Optimization

Màster de Fonaments de Ciència de Dades

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Lecture IX. Stochastic methods: Genetic algorithms

What nature does (approximately)

Consider a population of rabbits and foxes in an isolated medium.

- At any given time there is a population of rabbits, some of them are faster and/or smarter than other rabbits.
- These faster and/or smarter rabbits are less likely to be eaten by foxes, and therefore more of them survive to do what rabbits do best: make more rabbits.
- Of course, some of the slower and/or dumber rabbits will survive just because they are lucky.
- The surviving population of rabbits starts breeding. The breeding results in a good mixture of rabbit genetic material: some slow rabbits breed with fast rabbits, some fast with fast, some smart rabbits with dumb rabbits, and so on.
- And on the top of that nature, every once in a while, mutates some of the rabbit genetic material.
- The resulting baby rabbits will (on average) be faster and smarter than these in the original population because more faster, smarter parents survived the foxes. (It is a good thing that the foxes are undergoing similar process - otherwise the rabbits might become too fast and smart for the foxes to catch any of them).

Genetic Algorithms and Evolution Programs

Genetic Algorithms belong to a wider class of methods that has been developed during the last fifty years.

Genetic Algorithms are a particular kind of procedures based on principles of evolution and hereditary. They receive the generic name of Evolution Programs.

Some Evolution Programs, are:

1. **Genetic Algorithms** (John Holland 1970's),
2. **Evolution Strategies**,
3. **Evolutionary Programming**,
4. **Scatter Search techniques**.

Genetic algorithms

For low dimension problems, classical exhaustive methods usually suffice.

There are many optimization problems, that arise frequently in applications, for which no reasonably fast algorithms have been developed.

Genetic Algorithms (GA), developed by John Holland in the early 1970's, are among such techniques.

- Genetic Algorithms are stochastic search methods that mimic natural biological evolution.
- Genetic algorithms operate on a population of potencial solutions applying the principle of survival to generate improved estimations to a solution.
- At each generation, a new set of approximations is created by the process of selecting individuals according to their level of fitness and breeding them together, using genetic operators inspired by nature.
- This process leads to the evolution of better populations than previous populations.

Evolution programs. Main characteristics

- An **evolution program** is a probabilistic iterative algorithm which, at each iteration $t \to t+1$, **maintains** a population of individuals,

$$P(t) = (x_1^t, x_2^t, ..., x_n^t) \longrightarrow P(t+1) = (x_1^{t+1}, x_2^{t+1}, ..., x_n^{t+1}).$$

- The **new population**

$$P(t+1) = (x_1^{t+1}, x_2^{t+1}, ..., x_n^{t+1}),$$

  is formed at each **iteration**, $t \to t+1$, by **selecting the best fit individuals** in the select step.

- Each x_i^t represents a **potential solution** to the problem, and is **implemented as some data structure**. Often, the x_i^t are called **chromosomes**.

- **Each** potential solution $\boldsymbol{x_i^t}$ is evaluated to give some measure of its **fitness**.

Evolution programs. Main characteristics

- Some **members of the new population undergo transformations** by means of **"genetic operators"** to form new solutions:
  - There are transformations –**mutation type**– which create new individuals by a **small change in a single individual**, and
  - Higher order transformations –**crossover type**– which create new individuals by **combining parts from several (two or more) individuals**. These transformations produce information exchange between different potential solutions.

    For example, if the parents are represented by five-dimensional vectors
    $$x_m^{t+1} = (a_1, b_1, c_1, d_1, e_1) \text{ and } x_k^{t+1} = (a_2, b_2, c_2, d_2, e_2),$$
    then crossing the chromosomes would produce the offspring
    $$x_m^{t+1} = (a_1, b_1, c_2, d_2, e_2) \text{ and } x_k^{t+1} = (a_2, b_2, c_1, d_1, e_1).$$
- After **some (usually very large) number of generations** it is hoped that the program converges,and the best individual represents a near-optimum solution.

Structure of an evolution program

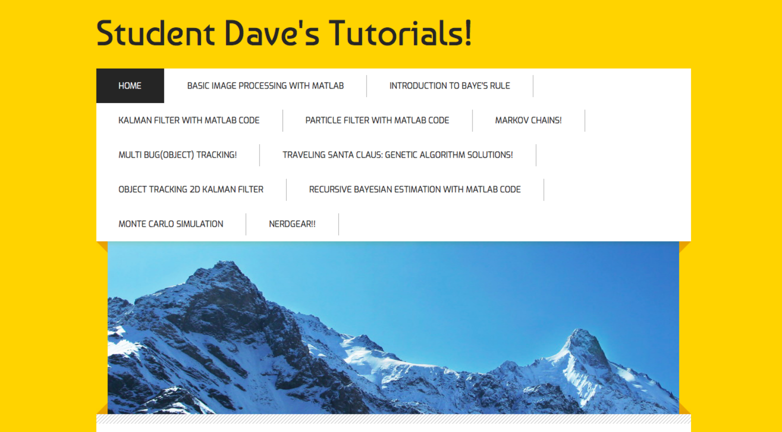
```
begin
    – $0 \rightarrow t$
    – initialize $P(t) = (x_1^t, x_2^t, ..., x_n^t)$
    – evaluate the fitness of the members
      of the population $P(t)$
    – while (not termination-condition) do
        – $t \rightarrow t + 1$
        – select the components of $P(t + 1)$ from $P(t)$
        – alter (mutation and crossover) $P(t + 1)$
        – evaluate the fitness of $P(t + 1)$
    – end do
end
```

Genetic algorithms. Example

Assume we search for a graph which should satisfy some requirements; for instance: we search for the optimal topology of a communication network accordingly to some criteria: cost of sending messages, reliability, etc.

- Each individual in the evolution program represents a potential solution to the problem, i.e., each individual is or represents a graph.
- The initial population of graphs $P(0)$ (either generated randomly or created as a result of some heuristic process) is a starting point ($t = 0$) for the evolution program.
- The evaluation function incorporates the problem requirements. The evaluation function returns the fitness of each graph, distinguishing between better and worse individuals.
- A few crossover operators can be considered which combine the structure of two (or more) graphs into one.
- Several mutation operators can be designed which would transform a single graph.
- Often such operators incorporate the problem-specific knowledge. For example, if the graph we look for is a connected tree, a possible mutation operator may delete an edge from the graph and add a new edge to connect two disjoint subgraphs.
- The other possibility would be to design a problem-independent mutation and incorporate this requirement into the evaluation function, penalizing graphs which are not trees.

Genetic algorithms. The travelling salesman problem for Santa Claus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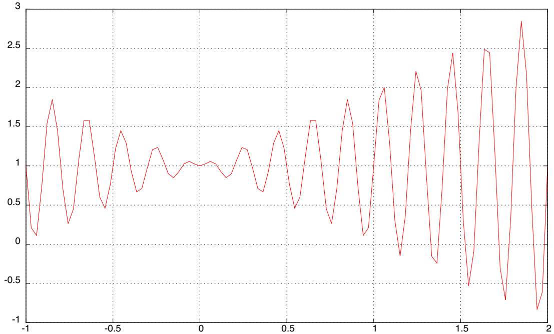
Optimization of a function

Problem: Find $x \in [-1, 2]$ that maximizes the function

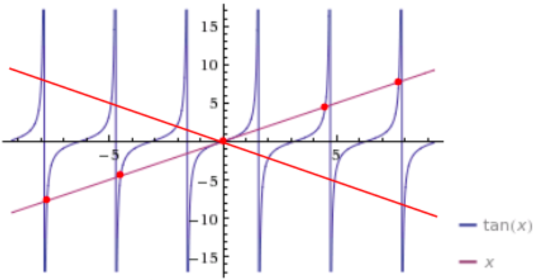
$$f(x) = x \sin(10\,\pi\, x) + 1.$$



The extrema of f are the zeros of

$$f'(x) = \sin(10\,\pi\, x) + 10\,\pi\, x \cos(10\,\pi\, x) = 0 \quad \Leftrightarrow \quad \tan(10\,\pi\, x) = -10\,\pi\, x.$$

Optimization of a function



The the zeros of $\tan(10\,\pi\,x) = -10\,\pi\,x$ are

$$\begin{aligned} x_i &= \frac{2i+1}{20} - \epsilon_i, \quad \text{for} \quad i = -1, -2, \ldots \\ x_0 &= 0 \\ x_i &= \frac{2i-1}{20} + \epsilon_i, \quad \text{for} \quad i = 1, 2, \ldots \end{aligned}$$

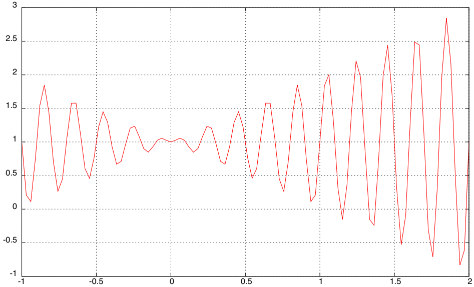
where $\{\epsilon_i\}$ is a decreasing sequence of real numbers approaching zero.

Optimization of a function

The function f reaches:

- its local maxima at x_i if i is odd,
- its local minima for x_i if i is even.

Since the domain of the problem is $[-1, 2]$, the function reaches its maximum for for $x_{19} = 37/20 + \epsilon_{19} \approx 1.85$, and the value of $f(x_{19})$ is approximately 2.28.



We are going construct a genetic algorithm to solve the above problem, i.e., to maximize the function f.

Optimization of a function. Representation

- We use a **binary vector** as a chromosome to represent real **values of the variable** x.
- The **length** of the vector depends on the **required precision**.
- In this example, the precision will be **six places after the decimal point**.
- The precision requirement implies that the range $[-1.0, 2.0]$ should be divided into, at least,

  $$3 \times 1\,000\,000 \;=\; 3\,000\,000$$

  equal size ranges.
- Since

  $$20\,971\,52 = 2^{21} < 3\,000\,000 < 2^{22} = 4\,194\,304,$$

  this means that **22 bits are required for each chromosome (value of x)**.

Optimization of a function. Representation

- The mapping from a binary string into a real number

$$(b_{21}b_{20}\ldots b_1 b_0)_2 \longrightarrow x \in [-1.0, 2.0],$$

  is done in two steps:

  - Convert the binary string $(b_{21}b_{20}\ldots b_1 b_0)_2$ from the base 2 to base 10:

$$(b_{21}b_{20}\ldots b_1 b_0)_2 = \sum_{i=0}^{21} b_i\, 2^i = b \in [0, 2^{22} - 1]$$

  - Find a corresponding real number x in the range $[-1, 2]$:

$$\begin{array}{ccc} [0, 2^{22} - 1] & \longrightarrow & [-1, 2] \\ b & \longrightarrow & x \end{array}$$

$$\frac{x - (-1)}{2 - (-1)} = \frac{b - 0}{2^{22} - 1 - 0} \quad \Rightarrow \quad \frac{x + 1}{3} = \frac{b}{2^{22} - 1} \quad \Rightarrow \quad x = \frac{3}{2^{22} - 1} b - 1.$$

Optimization of a function. Representation

- For instance, if the chromosome is $(1000101110110101000111)_2$, it represents the real number $x = 0.637196$, since

  $$b = (1000101110110101000111)_2 =$$

  $$= 2^0 + 2^1 + 2^2 + 2^6 + 2^8 + 2^{10} + 2^{11} + 2^{13} + 2^{14} + 2^{15} + 2^{17} + 2^{21} = 2\,288\,967$$

  and

  $$x = \frac{3}{4\,194\,303} 2\,288\,967 - 1.0 = 0.637196$$

- The chromosomes

  $$(0000000000000000000000)_2 \quad \text{and} \quad (1111111111111111111111)_2$$

  represent the boundaries of the domain, -1.0 and 2.0, respectively.

Optimization of a function. Initial population

The **initialization process of the GA** is simple:

- **Create a population** of chromosomes of a given population size.
- Each chromosome is a binary vector of 22 bits.
- All 22 bits for each chromosome are **initialized randomly.**

Optimization of a function. Evaluation function

The **fitness function** is the function f evaluated at the chromosomes (binary vectors b). We call it the **evaluation function**.

In the example, we want to maximize the function

$$f(x) = x \sin(10\,\pi\,x) + 1,$$

so, the evaluation function will be

$$\mathrm{eval}(b) = f(x) = x \sin(10\,\pi\,x) + 1,$$

where the chromosome b (in base 2) represents the real value x (in base 10).

The evaluation function plays the role of the environment, rating potential solutions in terms of their fitness.

Optimization of a function. Evaluation function

For example, the chromosomes

$$\begin{aligned} b_1 &= (1000101110110101000111)_2 \\ b_2 &= (0000001110000000010000)_2 \\ b_3 &= (1110000000111111000101)_2 \end{aligned}$$

correspond to values $x_1 = 0.637197$, $x_2 = -0.958973$, and $x_3 = 1.627888$, respectively.

Consequently, the evaluation function would rate them as follows:

$$\begin{aligned} \mathrm{eval}(b_1) &= f(x_1) = 1.586345 \\ \mathrm{eval}(b_2) &= f(x_2) = 0.078878 \\ \mathrm{eval}(b_3) &= f(x_3) = 2.250650 \end{aligned}$$

Clearly, the chromosome b_3, is the best of the three chromosomes, since its evaluation returns the highest value.

Optimization of a function. Genetic operations

- During the alteration phase of the genetic algorithm we would use the two genetic operators:
  - **mutation**
  - **crossover**
- **Mutation alters one or more genes** (positions in a chromosome) with a **probability** equal to a given **mutation rate**.
- Usually the mutation rate p_m is chosen to be very low (e.g., 0.01, 0.001).

Optimization of a function. Genetic operations

- Assume that the fifth gene from the b_3 chromosome was selected for a mutation (we will see how to do it). Since the fifth gene in this chromosome is 0, it would be flipped into 1. So the chromosome

$$b_3 = (1110000000111111000101)_2$$

after this mutation would be

$$b_3 \quad = \quad (1110100000111111000101)_2$$

- This chromosome represents the value

$$x_3' = 1.721638 \quad \text{and} \quad f(x_3') = -0.082257$$

This means that this particular mutation resulted in a significant decrease of the value of the chromosome b_3, since $f(x_3) = 2.250650$.

- On the other hand, if the 10th gene was selected for mutation in the chromosome b_3, then

$$b_3 \quad = \quad (1110000001111111000101)_2$$

Then

$$x_3'' = 1.630818 \quad \text{and} \quad f(x_3'') = 2.343555$$

and we get an improvement over the original value of $f(x_3) = 2.250650$.

Optimization of a function. Genetic operations

- Let us illustrate the **crossover** operator on chromosomes b_2 and b_3.
- Assume that the **crossover point** was **randomly** selected after the 5th gene:

$$\begin{aligned} b_2 &= (00000\,|\,01110000000010000)_2, \\ b_3 &= (11100\,|\,00000111111000101)_2. \end{aligned}$$

The two resulting offspring are

$$\begin{aligned} b_2' &= (00000\,|\,00000111111000101)_2, \\ b_3' &= (11100\,|\,01110000000010000)_2. \end{aligned}$$

The evaluation of these two offsprings gives

$$\begin{aligned} f(x_2') &= f(-0.998113) = 0.940865, \\ f(x_3') &= f(1.666028) = 2.459245. \end{aligned}$$

Note that the second offspring has a better evaluation than both of its parents (0.078878 and 2.250650).

Optimization of a function. Genetic operations

- For the **crossover** operator a **probability of crossover** p_c must be fixed.
- This probability **gives the expected number of chromosomes which undergo the crossover**.
- Usually, the probability of crossover p_c is chosen to be fairly high (e.g., $0.2 \sim 0.8$).

Optimization of a function. Experimental results

Consider the following simulation parameters for this problem:

- population size $pop.size = 50$,
- probability of crossover $p_c = 0.25$,
- probability of mutation $p_m = 0.01$.

The table provides the generation number (for 150 generations) for which there is an improvement in the evaluation function, together with the value of the function.

Generation number	Evaluation function
1	1.441942
6	2.250003
8	2.250283
9	2.250284
10	2.250363
12	2.328077
39	2.344251
40	2.345087
51	2.738930
99	2.849246
137	2.850217
145	2.850227

Optimization of a function. Experimental results

- The best chromosome, after 150 generations, was

  $$b_{max} = (1111001101000100000101)_2$$

  which corresponds to a value $x_{max} = 1.850773$.

- As expected, $x_{max} = 1.85 + \epsilon$, and $f(x_{max}) = 2.850227$ is slightly larger than 2.85.

Remark: In this example, we have not done any **selection process** before the mutation and the crossover operations.

How do GA work

- Suppose we wish to maximize a function of k variables

$$f(x_1, ..., x_k) : \mathbb{R}^k \rightarrow \mathbb{R}$$

- Suppose that each variable x_i can take values from a domain $D_i = [a_i, b_i] \subset \mathbb{R}$, and $f(x_1, ..., x_k) > 0$ for all $x_i \in D_i$.
- If the original f takes negative values, we can add some positive constant C to it, in order to make it positive
- We wish to optimize the function f with some required precision: suppose six decimal places for the values of the variables.

How do GA work

- It is clear that to achieve such precision each domain $D_i = [a_i, b_i]$ should be cut into $(b_i - a_i) \times 10^6$ equal size ranges.
- Denote by m_i the smallest integer such that $(b_i - a_i) \times 10^6 \leq 2^{m_i} - 1$. Then, a representation having each variable x_i coded as a binary string of length m_i clearly satisfies the precision requirement.
- The following formula gives the transformation from binary to decimal:

$$x_i = a_i + \frac{b_i - a_i}{2^{m_i} - 1} \text{decimal (binary string)}_2.$$

- Now, each chromosome (as a potential solution) is represented by a binary string of length

$$m = \sum_{i=1}^{k} m_i,$$

the first m_1 bits map into a value frorn the range $[a_1, b_1]$, the next group of m_2 bits map into a value from the range $[a_2, b_2]$, and so on.

How do GA work

- To **initialize a population**, we can simply set some number of chromosomes randomly in a bitwise fashion.
- If we do have some knowledge about the distribution of potential optima, we may use such information in arranging the set of initial potential solutions.
- The rest of the algorithm is straightforward:
  - in each generation we **evaluate each chromosome** (using the function f on the decoded sequences of chromosomes),
  - **select the new population** based on fitness values, and
  - **alter the chromosomes** in the new population by **mutation and crossover** operators.
- After some number of generations, when no further improvement is observed, the best chromosome represents an optimal solution (eventually the global).
- Often we stop the algorithm after a fixed number of iterations depending on speed and resource criteria.

The selection process

Selection of a new population

It can be done with different procedures: roulette wheel with slots, tournament selection, stochastic universal sampling,...

Roulette wheel with slots

We construct such a roulette wheel as follows:

- Calculate the **fitness value, $f(b_i)$, for each chromosome** b_i, for $i = 1, ..., pop.size$, where *pop.size* is the population size.
- Find the **total fitness** of the population

$$F = \sum_{i=1}^{pop.size} f(b_i).$$

- Calculate the **probability of a selection** p_i for each chromosome b_i

$$p_i = \frac{f(b_i)}{F}.$$

- Calculate a **cumulative probability** q_i for each chromosome b_i

$$q_i = \sum_{j=1}^{i} p_j, \quad \text{this is:} \quad q_1 = p_1, \; q_2 = p_1 + p_2, \; q_3 = p_1 + p_2 + p_3, \ldots$$

The selection process. The roulette wheel with slots

Roulette wheel with slots

The **selection process**, of the the roulette wheel with slots procedure, is based on **spinning the roulette wheel** *pop.size* **times**.

- Each time we select a single chromosome for a new population in the following way:
  - **Generate a random number** r in the range $[0, 1]$.
  - If $r < q_1$ then select the first chromosome b_1.
  - Otherwise **select the** $i - th$ **chromosome** b_i $(2 \leq i \leq pop.size)$ such that r **is between the two consecutive cumulative probabilities** q_{i-1} **and** q_i

$$q_{i-1} < r \leq q_i.$$

Obviously, some chromosomes would be selected more than once. This is in accordance with the "Schema Theorem": the best chromosomes get more copies, the average stay, and the worst die off.

When the selection process is finished, after *pop.size* selections, we are ready to apply the **mutation and crossover** operators to the individuals in the new population.

Other selection process. Tournament selection

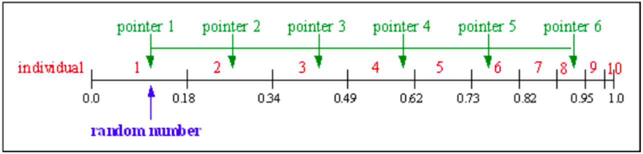
Tournament selection

- Tournament selection involves running several "tournaments" among a certain number of chromosomes (that depends on *pop.size*, and usually is not too large) chosen at random from the population.
- The winner of each tournament (the one with the best fitness) is selected for the new population.
- Selection pressure is easily adjusted by changing the tournament size.
- If the tournament size is large, weak individuals have a small chance to be selected.
- The procedure is repeated until a “new” population of *pop.size* individuals is generated (*pop.size* tournaments).

Other selection process. Stochastic universal sampling

Stochastic universal sampling

- In the stochastic universal sampling, the individuals b_i are first mapped to contiguous segments of a line, such that each individual's segment is equal in size to its fitness $f(b_i)$.



- The procedure makes a **single spin** of the roulette wheel, that **provides a starting position** (random number $r \in [0, 1]$) and the first selected individual.

- The **selection process** then proceeds by **advancing all the way around the wheel in equal sized steps**, where the step size is determined by the number of individuals to be selected. In this way, equally spaced pointers are placed over the line as many as there are individuals to be selected

Other selection process. Stochastic universal sampling

- Note that this does not mean that every candidate on the wheel will be selected.

  Some weak individuals will have very thin slices of the wheel and these might be stepped over completely depending on the random starting position.

- Stochastic universal sampling can have bad performance when a member of the population has a really large fitness in comparison with other members.

The crossover operator

- The **probability of crossover**, p_c, is one of the key parameters of a genetic algorithm.
- This probability **gives the expected number of chromosomes which undergo the crossover** operation.
- The value of p_c is chosen to be fairly high ($0.2 \sim 0.8$).

The crossover operator

The crossover operator proceeds in the following way:

- For each chromosome in the population:
    - Generate a random number r from the range $[0, 1]$.
    - If $r < p_c$ select the chromosome for crossover.
- Next we mate all the selected chromosomes randomly:
    - For each pair of selected chromosomes we generate a random integer number, *pos*, in the range $[1, ..., m-1]$ (m is the total length - number of bits - in a chromosome).
    - The number *pos* indicates the position of the crossing point.
    - Then each pair of selected chromosomes

      $$(b_1, b_2, ..., b_{pos}, b_{pos+1}, ..., b_m) \quad \text{and} \quad (c_1, c_2, ..., c_{pos}, c_{pos+1}, ..., c_m)$$

      are replaced by a pair of their offspring

      $$(b_1, b_2, ..., b_{pos}, c_{pos+1}, ..., c_m) \quad \text{and} \quad (c_1, c_2, ..., c_{pos}, b_{pos+1}, ..., b_m)$$

The mutation operator

- The **mutation** operator is performed on a bit-by-bit basis.
- The probability of mutation p_m, gives us the expected number of mutated bits p_m. Usually, p_m is chosen to be very low (e.g., 0.001).
- Every bit of the chromosomes in the whole population has an equal chance to undergo mutation, i.e., change from 0 to 1 or vice versa.
- The operator proceeds in the following way:
  - For each chromosome in the current population (i.e., after selection and crossover), and for each bit within the chromosome, generate a random number r in the range $[0, 1]$.
  - If $r < p_m$ mutate the bit.

The iterative procedure

- Following selection, crossover, and mutation, the new population is ready for its next evaluation.
- This evaluation is used to build the probability distribution (for the next selection process), i.e., for a construction of a roulette wheel with slots sized according to current fitness values.
- The rest of the evolution is just cyclic repetition of the above steps.

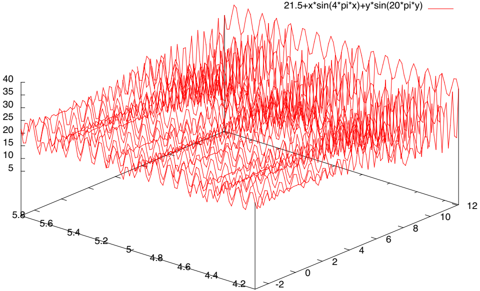
Example

We want to maximize the following function

$$f(x, y) = 21.5 + x\sin(4\,\pi\,x) + y\sin(20\,\pi\,y),$$

with

$$(x, y) \in [-3.0, 12.11] \times [4.5, 5.8]$$



We will use a GA with a population size $pop.size = 20$, and as probabilities of the genetic operators of crossover $p_c = 0.25$ and mutation $p_m = 0.01$.

Example (cont.)

- Assume that the required precision is four decimal places for each variable.
- The domain of variable "x", $[-3.0, 12.11]$, has length 15.1. The precision requirement implies that the x-range $[-3.0, 12.11]$ should be divided into at least 15.1×10^4 equal size ranges. This means that 18 bits are required as the first part of the chromosome:

$$2^{17} < 151\,000 \leq 2^{18}$$

- The domain of variable "y", $[4.1, 5.8]$, has length 1.7. The precision requirement implies that the range $[4.1, 5.8]$ should be divided into at least 1.7×10^4 equal size ranges. This means that 15 bits are required as the second part of the chromosome:

$$2^{14} < 17\,000 \leq 2^{15}$$

- The total length of a chromosome (solution vector) is then $m = 18 + 15 = 33$ bits; the first 18 bits code "x" and remaining 15 bits $(19 - 33)$ code "y".

Example (cont.)

- Let us consider an example chromosome

$$(010001001011010000\ 111110010100010)$$

- The first 18 bits

$$010001001011010000$$

represent

$$x = -3 + \frac{12.1 - (-3.0)}{2^{18} - 1} \text{decimal}(010001001011010000)_2 = 1.052426$$

The next 15 bits

$$111110010100010$$

represent

$$y = 4.1 + \frac{5.8 - 4.1}{2^{15} - 1} \text{decimal}(111110010100010)_2 = 5.755330$$

So the chromosome corresponds to $(x, y) = (1.052426, 5.755330)$.

- The fitness value for this chromosome is

$$f(1.052426, 5.755330) = 20.252640.$$

Example (cont.)

Assume that after the initialization process we get the following population:

$$
\begin{aligned}
b_1 &= (100110100000001111\ 111010011011111) \\
b_2 &= (111000100100110111\ 001010100011010) \\
b_3 &= (000010000011001000\ 001010111011101) \\
b_4 &= (100011000101101001\ 111000001110010) \\
b_5 &= (000111011001010011\ 010111111000101) \\
b_6 &= (000101000010010101\ 001010111111011) \\
b_7 &= (001000100000110101\ 111011011111011) \\
b_8 &= (100001100001110100\ 010110101100111) \\
b_9 &= (010000000101110100\ 010110101100111) \\
b_{10} &= (000001111000110000\ 011010000111011) \\
b_{11} &= (011001111110110101\ 100001101111000) \\
b_{12} &= (110100010111101101\ 000101010000000) \\
b_{13} &= (111011111010001000\ 110000001000110) \\
b_{14} &= (000010011000001010\ 100111100101001) \\
b_{15} &= (111011101101110000\ 100011111011110) \\
b_{16} &= (110011110000011111\ 100001101001011) \\
b_{17} &= (011010111111001111\ 010001101111101) \\
b_{18} &= (011101000000001111\ 010011110101101) \\
b_{19} &= (000101010011111111\ 110000110001100) \\
b_{20} &= (101110010110011110\ 011000101111110)
\end{aligned}
$$

Example (cont.)

During the evaluation phase we decode each chromosome and calculate the fitness function values from (x, y) values just decoded. We get:

$$\begin{array}{ll}
f(b_1) = 26.019600 & f(b_2) = 7.580015 \\
f(b_3) = 19.526329 & f(b_4) = 17.406725 \\
f(b_5) = 25.341160 & f(b_6) = 18.100417 \\
f(b_7) = 16.020812 & f(b_8) = 17.959701 \\
f(b_9) = 16.127799 & f(b_{10}) = 21.278435 \\
f(b_{11}) = 23.410669 & f(b_{12}) = 15.011619 \\
f(b_{13}) = 27.316702 & f(b_{14}) = 19.876294 \\
f(b_{15}) = 30.060205 & f(b_{16}) = 23.867227 \\
f(b_{17}) = 13.696165 & f(b_{18}) = 15.414128 \\
f(b_{19}) = 20.095903 & f(b_{20}) = 13.666916
\end{array}$$

It is clear, that the chromosome b_{15} is the best one, and the chromosome b_2 the worst.

Next, construct a roulette wheel with slots for the selection process.

The total fitness of the population is

$$F = \sum_{i=1}^{20} f(b_i) = 387.776822$$

Example (cont.)

The **probability of a selection** p_i for each chromosome is:

$$\begin{aligned}
p_1 &= f(b_1)/F = 0.067099 & p_2 &= f(b_2)/F = 0.019547 \\
p_3 &= f(b_3)/F = 0.050355 & p_4 &= f(b_4)/F = 0.044889 \\
p_5 &= f(b_5)/F = 0.065350 & p_6 &= f(b_6)/F = 0.046677 \\
p_7 &= f(b_7)/F = 0.041315 & p_8 &= f(b_8)/F = 0.046315 \\
p_9 &= f(b_9)/F = 0.041590 & p_{10} &= f(b_{10})/F = 0.054873 \\
p_{11} &= f(b_{11})/F = 0.060372 & p_{12} &= f(b_{12})/F = 0.038712 \\
p_{13} &= f(b_{13})/F = 0.070444 & p_{14} &= f(b_{14})/F = 0.051257 \\
p_{15} &= f(b_{15})/F = 0.077519 & p_{16} &= f(b_{16})/F = 0.061549 \\
p_{17} &= f(b_{17})/F = 0.035320 & p_{18} &= f(b_{18})/F = 0.039750 \\
p_{19} &= f(b_{19})/F = 0.051823 & p_{20} &= f(b_{20})/F = 0.035244
\end{aligned}$$

From the values of the probability of a selection we compute the **cumulative probability of each chromosome** q_i.

Example (cont.)

$q_1 = 0.067099$	$q_2 = 0.086647$	$q_3 = 0.137001$	$q_4 = 0.181890$
$q_5 = 0.247240$	$q_6 = 0.293917$	$q_7 = 0.335232$	$q_8 = 0.381546$
$q_9 = 0.423137$	$q_{10} = 0.478009$	$q_{11} = 0.538381$	$q_{12} = 0.577093$
$q_{13} = 0.647537$	$q_{14} = 0.698794$	$q_{15} = 0.776314$	$q_{16} = 0.837863$
$q_{17} = 0.873182$	$q_{18} = 0.912932$	$q_{19} = 0.964756$	$q_{20} = 1.000000$

Now we are ready to spin the roulette wheel 20 times.

Each time we select a single chromosome for a new population.

Assume that a (random) sequence of 20 numbers from the range $[0, 1]$ is:

0.513870	0.175741	0.308652	0.534534	0.947628
0.171736	0.702231	0.226431	0.494773	0.424720
0.703899	0.389647	0.277226	0.368071	0.983437
0.005398	0.765682	0.646473	0.767139	0.780237

– The first number $r = 0.513870$ is greater than q_{10} and smaller than q_{11}, meaning the chromosome b_{11} is selected for the new population.
– The second number $r = 0.175741$ is greater than q_3 and smaller than q_4, meaning the chromosome b_4 is selected for the new population, etc.

The new population consists of the following chromosomes:

Example (cont.)

$$\begin{aligned}
b'_1 &= (01100111111011010110000110111100 0) && (b_{11})\\
b'_2 &= (10001100010110100111100000111001 0) && (b_4)\\
b'_3 &= (00100010000011010111101101111101 1) && (b_7)\\
b'_4 &= (01100111111011010110000110111100 0) && (b_{11})\\
b'_5 &= (00010101001111111111000011000110 0) && (b_{19})\\
b'_6 &= (10001100010110100111100000111001 0) && (b_4)\\
b'_7 &= (11101110110111000010001111101111 0) && (b_{15})\\
b'_8 &= (00011101100101001101011111110001 01) && (b_5)
\end{aligned}$$

Example (cont.)

Now we are ready to apply the recombination operator, **crossover**, to the individuals in the new population (vectors b_i').

The probability of crossover $p_c = 0.25$, so we expect that (on average) 25% of chromosomes (i.e., 5 out of 20) undergo crossover.

We proceed in the following way:

- For each chromosome in the (new) population we generate a random number r from the range $[0, 1]$.
- If $r < p_c = 0.25$, we select a given chromosome for crossover.

Let us assume that the sequence of random numbers is:

0.822951	0.151932	0.625477	0.314685	0.346901
0.917204	0.519760	0.401154	0.606758	0.785402
0.031523	0.869921	0.166525	0.674520	0.758400
0.581893	0.389248	0.200232	0.355635	0.826927

This means that the chromosomes b_2', b_{11}', b_{13}' and $b_{18'}$ are selected for crossover.

We have been lucky: the number of selected chromosomes is even, so we can pair them easily. If the number of selected chromosomes were odd, we would either add one extra chromosome or remove one selected chromosome - this choice is made randomly as well.

Example (cont.)

Now we **mate selected crhromosomes randomly**: say, the first two (i.e., b'_2 and b'_{11}) and the next two (i.e., b'_{13} and b'_{18}) are coupled together.

For each of these two pairs, we generate a random integer number *pos* from the range [1 : 32] (33 is the total length - number of bits - in a chromosome).

The number *pos* indicates the position of the crossing point. The first pair of chromosomes is

$$\begin{aligned} b'_2 &= (100011000101101001111000001110010) \\ b'_{11} &= (111011101101110000100011111011110) \end{aligned}$$

and the generated random number is $pos = 9$. These chromosomes are cut after the 9th bit and replaced by a pair of their offspring:

$$\begin{aligned} b''_2 &= (111011101101101001111000001110010) \\ b''_{11} &= (100011000101110000100011111011110) \end{aligned}$$

Example (cont.)

The second pair of chromosomes is

$$\begin{aligned} b'_{13} &= (000101000010010101001010111111011) \\ b'_{18} &= (111011111010001000110000001000110) \end{aligned}$$

and the generated number $pos = 20$. These chromosomes are replaced by a pair of their offspring:

$$\begin{aligned} b''_{13} &= (111011111010001000111010111111011) \\ b''_{18} &= (000101000010010101000000001000110) \end{aligned}$$

The current population is now:

Example (cont.)

$$
\begin{aligned}
b'_1 &= (011001111110110101100001101111000)\\
b''_2 &= (111011101101101001111000001110010)\\
b'_3 &= (001000100000110101111011011111011)\\
b'_4 &= (011001111110110101100001101111000)\\
b'_5 &= (000101010011111111100000110001100)\\
b'_6 &= (100011000101101001111000001110010)\\
b'_7 &= (111011101101110000100011111011110)\\
b'_8 &= (000111011001010011010111111000101)\\
b'_9 &= (011001111110110101100001101111000)\\
b'_{10} &= (000010000011001000001010111011101)\\
b''_{11} &= (100011000101110000100011111011110)\\
b'_{12} &= (010000000101110100010110101100111)\\
b'_{13} &= (111011111010001000111010111111011)\\
b'_{14} &= (100001100001110100010110101100111)\\
b'_{15} &= (101110010110011110011000101111110)\\
b'_{16} &= (100110100000001111111010011011111)\\
b'_{17} &= (000001111000110000011010000111011)\\
b''_{18} &= (000101000010010101000000001000110)\\
b'_{19} &= (111011101101110000100011111011110)\\
b'_{20} &= (110011110000001111100001101001011)
\end{aligned}
$$

Example (cont.)

The next operator, **mutation**, is performed on a bit-by-bit basis.

- The probability of mutation is $p_m = 0.01$, so we expect that (on average) 1% of bits would undergo mutation.
- There are $m \times pop.size = 33 \times 20 = 660$ bits in the whole population, so we expect 6.6 mutations in each generation.
- Every bit has an equal chance to be mutated, so, for every bit in the population we generate a random number r in the range $[0, 1]$; if $r < 0.01$ we mutate the bit.
- This means that we have to generate 660 random numbers. In a sample run, only 5 of these numbers were smaller than 0.01.
- The the random number, the bit number, the chromosome number and the bit number within the chromosome are:

Random num.	Bit num.	Chromosome num.	Bit in chrom.
0.000213	112	4	13
0.009945	349	11	19
0.008809	418	13	22
0.005425	429	13	33
0.002836	602	19	8

Example (cont.)

The current version of the population is:

$$
\begin{array}{rcl}
b_1 & = & (011001111110110101100001101111000) \\
b_2 & = & (111011101101101001111000001110010) \\
b_3 & = & (001000100000110101111011011111011) \\
b_4 & = & (011001111110110101100001101111000) \\
b_5 & = & (000101010011111111110000110001100) \\
b_6 & = & (100011000101101001111000001110010) \\
b_7 & = & (111011101101110000100011111011110) \\
b_8 & = & (000111011001010011010111111000101) \\
b_9 & = & (011001111110110101100001101111000) \\
b_{10} & = & (000010000011001000001010111011101) \\
b_{11} & = & (100011000101110000100011111011110) \\
b_{12} & = & (010000000101110100010110101100111) \\
b_{13} & = & (000101000010010101001010111111011) \\
b_{14} & = & (100001100001110100010110101100111) \\
b_{15} & = & (101110010110011110011000101111110) \\
b_{16} & = & (100110100000001111111010011011111) \\
b_{17} & = & (000001111000110000011010000111011) \\
b_{18} & = & (000101000010010101000000001000110) \\
b_{19} & = & (111011101101110000100011111011110) \\
b_{20} & = & (110011110000011111100001101001011)
\end{array}
$$

Example (cont.)

We have just completed one iteration (i.e., one generation) of the while loop in the genetic procedure.

Let us examine the results of the evaluation process of the new population.

During the evaluation phase we decode each chromosome and calculate the fitness function values from (x, y) values just decoded. We get:

$$\begin{array}{ll}
f(b_1) = 23.410669 & f(b_2) = 18.201083 \\
f(b_3) = 16.020812 & f(b_4) = 23.1412613 \\
f(b_5) = 20.095903 & f(b_6) = 17.406725 \\
f(b_7) = 30.060205 & f(b_8) = 25.341160 \\
f(b_9) = 23.410669 & f(b_{10}) = 19.526329 \\
f(b_{11}) = 33.351874 & f(b_{12}) = 16.127799 \\
f(b_{13}) = 22.692462 & f(b_{14}) = 17.959701 \\
f(b_{15}) = 13.666916 & f(b_{16}) = 26.019600 \\
f(b_{17}) = 21.278435 & f(b_{18}) = 27.591064 \\
f(b_{19}) = 27.608441 & f(b_{20}) = 23.867227
\end{array}$$

The total fitness of the new population F is 447.049688, which is much higher than total fitness of the previous population, 387.776822.

Also, the best chromosome now (b_{11}) has a better evaluation (33.351874) than the best dmmosome (b_{15}) from the previous population (30.060205).

Example (cont.)

After 1000 generations the fitness values of the population are:

$$
\begin{array}{ll}
f(b_1) = 30.298543 & f(b_2) = 26.869724 \\
f(b_3) = 30.316575 & f(b_4) = 31.933120 \\
f(b_5) = 30.316575 & f(b_6) = 34.356125 \\
f(b_7) = 35.458636 & f(b_8) = 23.309078 \\
f(b_9) = 34.393820 & f(b_{10}) = 30.316575 \\
f(b_{11}) = 35.477938 & f(b_{12}) = 35.456066 \\
f(b_{13}) = 30.316575 & f(b_{14}) = 32.932098 \\
f(b_{15}) = 30.746768 & f(b_{16}) = 34.359545 \\
f(b_{17}) = 32.932098 & f(b_{18}) = 32.956664 \\
f(b_{19}) = 19.669670 & f(b_{20}) = 32.956664
\end{array}
$$

If we look carefully at the progress during the run, we may discover that in earlier generations the fitness values of some chromosomes were better than the value 35.477938 of the best chromosome after 1000 generations. For example, the best chromosome in generation 396 had value of 38.827553. This is due to the stochastic errors of sampling.

It is relatively easy to keep track of the best individual in the evolution process.

It is customary (in genetic algorithm implementations) to store "the best ever" individual at a separate location; in that way, the algorithm would report the best value found during the whole process (as opposed to the best value in the final population).

Stopping conditions

Some of the various stopping condition are:

- **Maximum generations.** The genetic algorithm stops when the specified number of generation's have evolved.
- **Elapsed time.**The genetic process will end when a specified (cpu) time has elapsed. Note: If the maximum number of generations has been reached before the specified time has elapsed, the process will end.
- **No change in fitness.**The genetic process will end if there is no change to the population's best fitness for a specified number of generations. *Note:* If the maximum number of generations has been reached before the specified number of generations with no changes has been reached, the process will end.
- **Stall generations.**The algorithm stops if there is no improvement in the objective function for a sequence of consecutive generations of length Stall generations.
- **Stall time limit.**The algorithm stops if there is no improvement in the objective function during an interval of cpu time in seconds equal to Stall time limit.

The Fundamental Theorem of Genetic Algorithms

The **Fundamental Theorem of Genetic Algorithms**, also called the Schema theorem, says, in short, that low-order schema with above-average fitness increase exponentially in successive generations. These particular schema are called building blocks.

Definitions:

A **schema** is a template that identifies a subset of strings with similarities at certain string positions.

The **order** of a schema is defined as the number of fixed positions in the template

The **defining length** is the distance between the first and last specific positions.

The **average fitness of a schema** is the average fitness of all strings matching the schema.

For example, consider a binary string of length 6:

- The schema $\begin{array}{|c|c|c|c|c|c|}\hline 1 & x & 1 & 0 & x & 1 \\ \hline\end{array}$ describes the set of all strings of length 6 with 1's at positions 1, 3 and 6, and a 0 at position 4.
- The "x' is a wildcard symbol, which means that positions 2 and 5 can have a value of either 1 or 0.
- The **order** of the schema is 4, and its **defining length** is $6 - 1 = 5$.

The Fundamental Theorem of Genetic Algorithms

Theorem.

For a given schema H, let:

- $m(H, t)$ be the relative frequency of the schema H in the population of the t^{th} generation,
- $f(H)$ be the mean fitness of the schema H,
- $o(H)$ be the order of the schema,
- l be length of the strings (chromosomes),
- $\delta(H)$ be the defining length of the string H,
- $\overline{f}$ be the average fitness of the current population,
- p_c be the crossover probability,
- p_m be the mutation probability.

Then, the espectation of $m(H, t+1)$ is

$$E[m(H, t+1)] \geq m(H, t)\frac{f(H)}{\overline{f}}\left[1 - p_c\frac{\delta(H)}{1-l}\right](1-p_m)^{o(H)}.$$

The above fundamental theorem states that schemas with mean fitness greater than the population average fitness $\left(m(H,t)\frac{f(H)}{\overline{f}}\right)$, short defining length $\left(1 - p_c\frac{\delta(H)}{1-l}\right)$, and lower order $\left((1-p_m)^{o(H)}\right)$ are more likely to survive.

Chromosome representations. The Traveling Salesman Problem (TSP)

The problem: *A traveling salesman must visit every city in his territory exactly once and then return to the starting point. Given the cost of travel between all cities, how should he plan his itinerary for minimum total cost of the entire tour?*

- To solve the problem with a GA, first, we should address an important question connected with the chromosome representation: should we leave a chromosome to be an integer vector, or rather we should transform it into a binary string?
- Until now, we represented a chromosome as a binary vector. This allowed us to use binary mutation and crossover; applying these operators we got legal offspring, i.e., offspring within the search space.
- This is not the case for the traveling salesman problem. In a binary representation of a n cities TSP problem, each city should be coded as a string of $\log_2 n$ bits: if there are 20 cities, we need 5 bits to represent a city.
- A chromosome will be a string of n ordered cities, this is of $n \log_2 n$ bits.

The Traveling Salesman Problem (TSP)

- A mutation can result in a sequence of cities which is not a tour, this is: we can get the same city twice in a sequence.
- Moreover, for a TSP with 20 cities some 5-bit sequences (for example, $(10101)_2 = 21$) do not correspond to any city. Similar problems are present when applying crossover operator.
- Clearly, if we use mutation and crossover operators as defined earlier, we would need some sort of a "repair algorithm"; such an algorithm would "repair" a chromosome, moving it back into the search space.
- It seems that the integer vector representation is better: instead of using repair algorithms, we can incorporate the knowledge of the problem into operators.
- In this particular approach we accept integer representation: a vector $v = (i_1, i_2, ..., i_n)$ represents a tour: from i_1 to i_2, etc., from i_{n-1} to i_n and back to i_1, where v is a permutation of $\{1, 2, ..., n\}$.

The Traveling Salesman Problem (TSP)

- For the **initialization** process we can either use some heuristics, or we can initialize the population by a random sample of permutations of $\{1, 2, ..., n\}$.

- The evaluation of a chromosome is straightforward: given the cost of travel between all cities, we can easily calculate the total cost of the entire tour.

- Given two parents, one can construct an offspring by choosing a subsequence of a tour from one parent and preserving the relative order of cities from the other parent. For example, if the parents are

  $$(1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12) \qquad (3, 7, 1, 11, 4, 12, 5, 2, 10, 9, 6, 8)$$

  and the chosen part is

  $$(4, 5, 6, 7)$$

  the resulting offspring is

  $$(1, 11, 4, 5, 6, 7, 12, 2, 10, 9, 8, 3)$$

Last exercise

Exercise 11. To be delivered before 14-I-2019 (`Ex11-YourSurname.pdf`)

Use a genetic algorithm to solve the example of page 38 with population size $pop.size = 50$.