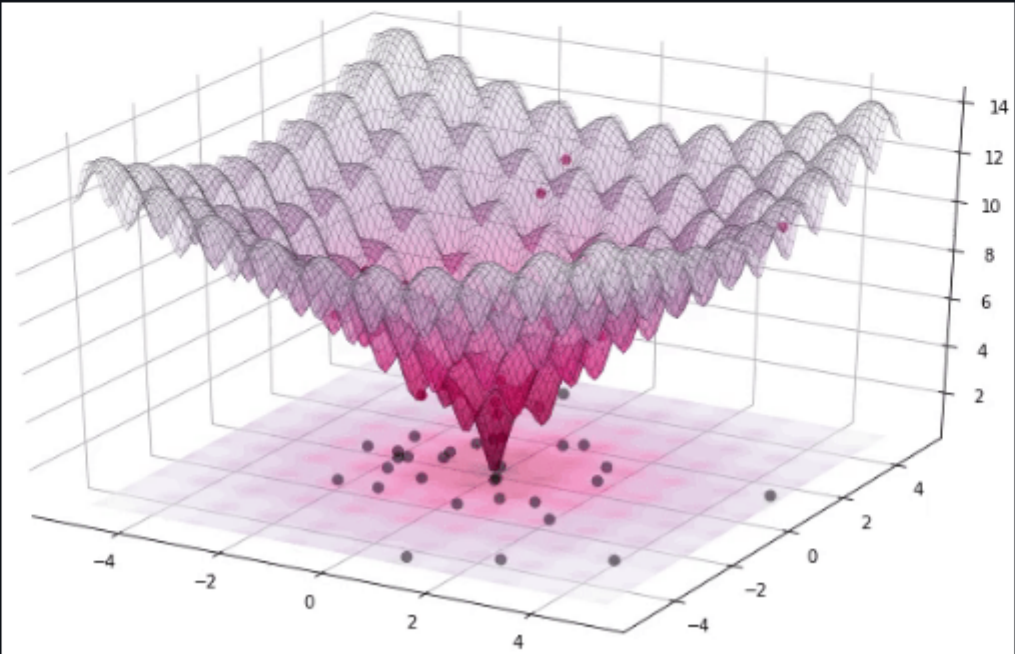
```
At the beginning
  Pheromones <- small value

Move the ants one by one
  Ants: move around the graph

When all the ants record the graph
  Pheromones: are updated
  Ants: deposit pheromones
  Pheromones: evaporate
```

## Evolutionary algorithms

### Differential evolution



#### Description

This is a robust algorithm and introduces the idea of mutating individuals based on 3 others, in order to work as a gravitational force into the minimums.

#### Types of problems

This algorithm solves continuous multidimensional optimization problems.

#### Representation

A vector of real values.

$$\vec{x}^i = \langle x_1^i, x_2^i, \dots, x_d^i \rangle$$

#### Mutation

This is the main operation of differential evolution.

For each individual  $x^i$ , another one called  $v^i$  is generated by performing the following operation.

$$v^i = x^{r1} + (x^{r2} - x^{r3})F$$
$$0 \leq F \leq 2$$

#### Crossover/Recombination

A new individual is created element by element, randomly picking values from the original one  $x^i$  or the mutated one  $v^i$ .

This is performed based on a Crossover probability  $0 \leq Cr \leq 1$ .

$$u_k^i = v_k^i \quad \text{if} \quad rand(0, 1) \leq Cr \quad \text{else} \quad x_k^i$$

#### Survivor selection

Tournament is used: The best individual between  $u^i$  and  $x^i$  is selected to be part of the next generation.

#### Pseudocode

##### Differential evolution

```
Parameters:
  N -> Population size
  G -> Maximum number of generations
  Cr -> Crossover probability

Return: the best individual

Begin
  Create the initial population of N individuals
  Calculate the population fitness
  While the number of generations is less than G or a good solution hasn't been found
    For each individual in the population.
      Mutation -> Create new individual
      Crossover -> Combine the individuals
      Calculate the fitness of the new one
      Selection -> Select the best between both
    End for
  End while
End
```

## Evolutionary algorithms

### Evolutionary programming

#### Description

The solutions represent species instead of individuals.

#### Types of problems

It has evolved to solve continuous multidimensional optimization problems.

#### Representation

The individual's solution is represented with a vector of  $d$  real values where  $d$  is the number of features to optimize. In addition to the values, a *mutation step size* is used to guide the change of each individual's mutation.

$$< \vec{x}_i, \vec{\sigma}_1 >$$

#### Mutation

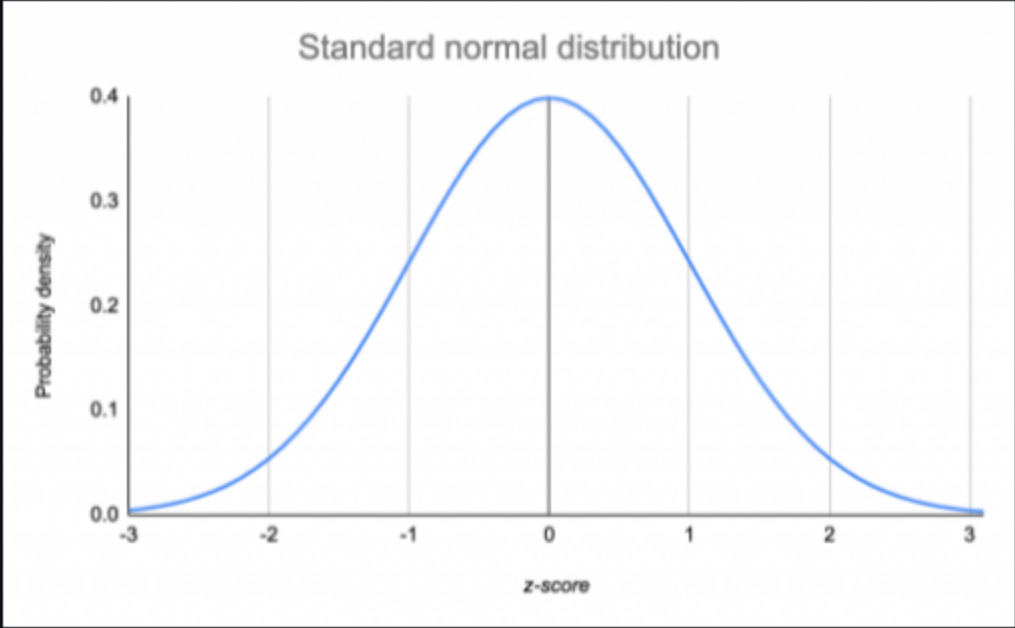
Each value is mutated with a random number based on its step size.

Step size is eventually updated as well.

$$\sigma'_i = \sigma_i(1 + N(0, \alpha))$$

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

$$\alpha \approx 0.2$$



#### Survivor selection

$(\mu + \lambda)$  selection: Where the best  $\mu$  individuals are selected out of the union of parents and offspring.

#### Pseudocode

##### Evolutionary programming

```
Parameters:
    μ -> Population size
    G -> Maximum number of generations

Return: the elite individual

Begin
    Create the initial population
    Calculate the population fitness
    Get the elite
    While the number of generations is less than G or a good solution hasn't beed found
        Mutation of all the species
        Calculate the population fitness
        Survivor selection
        Get the elite or include the elite in the population
    End while
End
```



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# Evolutionary algorithms

## Evolution strategies

### Description

The main characterisits of this algorithms is the *self-adaptation* of parameters, since they evolve with the individual itself.

### Types of problems

It's designed to solve continuous multidimensional optimization problems.

### Representation

The individual's solution is represented with a vector of  $d$  real values where  $d$  is the number of features to optimize. In addition to the values, a *mutation step size* is used to guide the change of each individual's mutation.

- If all the variables to be calculated are in the same range, a single step size can be used.

$$< \vec{x}_i, \sigma_1 >$$

- Otherwise, a size per featue is recommended.

$$< \vec{x}_i, \vec{\sigma}_1 >$$

### Parent selection technique

Completely random, this is because the whole population is seen as parent.

### Crossover/Recombination

Two variants are used:

- Intermediate recombination

$$\frac{\vec{p}_1 + \vec{p}_2}{2}$$

- Discrete recombination

$$RandomSelection \quad [\vec{p}_{1i}, \vec{p}_{2i}]$$

### Mutation

The mutation of the features consist of adding a random value based on a normal distribution zero-centered with a standard deviation equals to the corresponding  $\sigma$ .

$$x'_i = x_i + N(0, \sigma_1)$$

On the other hand, updating the step size depends of the chosen representation.

- With one step size

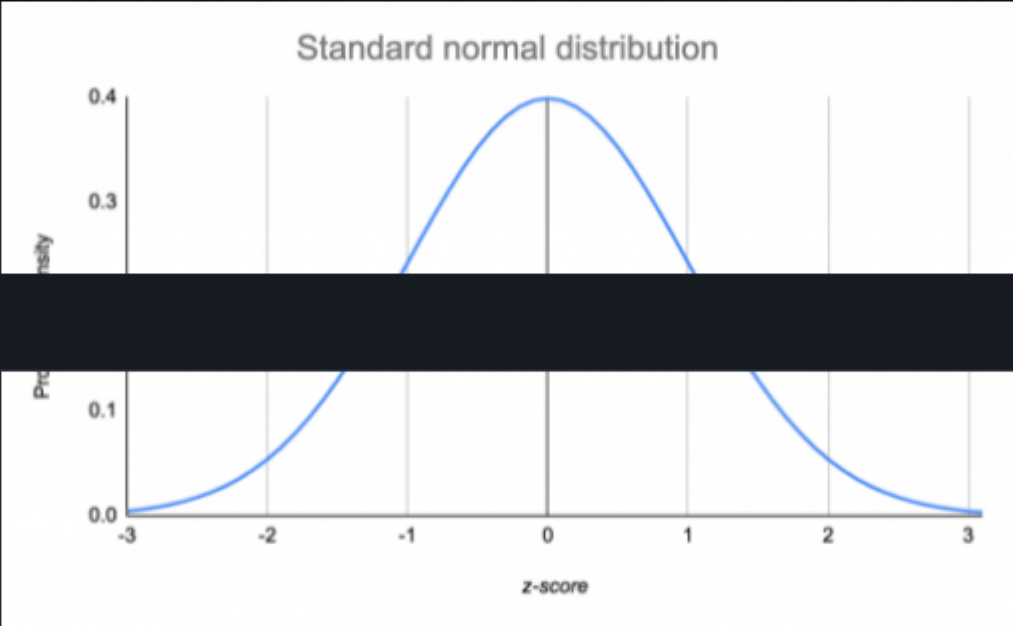
$$\sigma' = \sigma e^{N(0, \tau)}$$

Where  $\tau = \frac{1}{\sqrt{n}}$  and  $n$  is the population size.

- With  $d$  step sizes

$$\sigma' = \sigma e^{N(0, \tau_1) + N(0, \tau_2)}$$

Where  $\tau_1 = \frac{1}{\sqrt{n}}$ ,  $\tau_2 = \frac{1}{\sqrt{2\sqrt{n}}}$  and  $n$  is the population size.



Also, see the **1/5 sucess rule**.

### Survivor selection

After creating the offspring  $\lambda$  and calculating their fitness, the best  $\mu$  are deterministically chosen. There are two approaches.

- $(\mu, \lambda)$  selection: The best  $\mu$  individuals are selected out of the offspring.
- $(\mu + \lambda)$  selection: Where the  $\mu$  individuals are selected out of the union of parents and offspring.

### Pseudocode

#### Evolution strategies

```
Parameters:
  N -> Population size
  λ -> Offspring size
  G -> Maximum number of generations

Return: The elite individual

Begin
  Create the initial population
  Calculate the population fitness
  Get the elite
  While the number of generations is less than G or a good solution hasn't been found
    Recombination
    Mutation
    Calculate the population fitness
    Survivor selection (the best individuals)
    Get the elite or include the elite in the population
  End while
End
```

Evolutionary algorithms

Genetic algorithms

Description

Probably the most famous algorithm of its kind.

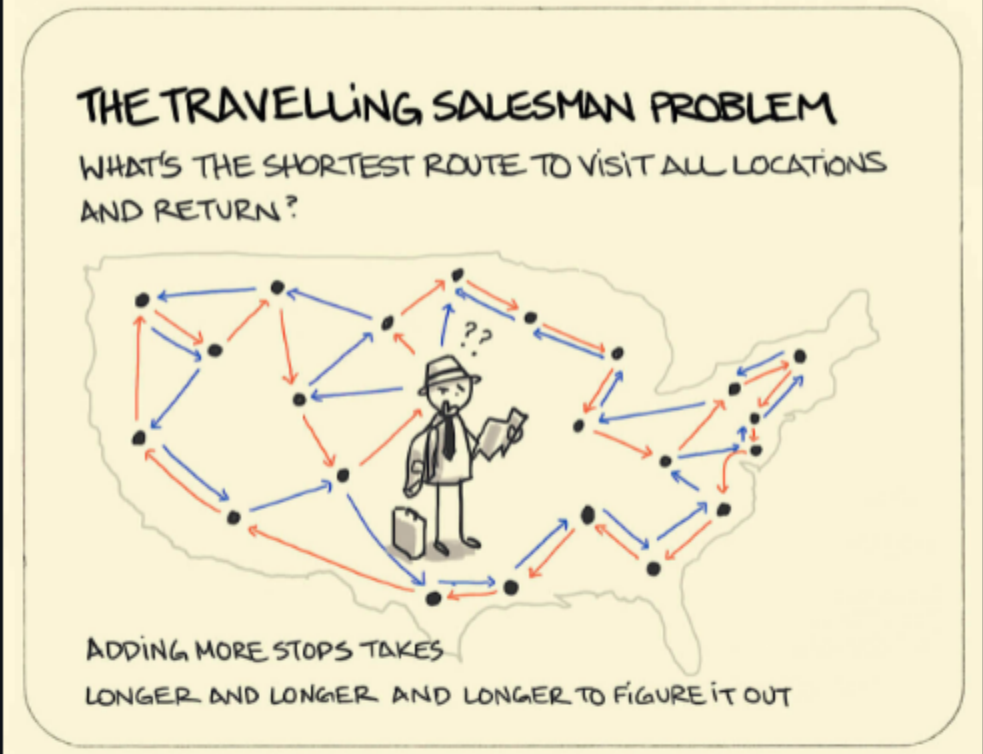
The inspiration comes from the DNA structures. Where there's a population with chromosomes and each one consists of genes.

Types of problems

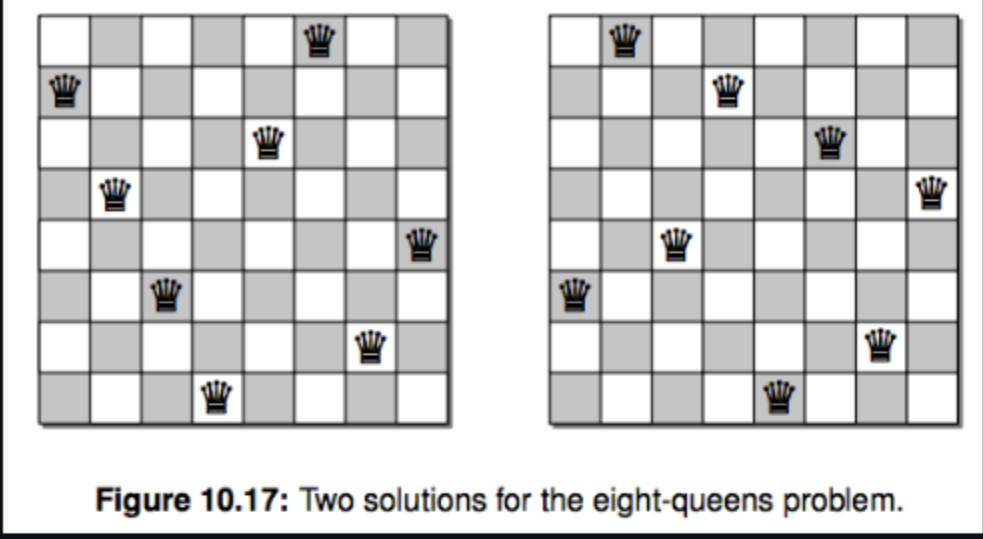
This algorithm can be used for *constrained* or *unconstrained* problems that are not usually suitable for standard optimization algorithms.

Some of the problems are:

- Traveling salesman problem.



- 8 queens problem.



Representation

There are several alternatives:

- Binary representation.

It's the original approach; the implementation is an array of bools.

- Integer representation.

Integer array.

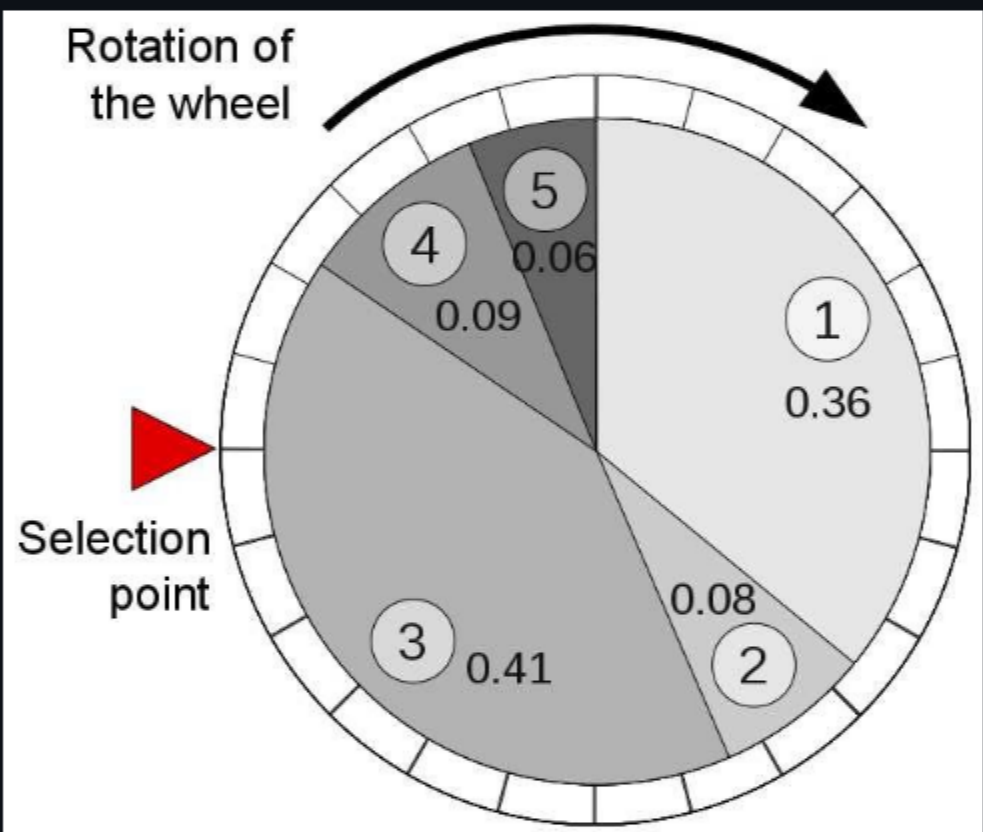
- Real representation.

Array  $x$  where each  $x_i$  is a real number.

Parent selection technique

- Roulette/Proportional selection

We can think of a roulette that has one slice per chromosome of the population. The size of the slice varies depending on the fitnesses; the better it is, the wider its corresponding slice is.



- Tournament selection

Consists of choosing k random elements and selecting the fittest one.

Crossover/Recombination

The goal is to generate an offspring combining the parents' properties. There are different approaches depending on the representation.

Binary and integer representation

- 1 point crossover.

Consists of choosing a random pivot point and the new individual will be generated with the left side of the first parent and the right side of the second.

- N points crossover.

Same idea as 1 point crossover but several sections are used.

- Uniform crossover.

The new individual is created element by element, randomly picking values from one parent or the other.

Real valued representation

- Discrete reproduction.

Same as uniform crossover.

- Asymmetric reproduction.

The offspring is generated with a weighted sum.

$$o_i = \alpha p_1 + (1 - \alpha) p_2$$

Where  $\alpha$  is a value between 0 and 1.

Mutation

The goal is to modify individuals in order to explore the search space. Some of the most used techniques are:

- Bitwise mutation.

Consists of choosing 1 or more genes and changing their values.

- Random resetting.

Consists of randomly choosing 1 or more genes and reset their values.

- Uniform mutation.

Consists of randomly choosing 1 or more genes and replace their values by a number within the constraints.

- Swap mutation.

Used for the permutation representation and consists of selecting two genes and swapping their values.

Pseudocode

Genetic algorithm

```
Parameters:
  N -> Population size
  G -> Maximum number of generations
  Pr -> Reproduction probability
  Pm -> Mutation probability
Return: The elite individual

Begin
  Create the initial population
  Calculate the population fitness
  Get the elite
  While the number of generations is less than G or a good solution hasn't been found
    Select the parents
    Apply crossover
    Apply mutation
    Calculate the population fitness
    Get the elite or include the elite in the population
  End while
End
```



# Evolutionary algorithms

## Genetic programming

### Description

The original goal was to evolve computational programs using syntax trees to solve a problem given a dataset.

This algorithm could instead be positioned in machine learning.

### Types of problems

Supervised learning problem.

### Representation

The individuals are usually represented as syntax trees.

So, the elements of each individual are:

- Terminals. Leaf nodes in the syntax tree.
- Functions. Internal nodes of a syntax tree, they can be seen as operations.

### Initial population

There are three ways to create the very first population.

- Full.

A set of trees are created with a given depth.
- Grow.

Each node randomly selects elements from either the set of Functions or the set of Terminals.
- Half-and-half.

As its name says, it's a mixture of full and grow.

### Parent selection technique

Tournament selection is the most used for this technique.

### Crossover/Recombination

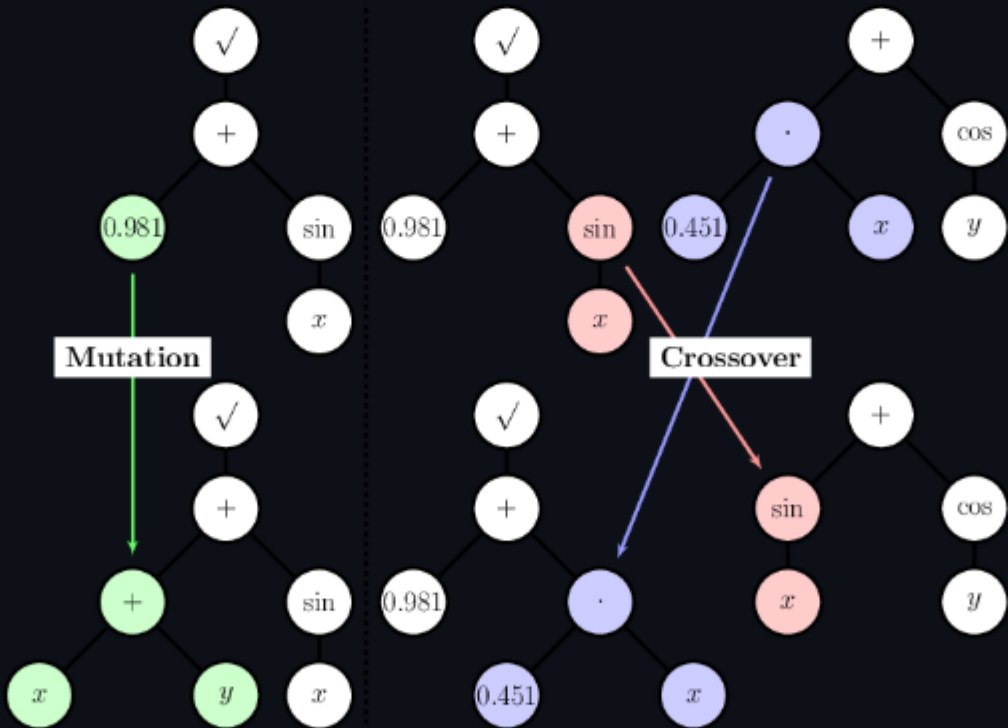
The classic crossover consists of randomly selecting a crossover point in each parent and using the subtree of the second parent instead of the first's.

### Mutation

- Subtree mutation

Randomly selects a mutation point in a tree and replaces the subtree for a random one.
- Point mutation

Consists of replacing a function F for another one with the same arity.



### Pseudocode

#### Genetic programming

```
Parameters:
N -> Population size

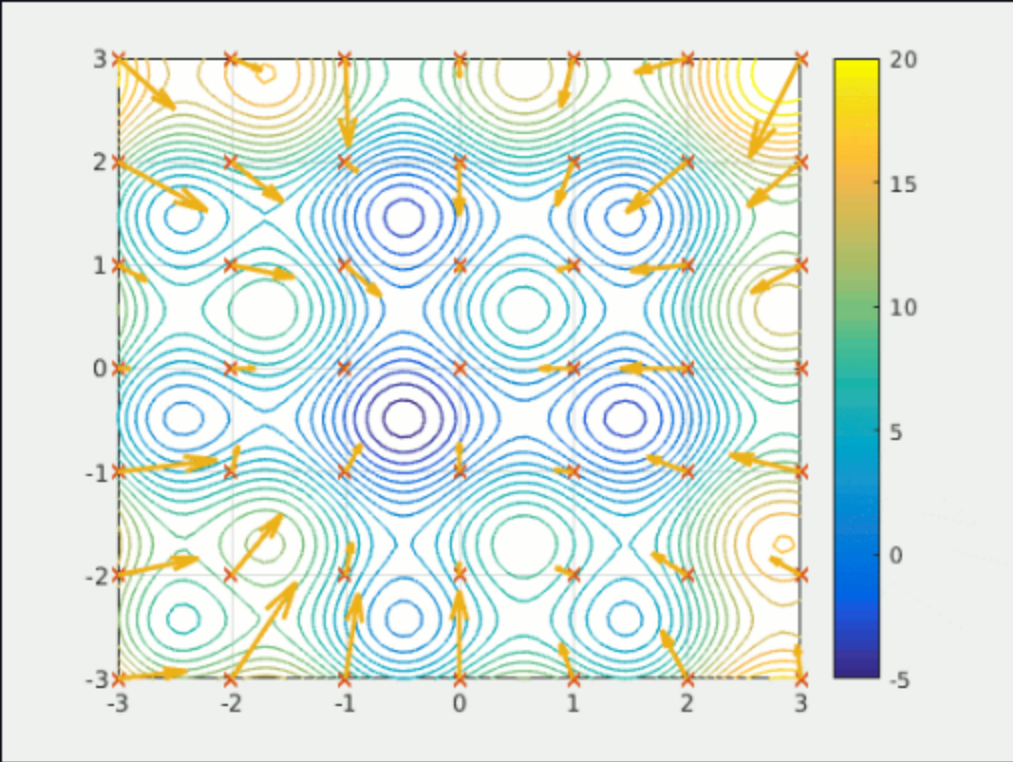
Return: Best program

Begin
  Create an initial population P of programs
  Calculate the fitness of all programs
  Get the best program
  While a termination criterion is not reached
    Parent selection
    Crossover
    Mutation
    Replace the worst one with the one just created
    Get new fitness
    if fitness(new) > fitness(best)
      Update best
    End if
  End while
End
```

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# Metaheuristics

## Particle swarm optimization



### Description

Inspired by the movement of a flock when searching for food.

### Types of problems

Continuous multidimensional problem optimization.

### Representation

Each particle represents a solution. And at the time  $t$ , a particle has a vector of positions and another one for velocities.

$$\vec{x^i(t)} = < x_1^i, x_2^i, \dots, x_d^i >$$
$$\vec{v^i(t)} = < v_1^i, v_2^i, \dots, v_d^i >$$

### Update

At each iteration, both the positions are updated.

Considering that  $P_{best}^i$  is the best position where a particle i has been,  $G_{best}^i$  is the global best location,  $r_1$  and  $r_2$  are random numbers between 0 and 1, and  $w$ ,  $c_1$  and  $c_2$  are hyper parameters that can be initiliazied at 0.9 and gradually reduced to 0.1.

$$v^i(t+1) = wv^i(t) + c_1r_1(P_{best}^i - x^i(t)) + c_2r_2(G_{best} - x^i(t))$$
$$x^i(t+1) = x^i(t) + v^i(t+1)$$

### Pseudocode

Particle swarm optimization

```
Parameters:
  N -> Number of particles
  maxIter -> Maximum number of iterations
  func -> Objective function
  bounds -> The search space

Return: the best position

Begin
  Initialize hyperparameters
  Create the particles positions and velocities randomly
  Calculate the objective function values
  Calculate the best position of each particle
  Calcule the best position
  While t < maxIter and a good solution hasn't been found
    For each particle i
      Update velocity
      Update position
      Calculate fitness
      Update best position of current particle
      Update best position
    End for
  End while
End
```