

Knowledge Engineering

Lecture Notes on Natural Computation

– 2004-2005 –

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Genetic Algorithms

– Introduction –

Terminology (From Biology)

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- Mutation: Error occurring during DNA replication from parents

From Biology to Genetic Algorithms

We can borrow some terms (and ideas) from biology . . .

- Chromosome: The coding of a possible solution for a given problem, usually represented with an array of bits or characters
- Gene: A single bit or a set of bits coding part of the solution
- Allele: One of the elements used to code the genes
- Fitness: Evaluation of the actual solution

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. . . to model a learning process as evolution:

- Crossover: Generate new solution by “mixing” two existing solutions
- Mutation: Random change in the solution

Genetic Algorithms: A Powerful Idea from Nature

Genetic Algorithms are a part of *evolutionary computing*, and they are inspired by Darwin's theory of evolution:

Problems are solved by an evolutionary process that mimics natural evolution in looking for a best (fittest) solution (survivor)

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We can trace a brief history of evolutionary computation:

1. 1960: Ingo Rechenberg introduces the idea of evolutionary computing in his work "Evolution strategies"
2. 1975: John Holland invents Genetic Algorithms and publish his book "Adaption in Natural and Artificial Systems"
3. 1992: John Koza has uses genetic algorithm to evolve programs to perform certain tasks. He called his method Genetic Programming
4. ...

Genetic Algorithm Applications

They have been used for many applications:

- Optimization (e.g., circuits layout, job shop scheduling, ...)
- Prediction (e.g., weather forecast, protein folding, ...)
- Classification (e.g., fraud detection, quality assessment, ...)
- Economy (e.g., bidding strategies, market evaluation, ...)
- Ecology (e.g., biological arm races, host-parasite coevolution, ...)
- Automatic programming
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In general they are best suited for

- Big search space, non unimodal, non smooth
- Noisy fitness function, usually not analytic
- We do not want to spend years looking for the global optimum, but we just want a good sub-optimum in a reasonable time

Outline of the Basic Genetic Algorithm

1. [Start] Generate random population of n chromosomes (suitable solutions)
2. [Fitness] Evaluate the fitness $f(x)$ of each chromosome x in the population
3. [New population] Create a new population by repeating following steps until the new population is complete
 - (a) [Selection] Select two parent chromosomes from a population according to their fitness (the better fitness, the bigger chance to be selected)
 - (b) [Crossover] With a crossover probability cross over the parents to form new offspring. If no crossover was performed, offspring is the exact copy of parents.
 - (c) [Mutation] With a mutation probability mutate new offspring at each locus
 - (d) [Accepting] Place new offspring in the new population
4. [Replace] Use new generated population for a further run of the algorithm
5. [Test] If the end condition is satisfied, return the best solution in current population
6. [Loop] Go to step 2

Two Comments to the Basic Genetic Algorithm

There are many parameters and settings that can be implemented differently in various problems:

- How to create chromosomes and what type of encoding choose
- How to select parents for crossover in the hope that the better parents will produce better offspring
- How to define crossover and mutation, the two basic operators of GA

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It seems there is some “black magic” behind genetic algorithms . . . Why do genetic algorithms work?

- It can be partially explained by the Schema Theorem
- They have been modeled using Monte Carlo Markov Chains

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But first of all we'll have a look to a simple example . . .

Example: Minimum of a Function

In this simple example we are looking for the extreme of a function defined over a search space.

1. Search Space: An interval of the real line
2. Fitness Function: The value of the function we are “exploring”

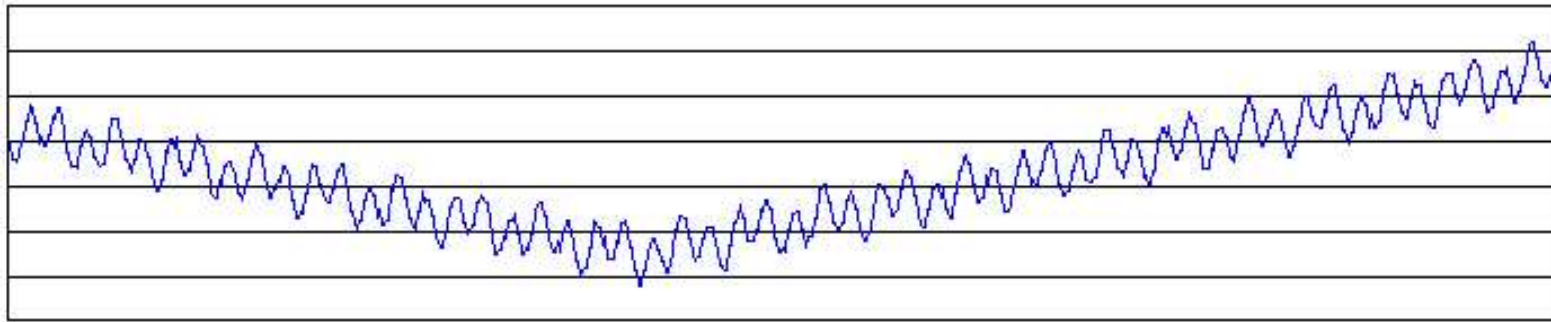
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Functions can get quite nasty ;)

Minimization Example: Chromosome Encoding

The first step in developing a genetic algorithm is defining a solution encoding:

- A chromosome should in some way contain information about solution that it represents
- The encoding depends mainly on the solved problem (e.g., integer or real numbers, permutations, parsing trees, ...)
- The most used way of encoding is a binary string; each bit in the string can represent some characteristics of the solution

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Our chromosome then could look like this:

Chromosome 1	1	1	0	1	1	0	0	1	0	0	1	1	0	1	1	0
Chromosome 2	1	1	1	0	1	1	1	0	0	0	0	1	1	1	1	0

Each chromosome is represented by the binary code of a real number

Minimization Example: Crossover Operator

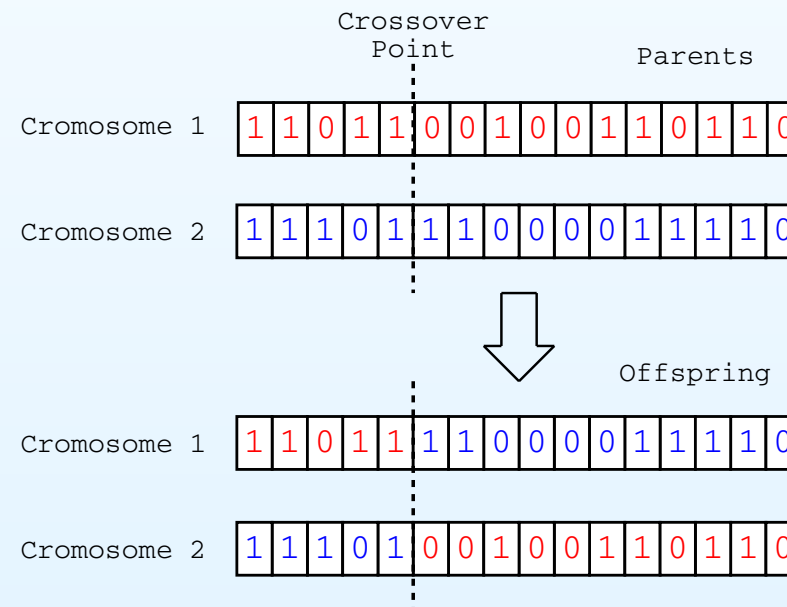
Crossover operates on selected genes from parent chromosomes and creates new offspring, the simplest way how to do that is:

1. Choose randomly some crossover point in the chromosome
2. Copy everything before this point from the first parent and then copy everything after the crossover point from the other parent

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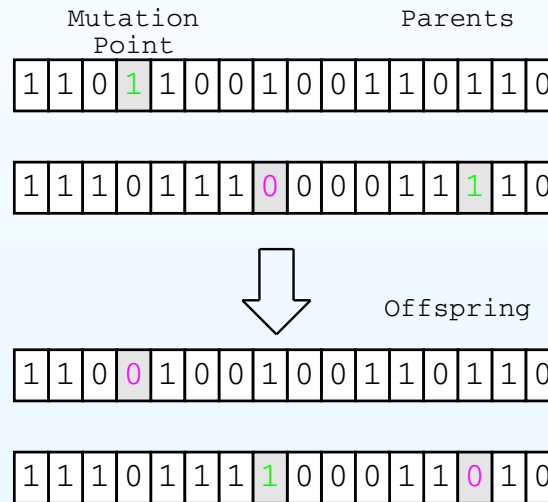


Note: Crossover depends mainly on the encoding of chromosomes. Specific crossover made for a specific problem can improve or reduce performance of the genetic algorithm

Minimization Example: Mutation Operator

After a crossover is performed, mutation takes place:

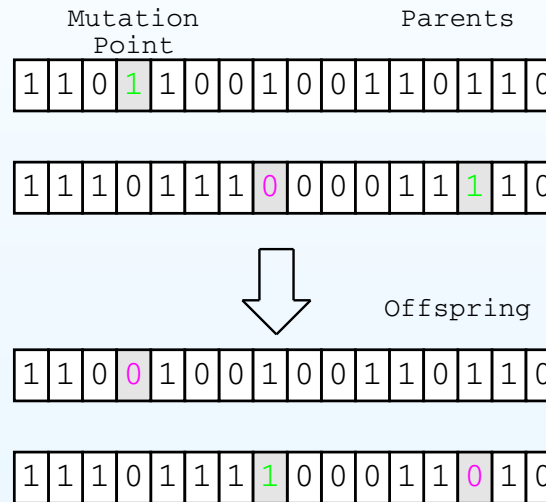
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Few notes on mutation:

- Mutation is intended to prevent falling of all solutions in the population into a local optimum
- Also mutation depends on the encoding of chromosomes (e.g., when we are encoding permutations, mutation could be performed as an exchange of two genes)

Minimization Example: Demo

Stolen from:
http://cs.felk.cvut.cz/~xobitko/ga/example_f.html

Genetic Algorithms

– Into the groove –

Genetic Algorithms Explained: Encoding (I)

Binary encoding is the most common one (mainly because the first research of GA used this type of encoding)

- In binary encoding, every chromosome is a string of bits (0 or 1)
- Simple Implementation of the genetic operators
- Not always natural for many problems

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Example of Problem: *Knapsack problem*

- There are things with given value and size. The knapsack has given capacity. Select things to maximize the value of things in knapsack, but do not extend knapsack capacity.
- Each bit says, whether the corresponding thing is in knapsack.

Genetic Algorithms Explained: Encoding (II)

Permutation encoding can be used in ordering problems

- Every chromosome is a string of numbers that represent a position in a sequence
- Crossover and mutation must be designed to leave the chromosome consistent (i.e. have real sequence in it)

Cromosome 1	1	5	7	8	3	5	13	10	11	11	6	12	1	14	2	4	6	9
Cromosome 2	2	9	14	1	11	5	8	15	13	6	12	16	7	3	10	4		

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Example of Problem: *Traveling salesman problem (TSP)*

- There are cities and given distances between them. Traveling salesman has to visit all of them, but he does not want to travel more than necessary. Find a sequence of cities with a minimal travelled distance.
- Chromosome describes the order of cities

Genetic Algorithms Explained: Encoding (III)

Direct value encoding can be used in problems where some more complicated values are required

- Every chromosome is a sequence of some values connected to the problem, such as (real) numbers, chars or any objects
- Good choice for some special problems, but necessary to develop some specific crossover and mutation

Chromosome	A	B	D	H	Y	V	S	V
Chromosome	2.5678	1.4361	3.3426	7.8761				
Chromosome	open	walk	back	close				

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Example of Problem: *Finding weights for a neural network*

- A neural network is given with defined architecture. Find weights between neurons to get the desired output from the network
- Real values in chromosomes represent weights in the neural network

Genetic Algorithms Explained: Encoding (IV)

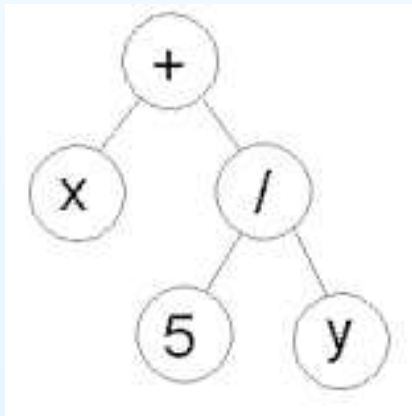
Tree encoding is used mainly for evolving programs or expressions (i.e., genetic programming)

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- Programming language LISP is often used for this purpose, so crossover and mutation can be done relatively easily.

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Chromosome (+ x (/ 5 y))

Example of Problem: *Finding a function that would approximate given pairs of values*

- Input and output values are given. The task is to find a function that will give the best outputs for all inputs.
- Chromosomes are functions represented in a tree

Genetic Algorithms Explained: Selection (I)

According to Darwin's theory of evolution the best chromosome survive to create new offspring. There are many methods in selecting the best chromosomes:

- Roulette wheel selection,
- Rank selection
- Tournament selection
- Boltzmann selection
- ...

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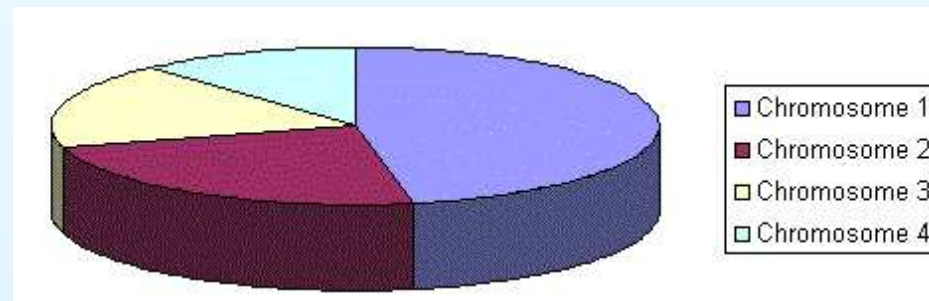
Elitism

When creating a new population by crossover and mutation, we have a big chance, that we will loose the best chromosome. Elitism is the name of the method that first copies the best chromosome (or few best chromosomes) to the new population. It can rapidly increase the performance, because it prevents a loss of the best found solution.

Genetic Algorithms Explained: Selection (II)

Roulette Wheel Selection: Parents are selected proportionally to their fitness. The better they are, the more chances to be selected they have.

1. Imagine a roulette wheel where all the chromosomes in the population are placed
2. The size of the section in the roulette wheel is proportional to the value of the fitness function of every chromosome - the bigger the value is, the larger the section is
3. A marble is thrown in the roulette wheel and the chromosome where it stops is selected



Genetic Algorithms Explained: Crossover/Mutation (I)

For binary encoding we have many operators:

- Single point crossover: one crossover point is selected, binary string from the beginning of the chromosome to the crossover point is copied from the first parent, the rest is copied from the other parent
- Two point crossover: two crossover points are selected, binary string from the beginning of the chromosome to the first crossover point is copied from the first parent, the part from the first to the second crossover point is copied from the other parent and the rest is copied from the first parent again
- Uniform crossover: bits are randomly copied from the first or from the second parent
- Arithmetic crossover: some arithmetic operation is performed to make a new offspring (e.g., logic AND)
- Mutation: inversion of selected bits

Genetic Algorithms Explained: Crossover/Mutation (II)

For permutation encoding we have to preserve consistency:

- Single point crossover: one crossover point is selected, the permutation is copied from the first parent till the crossover point, then the other parent is scanned looking for the other numbers

$$(1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9) + (4\ 5\ 3\ 6\ 8\ 9\ 7\ 2\ 1) = (1\ 2\ 3\ 4\ 5\ 6\ 8\ 9\ 7)$$

- Order changing mutation: two numbers are selected and exchanged

$$(1\ 2\ 3\ 4\ 5\ 6\ 8\ 9\ 7) \Rightarrow (1\ 8\ 3\ 4\ 5\ 6\ 2\ 9\ 7)$$

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For real value encoding we can reuse crossover from binary encoding:

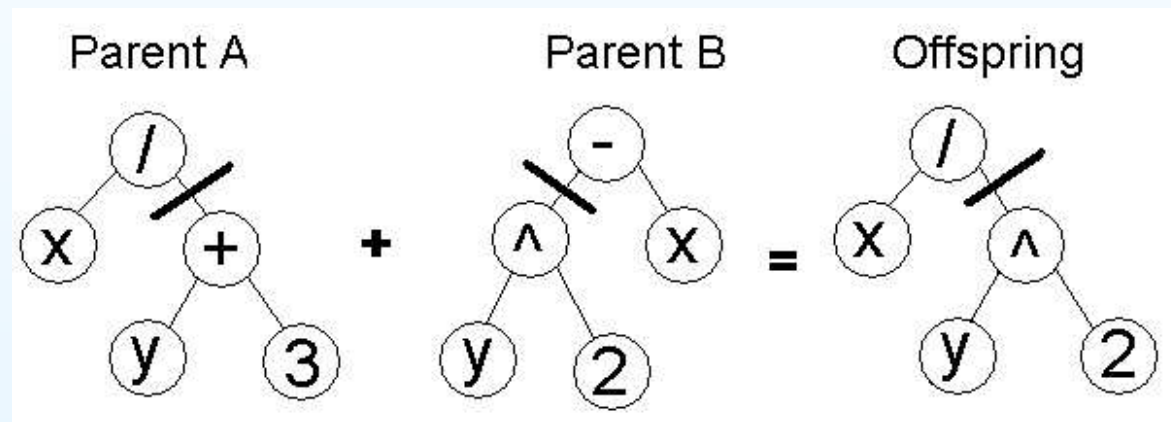
- Mutation: a small number is added (or subtracted) to selected values

$$(1.29\ 5.68\ 2.86\ 4.11\ 5.55) \Rightarrow (1.29\ 5.68\ 2.73\ 4.22\ 5.55)$$

Genetic Algorithms Explained: Crossover/Mutation (III)

Specific operators have to be selected also for tree encoding

- Tree crossover: one crossover point is selected in both parents, parents are divided in that point and the parts below crossover points are exchanged to produce new offspring



- Changing mutation: the operator, number, or variable in a randomly selected node is changed

Time for Another Demo

Stolen again from:
<http://cs.felk.cvut.cz/~xobitko/ga/tspexample.html>

Tips & Tricks

These “rules of thumb” are often results of empiric studies performed on binary encoding only, but they usually work fine . . .

- Crossover rate should be high generally, about 80% – 95% (However some results show that for some problems crossover rate about 60% is the best.)
- Mutation rate should be very low. Best rates seems to be about 0.5% – 1% per allele
- Very big population size usually does not improve performance (in the sense of speed of finding solution). Good population size is about 20 – 30, however sometimes sizes 50 – 100 are reported as the best
- Basic roulette wheel selection can be used, but sometimes rank selection can be better. Elitism should be used for sure if you do not use other method for saving the best found solution.

Understanding Genetic Algorithms: Building Blocks

Holland (1975) formalized the idea of building block and schema:

A string S will contain sub-strings. We can represent this as a 'similarity template string' (i.e., the schema) H which uses a 'wild card' symbol to mark positions not belonging to the sub-strings (they can take 1 or 0).

Example: schema $**11$ represents strings 1111, 0011, 1011 and 0111.
Alternatively, 1011 and 1101 contain common schemata $1***$, $***1$ and $1**1$.

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*Note: Since 2 strings have 3 common schemata each, making a total of 6 schemata; processing a string implicitly processes many more schemata.
In general, for a string of length l , there are 3^l schemata.*

This property is usually referred as implicit parallelism.

Understanding Genetic Algorithms: Schema Theorem

By evaluating many string we implicitly estimate the expected value of schemas, and working out a “little bit of math” we can approximate the expected number of schemas at next step:

$$M(H_i, t + 1) \geq M(H_i, t) \cdot \left[\frac{f(H_i)}{\bar{f}} \right] \cdot \left[1 - p_c \cdot \frac{\delta(H_i)}{l - 1} \right] \cdot \left[(1 - p_m)^{o(H_i)} \right].$$

- $f(H_i)$: Mean fitness of the i^{th} schema
- \bar{f} : Mean fitness of population
- $\delta(H_i)$: Length of the i^{th} schema
- l : Length of strings in the search space
- $o(H_i)$: Number of valid bits in the schema

Understanding Genetic Algorithms: What's going on?

The previous formula states two important concepts for the understanding of genetics algorithm:

Schema Theorem

Above average fitness, short, low-order schema will have a large survival probability. They will grow at least exponentially in the population.

Building Block Hypothesis

Short, highly fit, low order schemata are called building blocks; it is thought that they represent partial solutions to the problem and that processing them will build up the full solution.