Evolutionary algorithms

- Simple genetic algorithms
- Evolutionary Strategies
- Genetic Programming

Genetic algorithms

- Randomized search algorithms based on mechanics of natural selection and genetics
- Principle of natural selection through `survival of the fittest' with randomized search
- Search efficiently in large spaces
- Robust w.r.t. to the complexity of the search problem
- Many applications in hybrid systems (Fuzzy logic, neural networks)

Advantages of GAs

- Evolution and natural selection has proven to be a robust and flexible method for adaptation
- GAs can be used to represent complex problems relatively easily compared to traditional approaches
- GAs can be easily parallelized and run on multiple machines

Basic elements

- Solutions require encoding
- Encoding is called a chromosome or genotype
- Solution represented by chromosome is the phenotype
- A number of individuals form a population

- Population is updated iteratively; each iteration is called a generation
- Objective function is called the fitness function
- Evaluate multiple solutions (in parallel) for the next search step

Some definitions

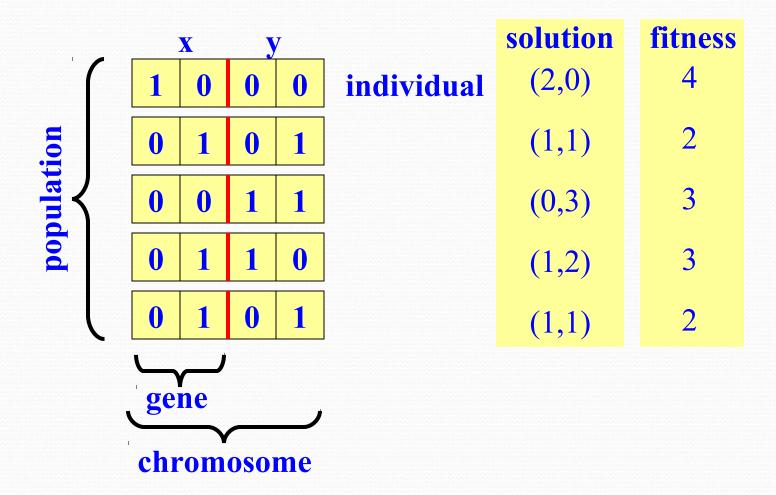
- Population: a collection of solutions for the studied (optimization) problem
- Individual: a single solution in a GA
- Chromosome (genotype): representation for a single solution
- Gene: part of a chromosome, usually representing a variable as part of the solution

Some definitions

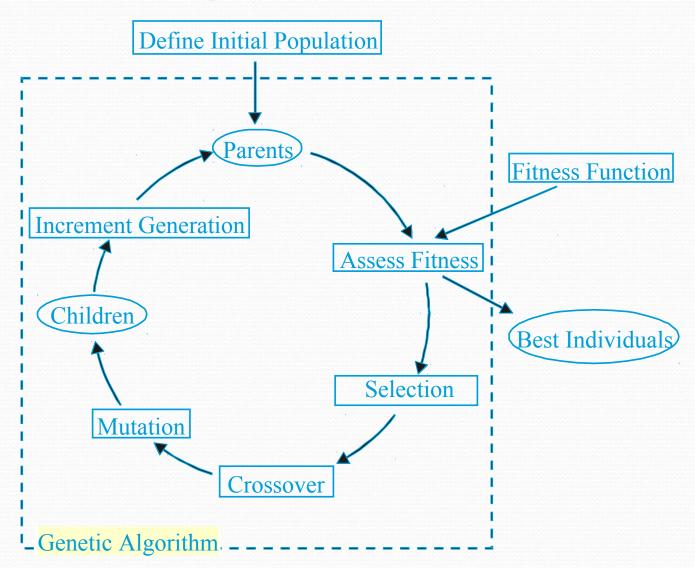
- **Encoding**: conversion of a solution to its equivalent representation (chromosome)
- Decoding: conversion of a chromosome (genotype) to its equivalent solution (phenotype)
- Fitness: scalar value denoting the suitability of a solution

GA terminology

Generation t



Genetic algorithm



Pseudo code

- Initialize population *P*:
 - E.g. generate random p solutions
- Evaluate solutions in *P*:
 - determine for all $h \in P$, Fitness(h)
- While terminate is FALSE
 - Generate new generation P using genetic operators
 - Evaluate solutions in P
- **Return** solution $h \in P$ with the highest Fitness

Termination criteria

- Number of generations (restart GA if best solution is not satisfactory)
- Fitness of best individual
- Average fitness of population
- Difference of best fitness (across generations)
- Difference of average fitness (across generations)

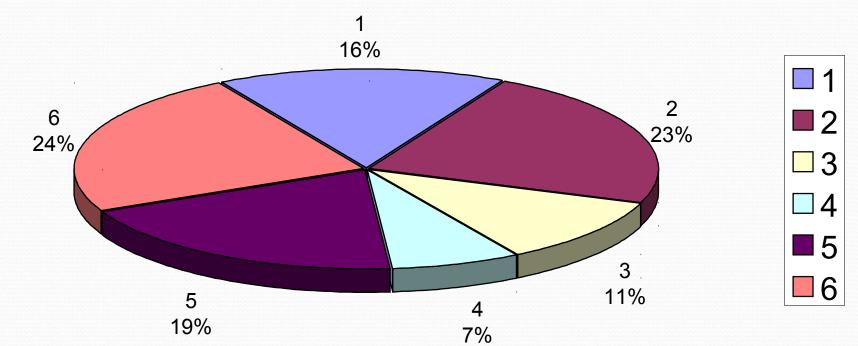
Reproduction

Three steps:

- Selection
- Crossover
- Mutation

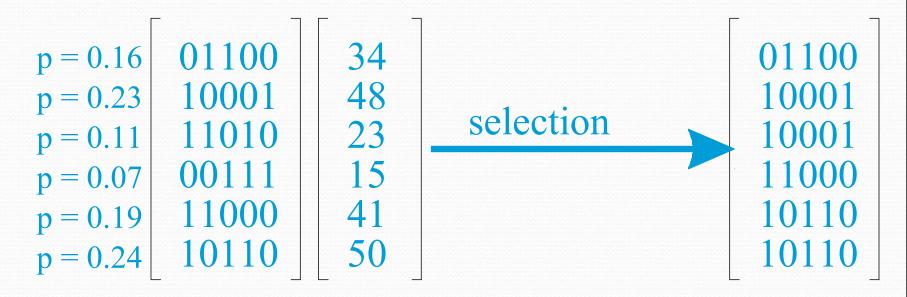
In GAs, the population size is often kept constant. User is free to choose which methods to use for all three steps.

Roulette-wheel selection



Roulette-wheel selection

individuals fitness



Sum = 211

Cumulative probability: 0.16, 0.39, 0.50, 0.57, 0.76, 1.00

Tournament selection

- Select pairs randomly
- Fitter individual wins
 - deterministic
 - probabilistic
 - constant probability of winning
 - probability of winning depends on fitness

It is also possible to combine tournament selection with roulette-wheel

Crossover

 Exchange parts of chromosome with a crossover probability (p_c is usually about o.8)

Select crossover points randomly

 One-point crossover:

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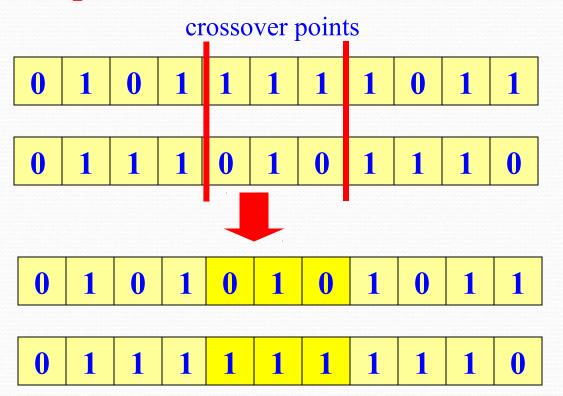
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N-point crossover

- Select N points for exchanging parts
- Exchange multiple parts

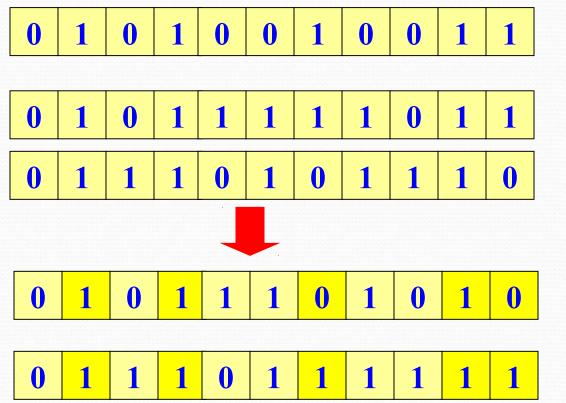
Two-point crossover:



Uniform crossover

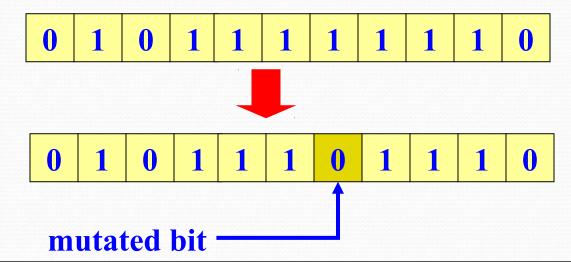
Exchange bits using a randomly generated mask

mask

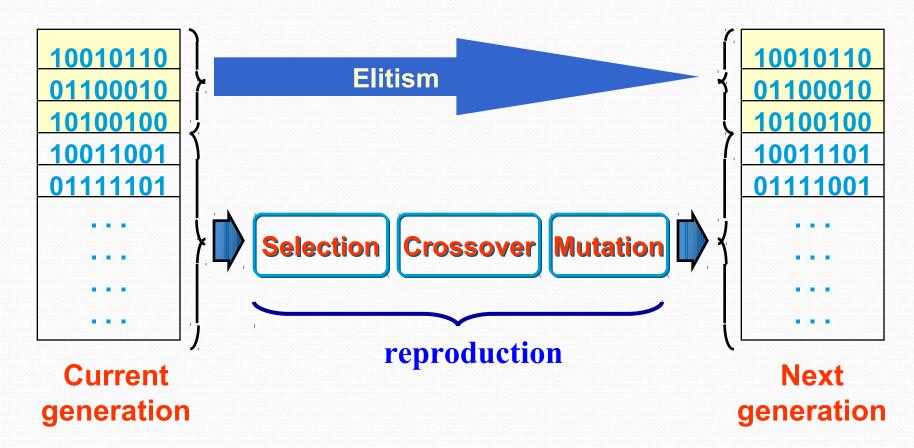


Mutation

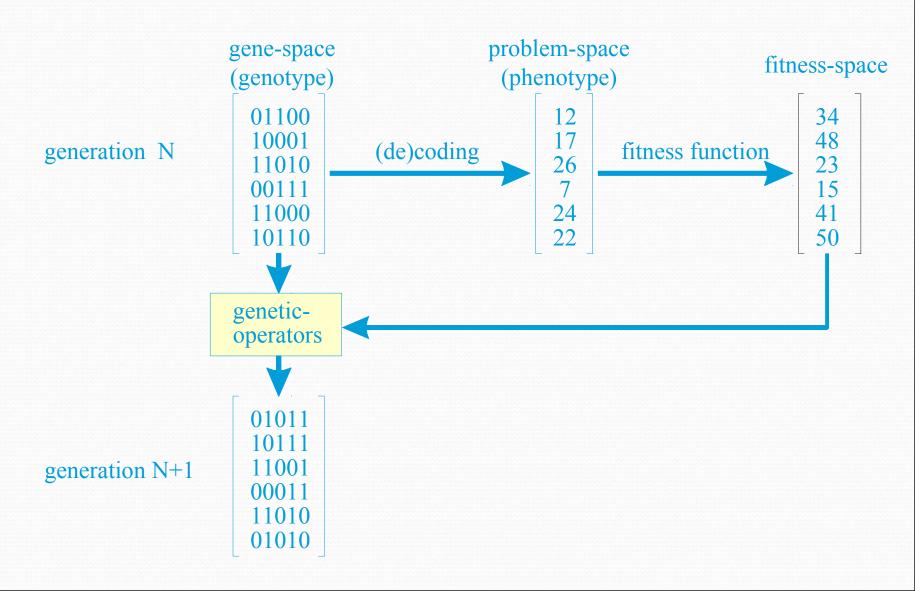
- Crossover is used to search the solution space
- Mutation is needed to escape from local optima
- Introduces genetic diversity
- Mutation is rare (p_m is about 0.005)
 Uniform mutation:



GA iteration



Spaces in GA iteration



Encoding and decoding

- Common coding methods for numbers
 - simple binary coding
 - Gray coding (binary)
 - real valued coding (evolutionary strategies)

Constraints

- Examples:
 - "A string of numbers should represent a permutation" (1,2,3) is valid; (1,1,3) is not
 - "The sum of numbers should not be lower than a threshold"
- Explicit handling: fitness function modification
 - setting fitness of unfeasible solutions to zero (search may be very inefficient due to unfeasible solutions)
 - penalty function (negative terms for violated constraints)
 - barrier function (already penalty if "close to" violation)

Constraints

- Implicit (preferred method): special encoding
 - GA searches always for allowed solutions
 - smaller search space
 - ad hoc method, may be difficult to find
- Example: permutations

- Insert mutation:
 - Pick two allele values at random
 - Move the second to follow the first, shifting the rest along to accommodate
 - Note: this preserves most of the order and adjacency information; changes the position of numbers a lot

Removed Adjancency: (2,3), (4,5), (5,6)

Added Adjacency: (2,5), (4,6), (5,3)

Removed orders: 3->5, 4->5

Added orders: 5->3, 5->4

Changed positions: 3, 4, 5

- Swap mutation:
 - Pick two alleles at random and swap their positions
 - Disrupts adjacency information and order more; preserves positions

Removed Adjancency:

Added Adjacency:

Removed order:

Added order:

Changed positions:

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

```
1 2 3 4 5 6 7 8 9
```

- Scramble mutation:
 - Pick a subset of genes at random (not necessarily consecutive)
 - Randomly rearrange the alleles in those positions

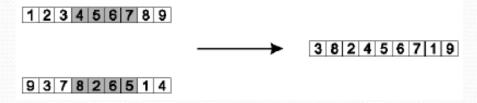
```
1 2 3 4 5 6 7 8 9
```

Crossover for Permutations

- Order one crossover:
 - Choose an arbitrary part from the first parent, copy this part to the first child



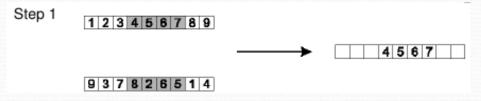
- Copy the numbers that are not in the first part, to the first child:
 - starting right from cut point of the copied part,
 - using the order of the second parent and wrapping around at the end



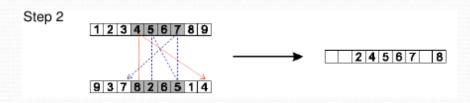
Analogous for the second child, with parent roles reversed

Crossover for Permutations

- Partially Mapped Crossover (PMX):
 - Choose random segment and copy it from P1

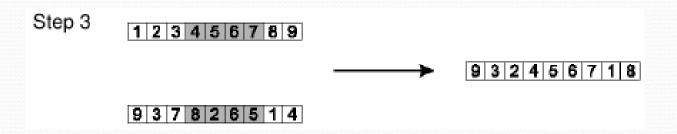


- Starting from the first crossover point look for elements in that segment of P2 that have not been copied
- For each of these i look in the offspring to see what element j has been copied in its place from P1
- Place i into the position occupied j in P2, since we know that we will not be putting j there (as is already in offspring)
- If the place occupied by j in P2 has already been filled in the offspring k, put i in the position occupied by k in P2



Crossover for Permutations

- Partially Mapped Crossover (PMX):
 - Having dealt with the elements from the crossover segment, the rest of the offspring can be filled from P2.

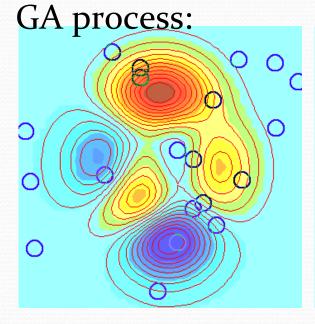


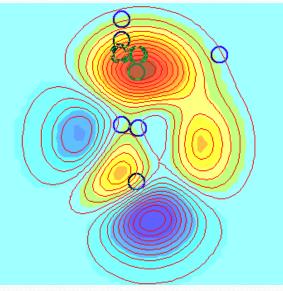
Idea: maintain position

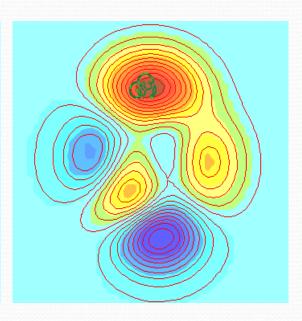
Order vs Position in Permutations

- Order, but not position of numbers is important in problems such as the traveling salesman problem (visiting all cities in a certain order)
- Position, but not order of numbers is important in problems such as allocating visitors in hotels to rooms (visitors have to be allocated once to one room, but the order of the allocation does not matter)

Example





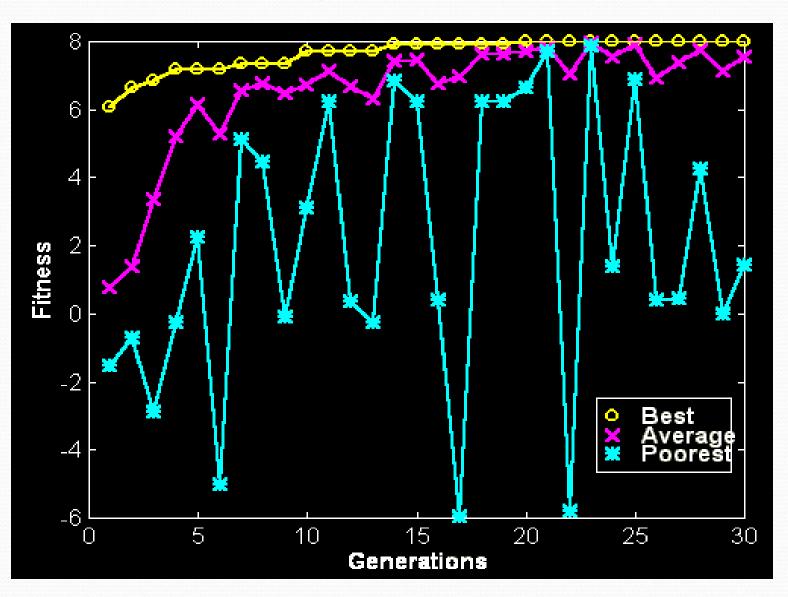


Initial population

5th generation

10th generation

Performance profile

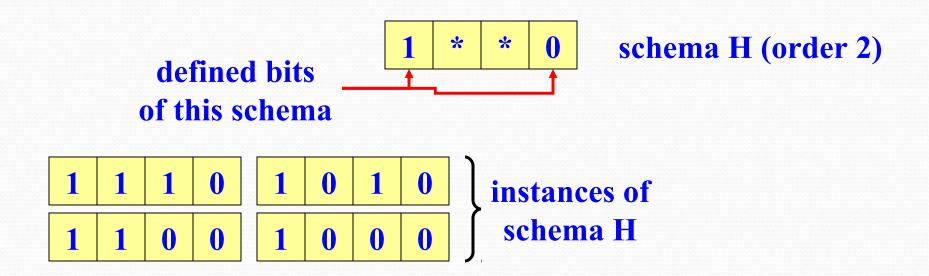


Schema Theory

- Why do genetic algorithms work?
- We will prove that genetic algorithms focus their search on high-quality combinations of high-quality building blocks

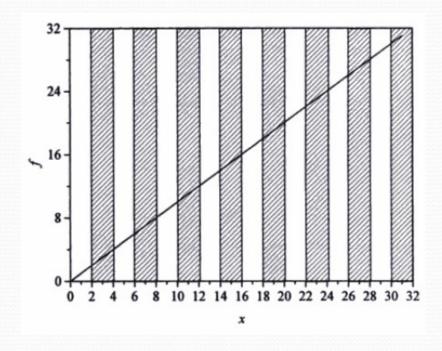
Schema

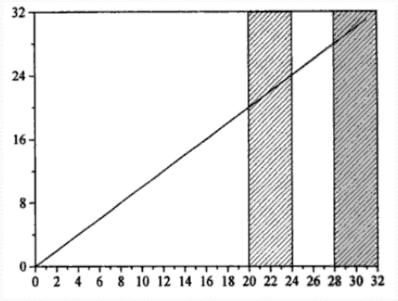
- A schema is a bit string with 1's, 0's and don't cares (*)
- It represents parts of a chromosome
- Order of schema: number of defined bits in the schema



Schema Examples

• f(x)=x, "standard" binary encoding





Schema ***1*
(Mediocre fitness)

Schema 1*1**
(Good fitness)

- Given $\xi(S,t)$, the number of strings in a population at time *t* matched by schema *S*
- Estimate $\xi(S, t+1)$
- Step 1: Selection
 - Let $\bar{f}(P) = \sum f(h)/|P|$ (Average fitness of population)
 - Let $\bar{f}(S, P) = \sum f(h)/|P'|$ (Average fitness schema) $h \in P'$

(after selection only)

where
$$P'$$
 is the set of individuals in P matched by S

Then it is expected that $\xi(S,t+1) = \xi(S,t) \frac{\bar{f}(S,P)}{\bar{f}(P)}$

- Step 2: Crossover
 - Let $\delta(S)$ be the defining length of the schema, i.e. the distance between the first and last defined elements

$$**1**1* \rightarrow 6 - 3 = 3$$

 $1*****1 \rightarrow 7 - 1 = 6$

- Let *n* be the length of the strings in the population
- Then crossover will "destroy" a schema with probability

$$p_c \cdot \frac{\delta(S)}{n-1}$$

- Step 3: Mutation
 - Let o(S) be the order of schema S
 - Then the schema remains unchanged with probability $(1-p_m)^{o(S)}$

 Overall, after selection, crossover and mutation, the expected number of instances of a schema is

$$\xi(S, t+1) = \xi(S, t) \frac{\bar{f}(S, P)}{\bar{f}(P)} (1 - p_c \frac{\delta(S)}{n-1}) (1 - p_m)^{o(S)}$$

Schema Theorem
 Short, low-order, above average schemata receive exponentially increasing trials in subsequent generations of a genetic algorithm

$$\xi(S, t+1) = \xi(S, t) \frac{\bar{f}(S, P)}{\bar{f}(P)} (1 - p_c \frac{\delta(S)}{n-1}) (1 - p_m)^{o(S)}$$

Building Block Hypothesis

A genetic algorithm seeks near-optimal performance through combination of short, low-order, highperformance schemata, called the building blocks

Implicit Parallelism

• A population of size |P| with individuals of length n represents between 2^n and $2^{|P|n}$ schemata

 Hence, many schemata are implicitly considered at the same time

Evolutionary Strategies

- Main idea: individuals consist of vectors of real numbers (not binary)
- Redefinitions of
 - selection
 - crossover
 - mutation
- Operations executed in the order crossover → mutation → selection

ES: Selection

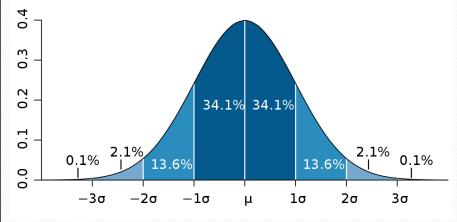
- Not performed before mutation and crossover, but <u>after</u> these operations
- It is assumed mutation (& crossover) generate $\lambda > \mu$ individuals (where μ is population size) (typically $\lambda \approx 7\mu$)
- <u>Deterministically</u> eliminate worst individuals from
 - children only: (μ, λ) -ES \rightarrow escapes from local optima more easily (Notational convention)
 - parents and children: $(\mu+\lambda)$ -ES \rightarrow doesn't forget good solutions ("elitist selection")

ES: Basic Mutation

- An individual is a vector $\vec{h} = (x_1, \dots, x_n)$
- Mutate each x_i by sampling a change from a normal distribution:

$$x_i \leftarrow x_i + \Delta x_i$$
 where $\Delta x_i \sim N(0, \sigma)$

"sampled from"



Simple modification: mutation rate for each x_i

Major question: How to set σ or σ_i ?

MAIN IDEA: make search more efficient by increasing mutation rate if this seems safe

ES: Basic Mutation

- An algorithm for setting global σ : Improved fitness
 Count the number G_s of successful
 - mutations
 - Compute the ratio of successful mutations $p_s = G_s / G$
 - Update strategy parameters according to

$$\sigma_{i} = \begin{cases} \sigma_{i}/c & \text{if } p_{s} > 0.2 \\ \sigma_{i} c & \text{if } p_{s} < 0.2 \\ \sigma_{i} & \text{if } p_{s} = 0.2 \end{cases}$$

$$c \in [0.8,1.0]$$
Increase mutation rate as we are are successful

until termination

"1/5 rule"

Basic (1+1) ES

Common use of the 1/5 rule

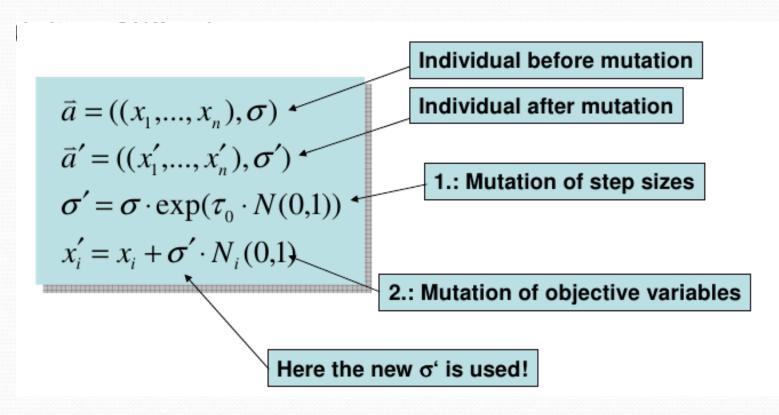
```
t := 0;
initialize P(0) := {\vec{x}(0)} \in I, I = IR^n, \vec{x} = (x_1, \dots, x_n);
evaluate P(0): \{f(\vec{x}(0))\}
while not terminate(P(t)) do
     mutate: \vec{x}'(t) := m(\vec{x}(t))
          where x_i' := x_i + \sigma(t) \cdot N_i(0,1) \ \forall i \in \{1,\ldots,n\}
     evaluate: P'(t) := \{\vec{x}'(t)\} : \{f(\vec{x}'(t))\}
     select: P(t+1) := s_{(1+1)}(P(t) \cup P'(t));
     t := t + 1:
     if (t \mod n = 0) then
         \sigma(t) := \left\{ egin{array}{ll} \sigma(t-n)/c & , & 	ext{if } p_s > 1/5 \ \sigma(t-n) \cdot c & , & 	ext{if } p_s < 1/5 \ \sigma(t-n) & , & 	ext{if } p_s = 1/5 \end{array} 
ight.
          where p_s is the relative frequency of successful
                     mutations, measured over intervals of,
                     say, 10 \cdot n trials;
                    0.817 < c < 1;
          and
     else
          \sigma(t) := \sigma(t-1);
     fi
od
```

ES Mutation:

Strategy Parameters

- An individual is a vector $\vec{h} = (x_1, \dots, x_n, \sigma)$ or $\vec{h} = (x_1, \dots, x_n, \sigma_1, \dots, \sigma_n)$ where the σ_i are the standard deviations
- Mutate strategy parameter(s) first Order is important!
- If the resulting child has high fitness, it is assumed that:
 - quality of phenotype is good
 - quality of strategy parameters that led to this phenotype is good

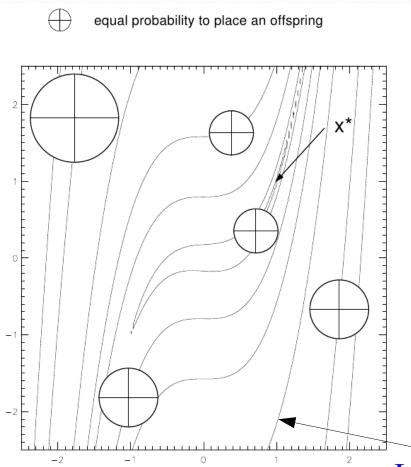
Mutation of one strategy parameter



- Here τ_0 is the mutation rate
 - τ_0 bigger: faster but more imprecise
 - τ_0 smaller: slower but more imprecise
- Recommendation for setting τ_0 :

$$\tau_0 = \frac{1}{\sqrt{n}}$$

*H.-P. Schwefel: Evolution and Optimum Seeking, Wiley, NY, 1995.



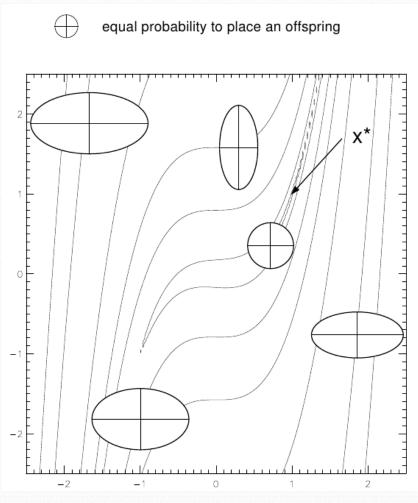
One parameter for each individual

2 dimensional genotype

$$\vec{h} = (x_1, x_2, \sigma)$$

5 individuals

Line indicates points with equal fitness



- One parameter for each dimension
- 2 dimensional genotype

$$\vec{h} = (x_1, x_2, \sigma_1, \sigma_2)$$

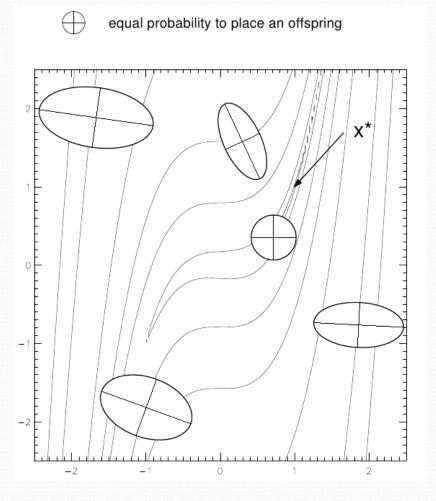
5 individuals

Mutation of all strategy parameters

$$\sigma'_{i} = \sigma_{i} \cdot \exp(\tau' \cdot N(0, 1) + \tau \cdot N_{i}(0, 1))
x'_{i} = x_{i} + \sigma'_{i} \cdot N_{i}(0, 1)$$

Sample from normal distribution, the same for all parameters

Update for this specific parameter



An individual is a vector

$$\vec{h} = (x_1, \dots, x_n, \sigma_1, \dots, \sigma_n, \alpha_1, \dots, \alpha_m)$$

where α_i encode angles

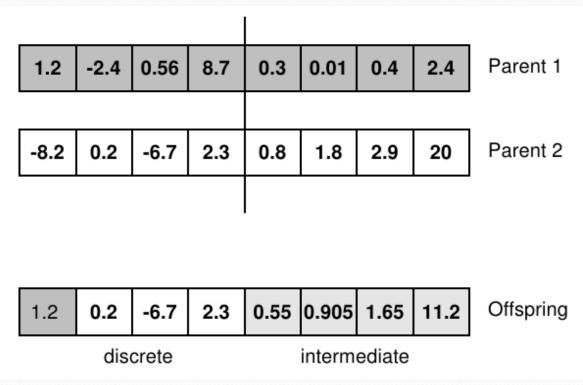
- Also here mutation can be defined
- Mathematical details skipped

ES Crossover / Recombination

- Application of operator creates one child (not two)
- Is applied λ times to create an offspring population of size λ (on which then mutation and selection is applied)
- Per offspring gene two parent genes are involved
- Choices:
 - combination of two parent genes:
 - average value of parents (intermediate recombination)
 - value of one randomly selected parent (*discrete recombination*)
 - choice of parents:
 - a different pair of parents for each gene (*global recombination*)
 - the same pair of parents for all genes

ES Crossover / Recombination

 Default choice: discrete recombination on phenotype, intermediate recombination on strategy parameters



GAs vs. ES

Genetic algorithms

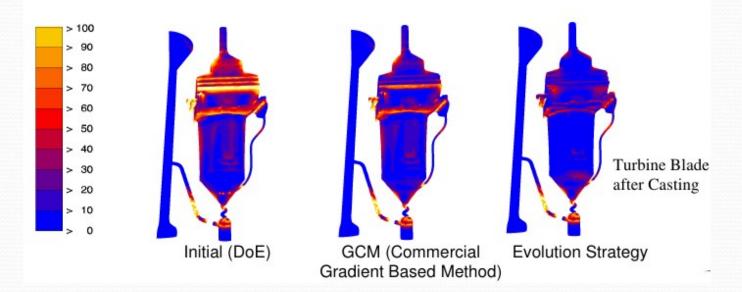
- Crossover is the main operator
- Uses also mutation
- Encoding for problem representation
- Biased selection of the parents
- Algorithm parameters often fixed
- Selection → Crossover → Mutation

Evolution strategies

- Mutation is the main operator
- Uses also crossover (recombination)
- No encoding needed for problem representation
- Random selection of the parents
- Adaptive set of algorithm parameters (strategy parameters)
- Crossover → Mutation → Selection

Example

- Casting of blased in gas turbine manufacturing
 - Objective: Max. homogeneity of workpiece after Casting Process
 - Variables: 18 continuous speed variables for Casting Schedule
 - Computationally expensive simulation (up to 32h simulation time)



Example

Traffic light control optimization



- Objective: Minimization of total delay / number of stops
- Variables: Green times for next switching schedule
- Dynamic optimization, depending on actual traffic
- Better results (3-5%)
- Higher flexibility than with traditional controllers

Genetic Programming

- Main idea: individuals are (simple) computer programs of arbitrary size
- Redefinitions of
 - selection
 - crossover
 - mutation

Program Trees / Parse Trees

- Representation of
 - Arithmethic formulas

$$2 \cdot \pi + \left((x+3) - \frac{y}{5+1} \right)$$

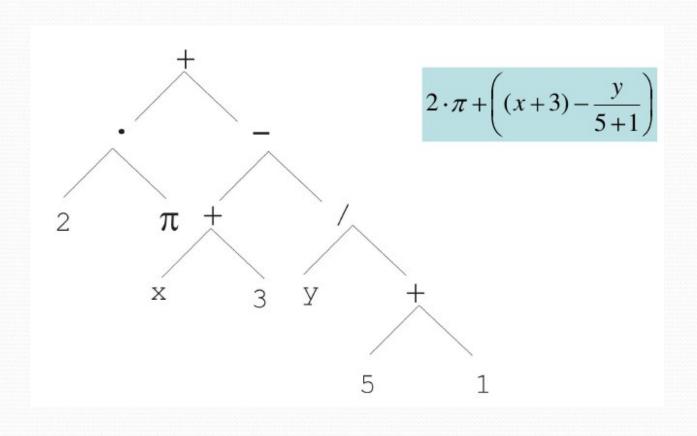
Logical formulas

$$(x \land true) \rightarrow ((x \lor y) \lor (z \longleftrightarrow (x \land y)))$$

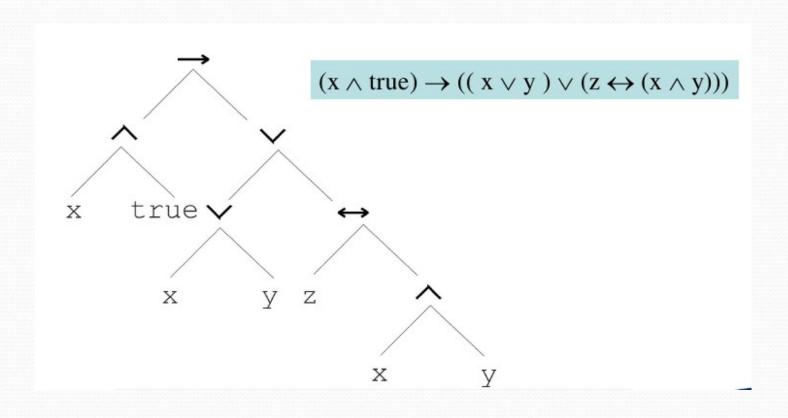
Computer programs

```
i = 1;
while (i < 20)
{
i = i + 1
}
```

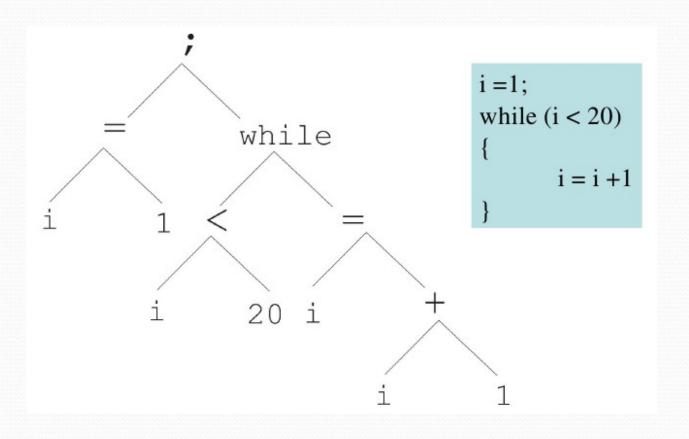
Representation of Arithmetic Formula



Representation of Logical Formula



Representation of Computer Programs



Representation

- Trees consisting of:
 - terminals (leaves)
 - constants
 - variables (inputs to the program/formula)
 - functions of fixed arity (internal nodes)

Representation Issues

 Closure: any function should be well-defined for all arguments

Example: $\{ *, / \}$ is not closed as division is not well defined if the second argument is $o \rightarrow redefine /$.

• **Sufficiency:** the function and terminal set should be able to represent a desirable solution

Evolutionary Cycle

- Fixed population size
- Create a new population by randomly selecting an operation to apply, each of which adds one or two individuals into the new population, starting from one or two fitness proportionally selected individuals:
 - reproduction (copying)
 - one of many crossover operations
 - one of many mutation operations

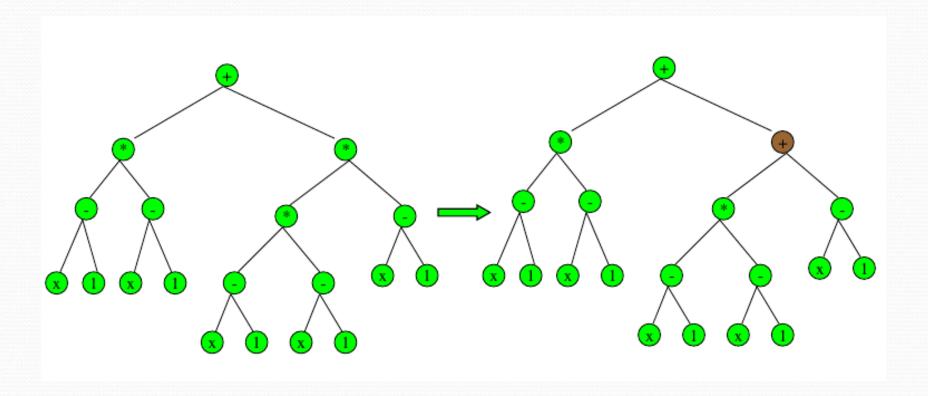
Initialization

- ullet Given is a maximum depth on trees $D_{\scriptscriptstyle{ ext{max}}}$
- Full method:
 - for each level $< D_{max}$ insert a node with function symbol (recursively add children of appropriate types)
 - for level D_{max} insert a node with a terminal
- Grow method:
 - for each level $< D_{\max}$ insert a node with either a terminal or a function symbol (and recursively add children of appropriate types to these nodes)
 - for level D_{max} insert a node with a terminal
- Combined method: half of the population full, the other grown

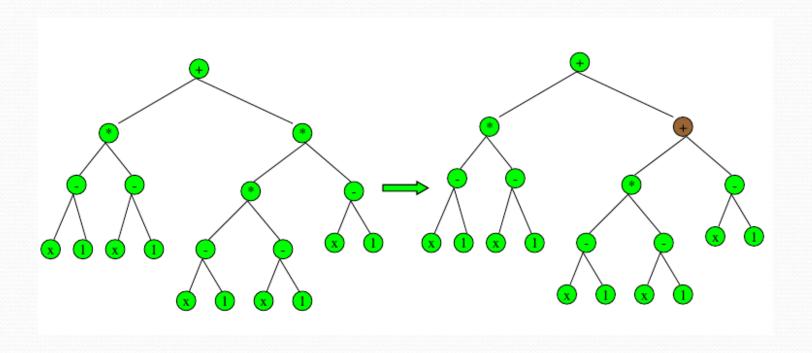
Mutation

Operator name	Description
Point mutation	single node exchanged against random node of same class
Permutation	arguments of a node permuted
Hoist	new individual generated from subtree
Expansion	terminal exchanged against random subtree
Collapse subtree	subtree exchanged against random terminal
Subtree mutation	subtree exchanged against random subtree

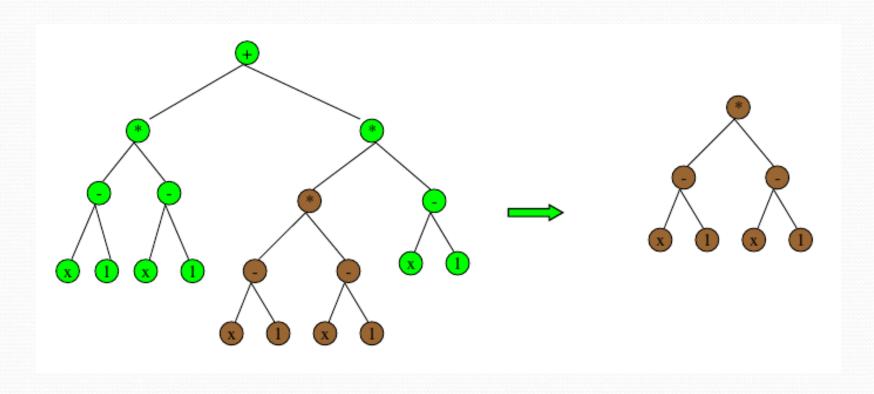
Point Mutation



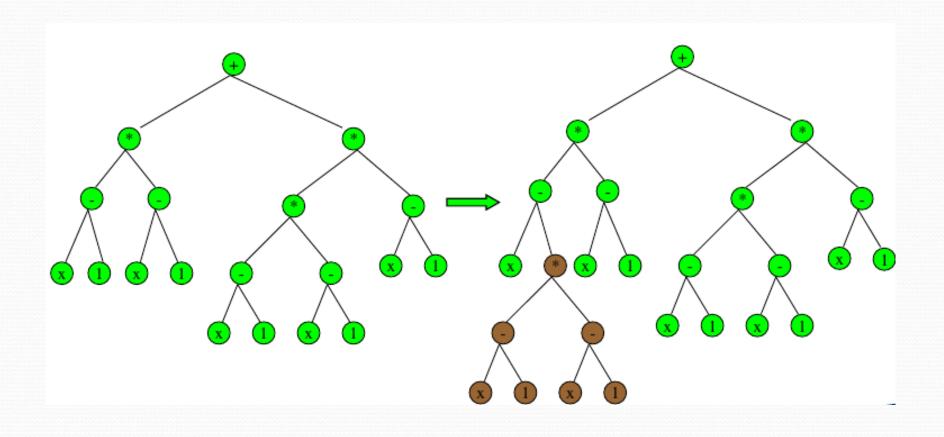
Permutation



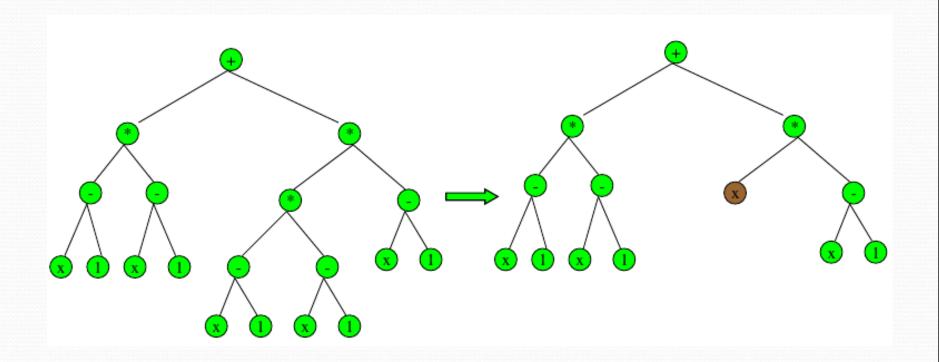
Hoist



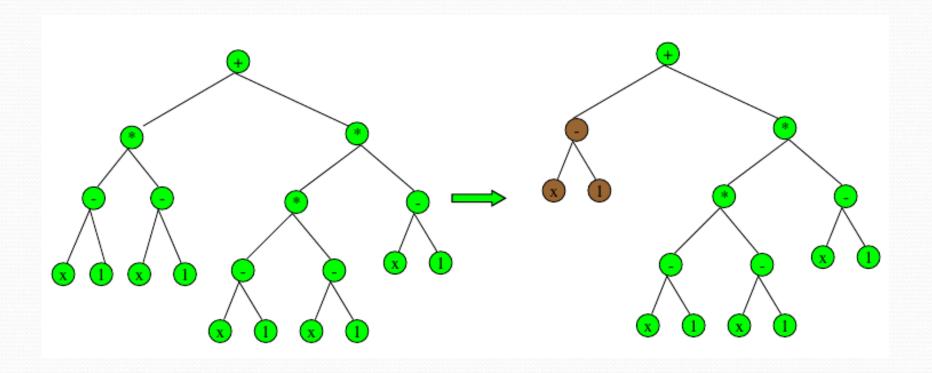
Expansion Mutation



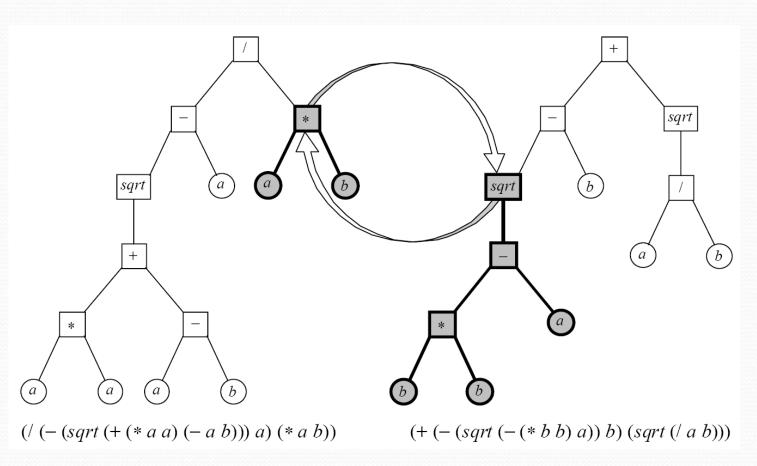
Collapse Subtree Mutation



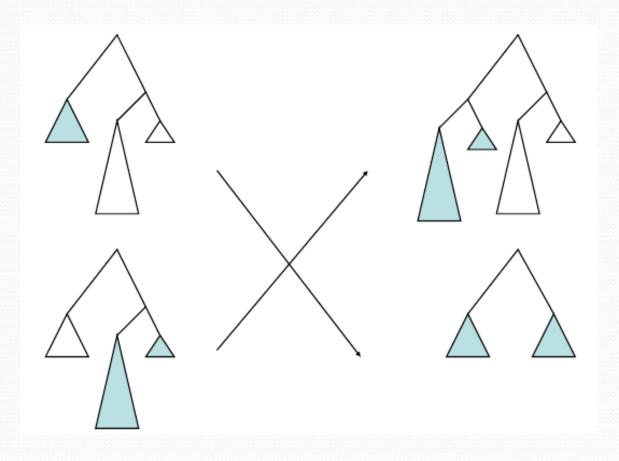
Subtree Mutation



Crossover



Self-Crossover



Bloat

- "Survival of the fattest", i.e. the tree sizes in the populations increase over time
- Countermeasures:
 - simplification
 - penalty for large trees
 - hard constraints on the size of trees resulting from operations

Editing Operator

- An operation that simplifies expressions
- Examples:
 - $X \text{ AND } X \rightarrow X$
 - \bullet X OR X \rightarrow X
 - $NOT(NOT(X)) \rightarrow X$
 - $\bullet X + o \rightarrow X$
 - \bullet X . 1 \rightarrow X
 - \bullet X. $o \rightarrow o$
 -

Preparatory steps to apply GP

- Determine the set of terminals
 - Atoms of the language (inputs of the program, constants)
- Select the set of primitive functions
 - Basic functions of (programming) language
- Define the fitness function
- Decide on control parameters
 - Similar to GA parameters: population size, stopping condition, crossover rate, etc.
- Choose method to designate the result of a run
 - Usually, best individual encountered

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Example – <u>Symbolic</u> Regression Pythagorean Theorem

Not (necessarily) linear

Underlying function: $c = \sqrt{a^2 + b^2}$

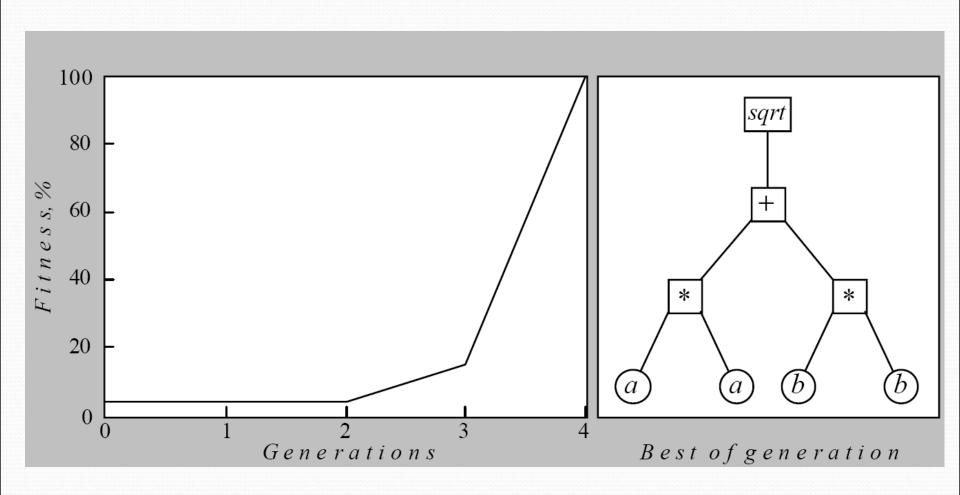
Negnevitsky 2004

Fitness cases:

Side <i>a</i>	Side b	Hypotenuse c	Side <i>a</i>	Side <i>b</i>	Hypotenuse c
3	5	5.830952	12	10	15.620499
8	14	16.124515	21	6	21.840330
18	2	18.110770	7	4	8.062258
32	11	33.837849	16	24	28.844410
4	3	5.000000	2	9	9.219545

Language elements: +, -, *, /, sqrt, a, b

Results

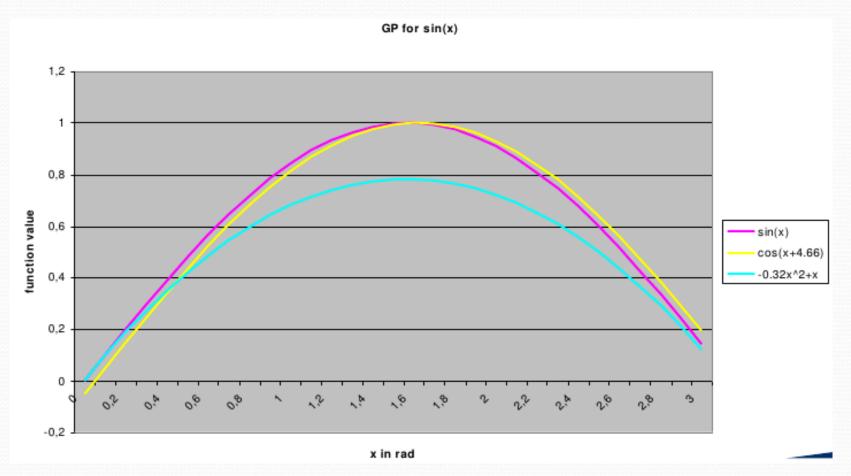


Example – Symbolic Regression Approximation of sin(x)

- **Given** examples $(x, \sin(x))$ with x in $\{0,1,...,9\}$
- **Find** a good approximation of sin(x)

Function Sets	Result	Generation	Error (final)
F ₁ : { +, -, *, /, sin }	sin(x)	0	0.00
F ₂ : { +, -, *, /, cos }	cos(x + 4.66)	12	0.40
F ₃ : { +, -, *, / }	$-0.32 x^2 + x$	29	1.36

Example – Symbolic Regression Approximation of sin(x)



GAs vs. GP

Genetic algorithms

- Chromosomes represent coded solutions
- Fixed length chromosomes
- A small set of welldefined genetic operators
- Conceptually simple

Genetic programming

- Chromosomes represent executable code
- Variable length chromosomes
- More complex genetic operators required
- Conceptually complex