Evolutionary Algorithms

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Universidad Carlos III de Madrid
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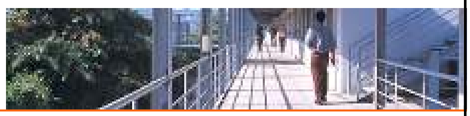
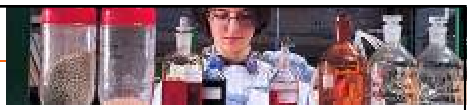


RESEARCH CENTERS



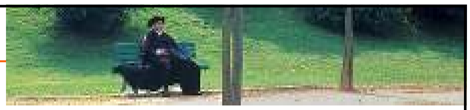
Engineering

- 3 B's - Research Group - Biomaterials, Biodegradables and Biomimetics
- Algoritmi Centre (CALG)
- Centre of Biological Engineering (CEB)
- Computer Science and Technology Center (CCTC)
- Centre for Textile Sciences and Technology (CCTT/2C2T)
- Centre for Mechanical and Materials Technology (CT2M)
- Territory, Environment and Construction Centre (C-TAC)
- Institute for Sustainability and Innovation in Structural Engineering (ISISE)
- **Institute for Polymers and Composites (IPC)**
- Interdisciplinary Center for Production Technology and Energy (CITEPE)

Associate Labs

- IBB - Institute of Biotechnology and Bioengineering
- **I3N - Institute of Nanostructures, Nanomodelling and Nanofabrication**

TEACHING



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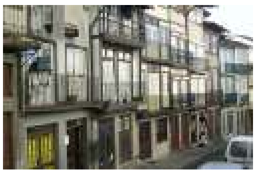
GUIMARÃES

HISTORIC CITY CENTRE – Intramural Area (Classified UNESCO World Heritage Site)



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GUIMARÃES

The city of Guimarães has a great variety of historical and cultural offers. It was the birthplace of Portugal and was considered by Unesco a **world heritage site**: http://whc.unesco.org/en/list/1031.

The city was selected as **2012 European Capital of Culture**.

Recently the **New York Times Journal** designated Guimarães as the **26th place (from 41) to visit in 2011**: http://www.nytimes.com/2011/01/09/travel/09where-to-go.html?_r=2&pagewanted=3&sq=Guimarães&st=cse&scp=1.

More information can be found at: http://www.cm-guimaraes.pt/PageGen.aspx?WMCM_PaginaId=4194.

CONTENTS

Lesson 1: Introduction to Evolutionary Algorithms

- Bibliography
- Motivation
- Evolutionary Theory
- Evolutionary Algorithms
- Schema Theorem
- Application Example
- Conclusions

CONTENTS

Lesson 2: How to "build" a Genetic Algorithm

- Global Structure of the Algorithm
- Population Initialization
- Evaluation
- Selection
- Mutation
- Recombination (Crossover)
- Inversion
- Final Notes
- Other Algorithms

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CONTENTS

Lesson 3: Multi-Objective Evolutionary Algorithms

- Concepts and Definitions
- Classical Methods
- EMO Methods
- State-of-the-art EMO
- NSGA-II
- RPSGA
- Application Example
- Niching and Speciation

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CONTENTS

Lesson 4: Extending MOEAs to Solve Complex Engineering Problems

- Motivation
- Multi-Objective Evolutionary Algorithm
- Decision Making
- Robustness
- Hybrid Algorithms
- Number of Objectives Reduction
- Case Study
- Global Conclusions

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CONTENTS

Lesson 5: Examples of Application of MOEAs

- Design of Shading Devices
- Polymer Extrusion
  (single and twin-screw extruders)
- Scale-up
- Feature Selection
  (bankruptcy prediction and cardiac SPEC diagnosis)

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PEOPLE

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Armando Vieira
José António Covas
Fernando Mendes
Dirk Loyens
Lino Costa
Bruno Vergnes
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Lesson 1:

Introduction to Evolutionary Algorithms

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OUTLINE

- **Bibliography**
- **Motivation**
- **Evolutionary Theory**
- **Evolutionary Algorithms**
- **Schema Theorem**
- **Application Example**
- **Conclusions**

BIBLIOGRAPHY

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2- Zbigniew Michalewicz, “Genetic algorithms + data structures = evolution programs”, 3rd ed., Springer , 1996:

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4- Melanie Mitchell, “ An introduction to genetic algorithms”, Bradford Book, 1996:

5- Kalyanmoy Deb, ”Multi-objective optimization using evolutionary algorithms”, John Wiley & Sons, 2001:

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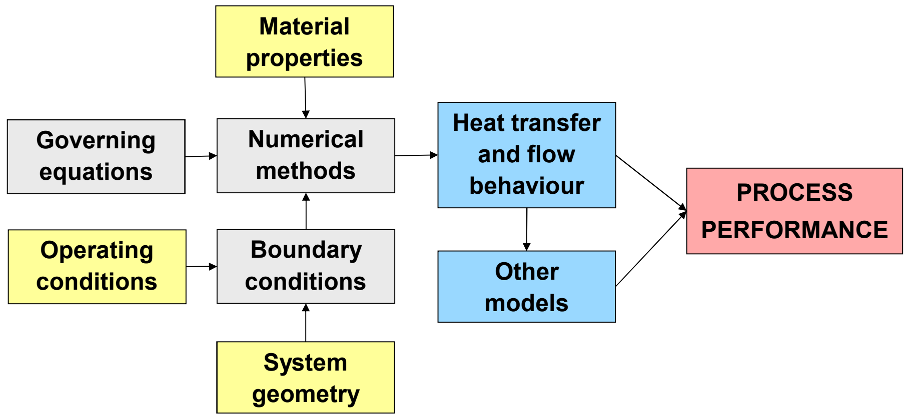
Sophisticated mathematical models are able to describe adequately a specific process



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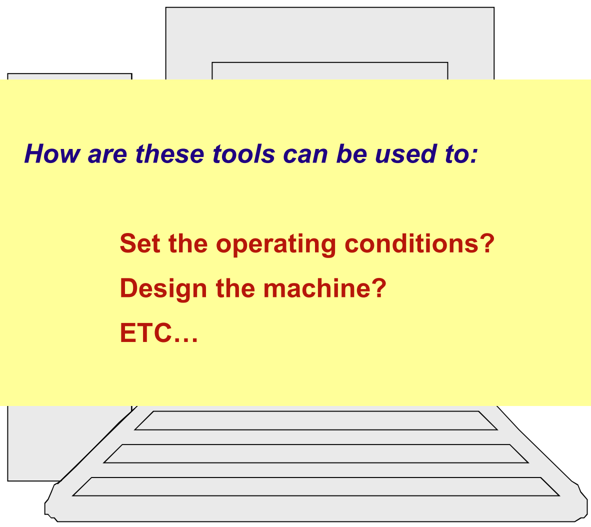
MOTIVATION



How are these tools can be used to:

Set the operating conditions?

Design the machine?

ETC…

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MOTIVATION

Approaches to optimize the processes (e.g., set the operating conditions, design machines, etc…):

- **Use empirical knowledge;**
- **Use computational tools on a trial and error basis;**
- **Solve the inverse problem;**
- **Perform a partial process optimization;**
- **Develop a global optimization procedure.**

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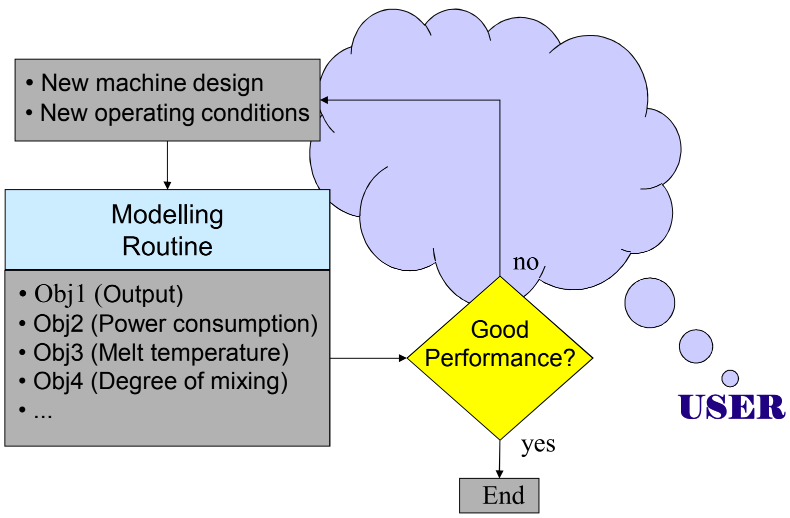
Use computational tools on a trial and error basis



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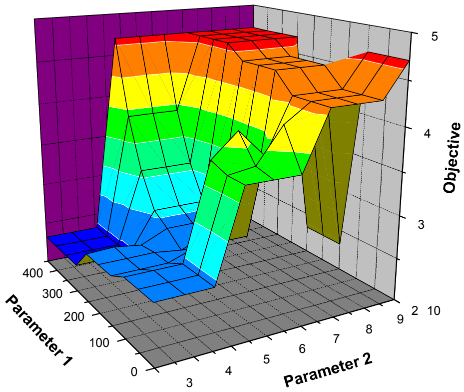
Use computational tools on a trial and error basis



A good performance may be distinct from the best performance

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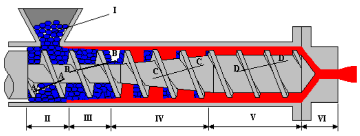
Solve the inverse problem



***Direct problem*:**

- Geometry
- Material properties
- Operating conditions

Governing equations →

- Output
- Power consumption
- Melt temperature
- Degree of mixing
- ...

***Inverse problem*:**

- Material properties
- Output
- Power consumption
- Melt temperature
- Degree of mixing
- ...

Governing equations →

- Geometry
- Operating conditions
- ...

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Perform a partial process optimization

1. Optimizing for output

- ***Melt conveying***
- ***Melting*** **(helix angle, number of flights, flight clearance, compression ratio)**
- ***Solids conveying*** **(channel depth, helix angle, number of flights, flight clearance)**

2. Optimizing for power consumption

(helix angle, flight clearance, flight width)

EXAMPLE: Optimizing for output *(Melt conveying)*

$$H_{opt} = \left[\frac{6(\pi DN)^n k(\Delta L)}{(n+2)(\Delta P)\tan\theta} \right]^{\frac{1}{n+1}} \qquad \sin\theta_{opt} = \left(\frac{n}{2n+2}\right)^{1/2} + \frac{pW}{\pi D}\left(\frac{n+2}{4}\right)$$

C. Rauwendaal, *Polymer Extrusion*, Hanser (2001)

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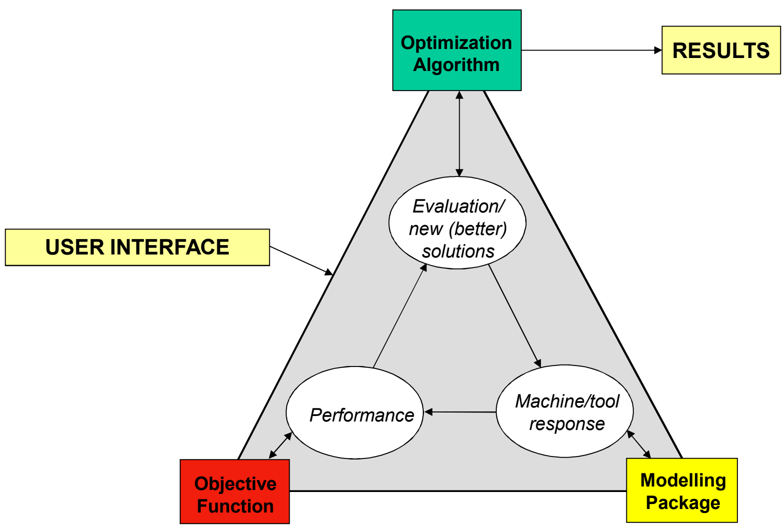
Develop a global optimization procedure



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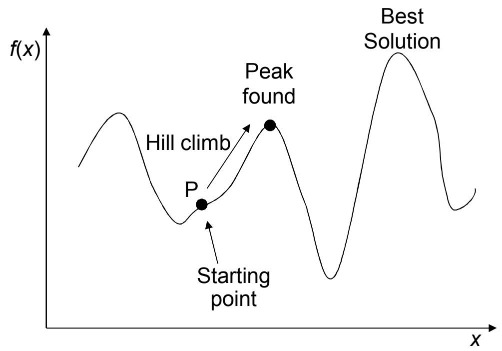
Develop a global optimization procedure



In most optimization algorithms:

- **The search is local**
- **If one local peak is found the search stops**

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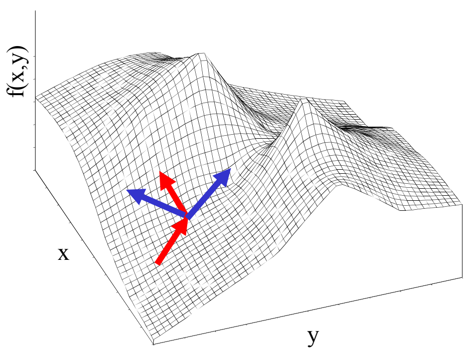

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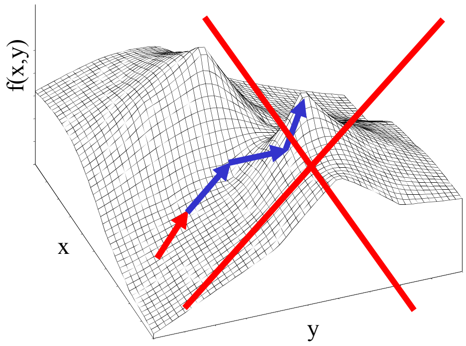

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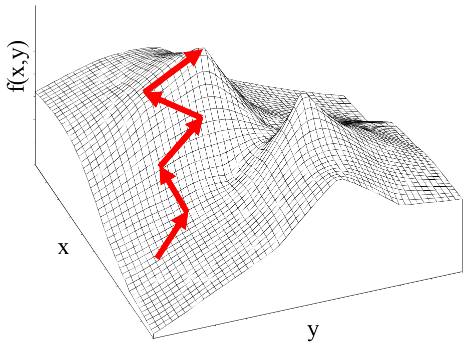

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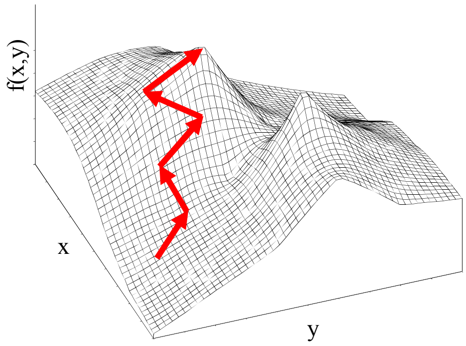

OPTIMIZATION ALGORITHMS

- Random search
- Gradient methods
- Simulated annealing
- Neural networks
- Expert systems
- Sensitivity analysis
- Statistical methods
- ANT colony optimization
- Evolutionary algorithms

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RANDOM SEARCH

- This technique consists simply in **selecting randomly** points from the search space and evaluating them.
- This technique has the limitation of working with **one point each time**, which does not provide an amplifying overview of the search space.
- **Search is very slow** since the technique does not use any available information on the problem.

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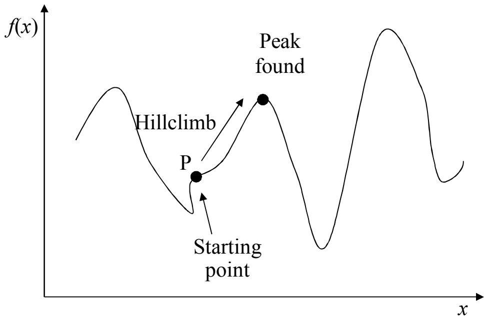
GRADIENT METHODS

These methods use information about the objective function gradient in order to establish the search direction.

y = f(x1,x2)
starting point P(x1(0),x2(0))

$$grad\ f = \left\{ \frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right\}$$



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SIMULATED ANNEALING

- Simulated annealing makes a parallelism with the **way liquids freeze or metals recrystallize** during the annealing process.
- When a melt initially at high temperature and disordered is slowly cooled down, the system at any time is approximately under **thermodynamic equilibrium**.
- The system becomes **progressively ordered** and approaches a frozen ground state.
- By analogy, simulated annealing optimization starts from **one point randomly selected** from the search space and makes a random movement.
- This movement will be accepted if **improvement is obtained** and accepted with a determined probability in the opposite case.

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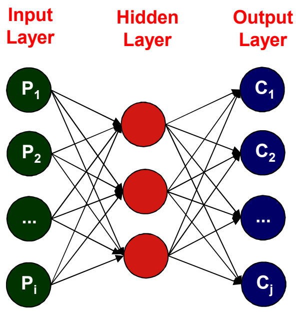
ARTIFICIAL NEURAL NETWORKS

- ANN implemented by a Multilayer Perceptron is a flexible scheme capable of **approximating an arbitrary complex function**;
- The ANN **builds a map** between a set of inputs and the respective outputs;
- A feed-forward neural network consists of an array of **input** nodes connected to an array of **output** nodes through successive **intermediate layers**;
- Each connection between nodes has a **weight**, initially random, which is adjusted during a **training** process;
- The output of each node of a specific layer is a **function** of the sum on the weighted signals coming from the previous layer;



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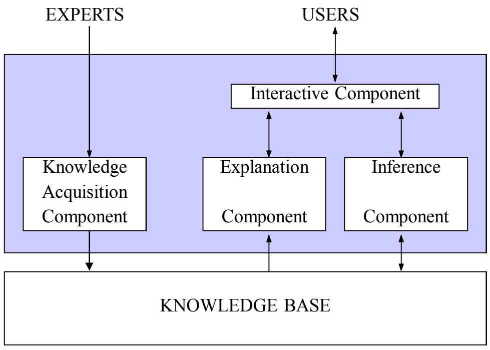
EXPERT SYSTEMS

- An expert system simulates the interaction of the user with a specialist to solve a problem.
- It comprises a knowledge base, a knowledge acquisition component, an interactive component, an explanation component, and an inference component.
- All facts, rules and know-how are collected in the knowledge base.
- The knowledge acquisition component provides communication between the specialists of the process and the knowledge base.
- New information is incorporated in the base.
- A lot of interaction with the specialists is thus necessary.
- The interactive component is the link between the final users and the knowledge base, either by solving the problem (inference component) or by explaining the solutions (explanation component) and the decision-making process to the user.



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SENSITIVITY ANALYSIS

A sensitivity analysis is generally used to quantify the relationship between variations of the parameters to optimize (independent variables) and variations of the objective function (dependent variables).

$$F(x) = G(f(x), x) \qquad \nabla F(x) = \frac{DF}{Dx}(x) = \frac{DG}{\partial f}(f(x), x)\frac{Df}{Dx}(x) + \frac{DG}{\partial x}(f(x), x)$$

Once this sensitivity is known, the effects of a variation of the parameter δx on the objective function can be estimated using e.g. finite differences (forward differences):

$$\frac{DF}{Dx}(x) = \frac{F(x+\delta x) - F(x)}{\delta x}$$

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STATISTICAL METHODS

- The aim here is to **evaluate data**, obtained either by computer modelling or by experimental means, through the use of an **objective function**.
- Several experimental designs are available, such as full factorial, central composite, Latin square, Plackett-Burman, Box-Behnken, Taguchi and simplex design.
- The choice of a method depends on the characteristics of the problem under study, namely the number of factors and levels for each factor, the factors type (continuous or discrete), the type of response variable to study, the sample size (number of replicates) and the restrictions involved.

$$f_j(N, T_b) = a_0 + a_1\, N + a_2\, T_b + a_{11}\, N^2 + a_{22}\, T_b^2 + a_{12}\, N\, T_b$$

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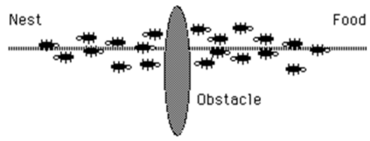
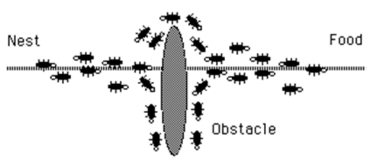
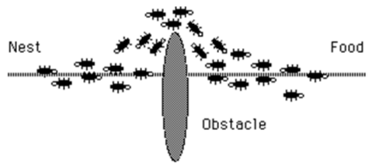
ANT COLONY OPTIMIZATION

Real ants are capable of finding shortest path from a food source to the nest without using visual clues.



Also, they are capable of adapting to changes in the environment, for example finding a new shortest path once the old one is no longer feasible due to a new obstacle.





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ANT COLONY OPTIMIZATION

- Ant Colony Optimization (ACO) is a metaheuristic approach proposed by Dorigo et al.
- The inspiring source of ACO is the foraging behavior of real ants. This behavior enables ants to find shortest paths between food sources and their nest. While walking from food sources to the nest and vice versa, ants deposit a substance called pheromone on the ground. When they decide about a direction to go, they choose with higher probability paths that are marked by stronger pheromone concentrations.
- This basic behavior is the basis for a cooperative interaction which leads to the emergence of shortest paths.

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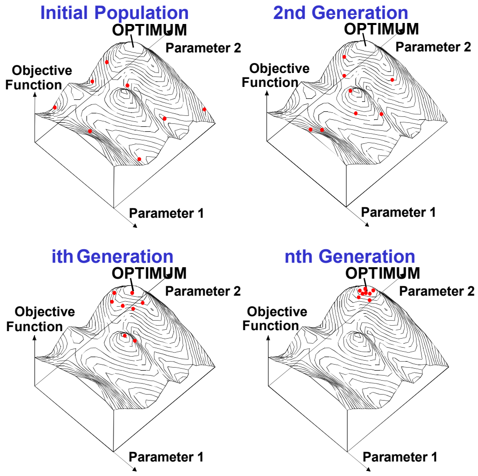
EVOLUTIONARY ALGORITHMS



- **Search uses a population of points**
- **Able to distinguish between local and absolute maxima**
- **Do not require derivatives nor other knowledge on the process (BLACK BOX)**
- **Require significant computation resources**

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The role of optimisation is to find the best set of parameters that optimise an objective function, particularly by improving the performance in the direction of some optimal point or points:

$$
\begin{array}{lll}
\text{maximise}_{x\in\Omega} & f(x_i) & i=1,\ldots,n \\
\text{subject to} & g_j(x_i)\geq 0 & j=1,\ldots,J \\
 & h_k(x_i)=0 & k=1,\ldots,K
\end{array}
$$

where x is a vector of n and $\Omega \subset \Re^n \left(\Omega = \{x \in \Re^n : l \leq x \leq u\}\right)$

f **is the objective function of the** ***n*** **parameters** x_i, g_j **are the** ***J*** **(*J*≥0) inequality constraints, and** ***k*** **are the** ***K*** **(*K*≥0) equality constraints.**

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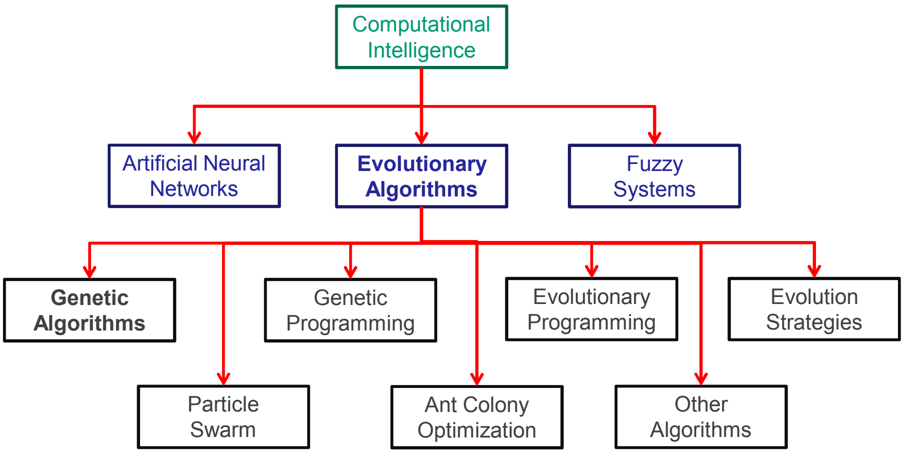
Computational Intelligence



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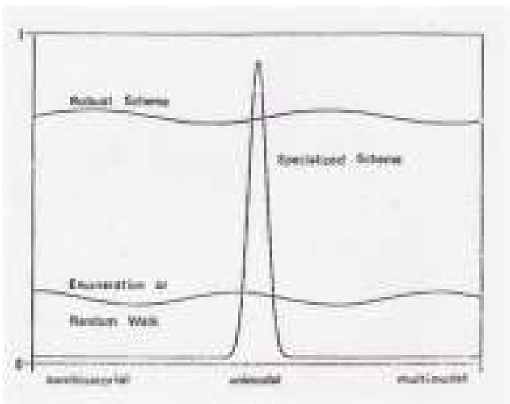
Robust Search Methods



(Goldberg, 1989)

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Genes and DNA

- DNA **encodes the information** needed to define a living organism;
- Most genetic material is **identical** in all individuals inside the same species;
- **Small changes** in the genetic material give rise to small changes in the organisms:

  -For example: height, hair colour, etc. ...

Genes and DNA

- DNA is a large molecule consisting of several fragments. Each one of these fragments acts as a letter in a coded message:

  -A-B-A-D-C-B-B-C-C-A-D-B-C-C-A-

- Certain groups of “letters” are only useful when they are together (similarly as words);
- These groups are designated as GENES;
- DNA is composed of GENES and "waste".

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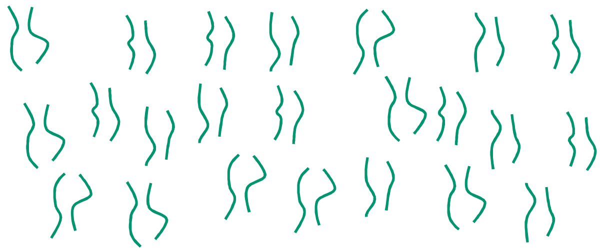
Human Reproduction

- The human DNA is organized into **chromosomes**;
- Most human cells contain 23 pairs of chromosomes, defining together the **physical attributes** of the individual:

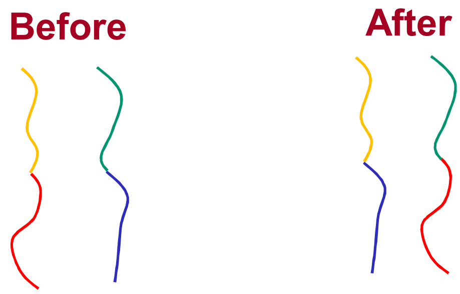


Reproductive Cells

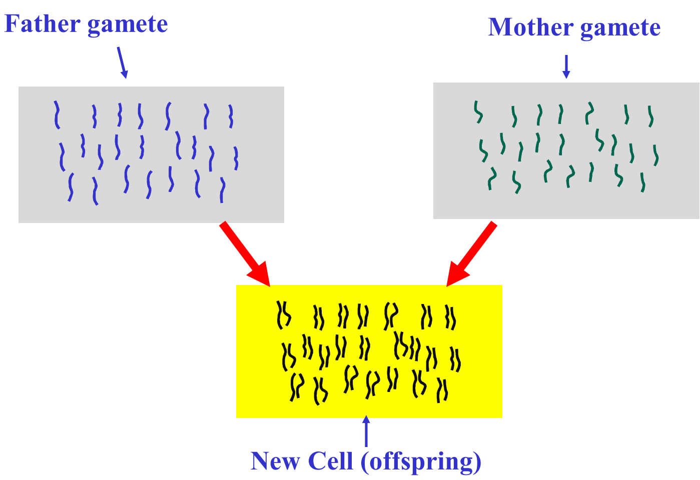
- Male and female gametes have 23 individual chromosomes (and not 23 pairs);
- The reproductive cells are formed by half of chromosomes;
- During this process the pairs of chromosomes carry out an operation called "crossover".

Crossover

The crossover process consists in exchange of information between chromosomes using only parts of themselves.



Fertilization



Mutation

- During this process the genetic material may change slightly due to an sporadic **mutation** of some gene(s);
- This signifies the introduction, in the offspring's, of genetic material that was **not inherited** directly from parents;
- The probability of occurring mutation is **very low**;
- This can constitute a problem (or an advantage).

Evolutionary Theory

Mutation Crossover → New genetic material

- Usually less able to survive and reproduce
- Occasionally more able to survive and reproduce

More reprodution → More “improved” genetic material

- A "Good" set of genes implies more reproduction
- A "Bad" set of genes implies less reproduction
- The set of “organisms” (of this specie) becomes increasingly able to survive in their environment

Evolutionary Theory

The evolutionary theory allows to explain that this slow change of genetic material through reproduction and mutation (and possibly crossover) enabled the possibility of generating all species of plants and animals

Evolutionary Algorithms

- Evolutionary Algorithms (*EAs*) are stochastic search and optimisation methods that mimic natural evolution through genetic operators like crossover and mutation.
- They work with a population of points, each one representing a possible solution in the search space.
- Each individual has a value associated to it (fitness or objective function), which is a measure of its performance on the system.
- Individuals with greater performance have a bigger opportunity for reproduction, i.e. to pass their characteristics to future.

Evolutionary Computation – THE METAPHOR

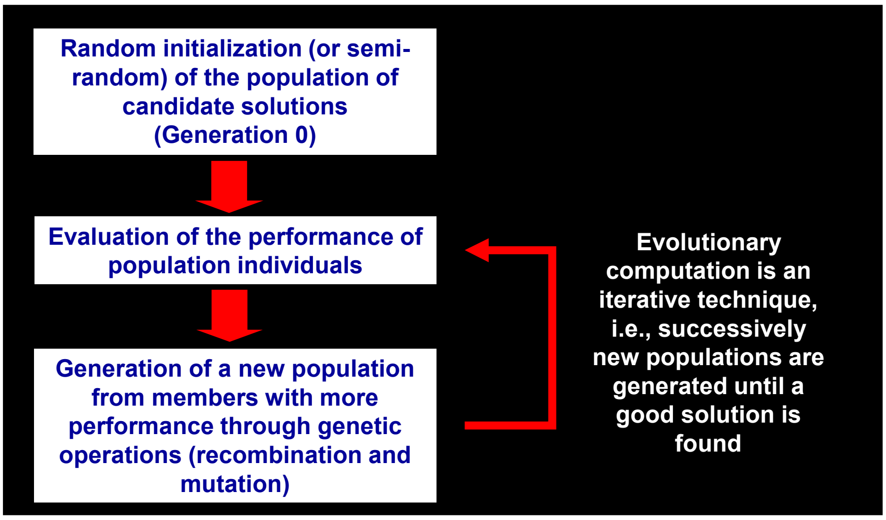
Natural Evolution		Evolutionary Computation
Individual	⟷	Solution
Performance	⟷	Quality
Environment	⟷	Problem

Evolutionary Equation

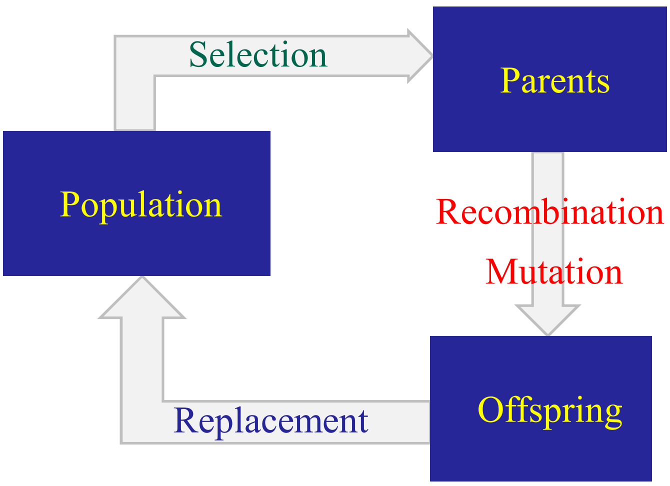
- The term *evolutionary computation* refers to the study of the foundations and applications of certain heuristics based on the principles of natural evolution.
- In spite of the fact that these techniques can be classified into four main categories.
- This classification is based in some details and historical development facts rather than in major functioning differences.
- In fact, their biological basis is essentially the same.

EC	=	GA	+	ES	+	EP	+	GP
Evolutionary Computing		*Genetic Algorithms*		*Evolution Strategies*		*Evolutionary Programming*		*Genetic Programming*
		(Holland, 1975)		(Rechenberg, 1973)		(Fogel, Owens, Walsh, 1966)		(Koza, 1992)

The Computational Cycle



The Evolutionary Cycle



Schema Theorem: John Holland

- **Objective** – to provide a formal model for the effectiveness of the GA search process.
- In the following we will first approach the problem through the framework formalized by Holland and popularized by Goldberg.
- This concentrates on providing a model for the expectation of schema survival, where this naturally represents a limitation in itself.

Consider the case of a canonical GA:

- Binary alphabet;
- Fixed length individuals, l;
- Fitness Proportional Selection;
- Single Point Crossover;
- Gene wise mutation.

Definition 1 – Schema, *H*:

- A schema is a subset of the space of all possible individuals for which all the genes match the template for schema *H*.
- If *A* denotes the alphabet of gene alleles then $A \cup *$ is the schema alphabet, where * is the 'wild card' symbol matching any allele value.
- E.g. for the binary alphabet $A \in \{0, 1, *\}$ where $* \in \{0, 1\}$

SCHEMA THEOREM

Example

- For a binary individual with the gene sequence {0 1 1 1 0 0 0}, then it follows that one (of many) matching schema might have the form, H = [* 1 1 * 0 * *]
- The schema H = [0 1 * 1 *] identifies the chromosome set,

0 1 0 1 0

0 1 0 1 1

0 1 1 1 0

0 1 1 1 1

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SCHEMA THEOREM

Definition 2 – Schema Order, $o(H)$:

Schema order, $o(.)$, is the number of non '*' genes in schema H.

Example,

$o(* * * 0 * * *) = 1$

Definition 3 – Schema Defining Length, $\delta(H)$:

Schema Defining Length, $\delta(H)$, is the distance between first and last non '*' gene in schema H.

Example,

$\delta(* * * 0 * * *) = 4 - 4 = 0$

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SCHEMA THEOREM

Schemata theory

The improvement in performance throughout the various generations can be explained with the aid of the Schemata Theory

DEFINITIONS:

scheme $H = 0**$ —represents→ chromossomes: 000, 001, 010 and 011

***o*(*H*) - Scheme order (*number of fixed positions*):**

$o(1*01*) = 3$ and $o(*1**0) = 2$

$\delta(H)$ - Scheme length (*distance between the first and the last fixed positions*)

$\delta(1*01*) = 3$ and $\delta(*1**0) = 3$

SCHEMA THEOREM

Schemata theory

The expected number of copies of the scheme *H*, included in the next generation (*t*+1), is given by:

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

- $m(H, t+1)$ and $m(H, t)$ are the number of copies of the scheme H on the generations t+1 e t;
- $f(H)$ is the mean value of the objective function of all individuals of generation t which are represented by the scheme H;
- $\bar{f}$ is the mean value of the objective function of the entire population;
- p_c and p_m are the probabilities of crossover and mutation respectively.

GEOMETRIC PROGRESSION → exponential increase of the best individuals on future generations.

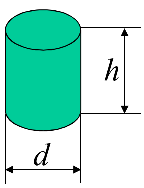
APLICATION EXAMPLE

EXAMPLE OF APPLICATION:

To minimize the cost of material used to manufacture a can

APLICATION EXAMPLE

To minimize the cost of material used to manufacture a can



Caracteristic dimensions:

- ***h*- heigth**
- ***d*- diameter**

Problem Formulation:

$$\begin{cases} Minimize \quad f(d,h) = c\left(\dfrac{\pi d^2}{2} + \pi d h\right), \\ Subject\ to \quad g(d,h) \equiv \dfrac{\pi d^2 h}{4} \geq 300 \\ \qquad d_{\min} \leq d \leq d_{\max}, \quad 1 \leq d \leq 20\ cm \\ \qquad h_{\min} \leq h \leq h_{\max}, \quad 1 \leq h \leq 20\ cm \\ c = 0.1\,€/cm^2 \\ \textbf{\textit{c} is the cost of can material per squared cm} \end{cases}$$

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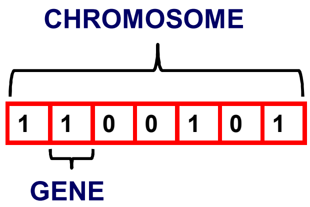
APLICATION EXAMPLE

Chromosome Representation

An array of bits - one for each parameter



Create 100 random bit strings for the initial population

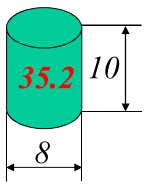
APLICATION EXAMPLE

Solution Representation

Codification types :
- *Real*
- *Binary*
- *Etc.*

(d, h) = (8, 10) cm

Chromosome = 0 1 0 0 0   0 1 0 1 0
d   *h*



Example – binary codification:

- **d [5.0, 15.0] with a single decimal place (*c*)**
- **length: *l* = 15 - 5 = 10**
- **number of intervals (*Nl*) = *l* * 10^*c* = 10 * 10^1 = 100**
- **number of bits (n_b): [8] 2^6 = 64 < 100 < 2^7 = 128**
- **5.0 is represented by (00 000 000)**
- **15.0 is represented by (11 111 111)**
- **using a direct binary representation 8.0 (80) is (01 010 000)**
- **while using the present representation (01 010 000) is 8.1**

→ "GRAY Coding"

APLICATION EXAMPLE

Conversion of binary string from base 2 to base 10

$$x' = \sum_{i=0}^{n_b-1} b_i.2^i$$

$$x = V_{min} + x' \frac{l}{2^{n_b}-1}$$

Example:

- *d [5.0, 15.0]*
- *l* = 10
- *Nl* = 100
- n_b = 8
- x´ = (01 100 001) = 97
- x = 8.803922

gene								x'	x
0	0	0	0	0	0	0	0	0	5.00
0	0	0	0	0	0	0	1	1	5.04
0	0	0	0	0	0	1	0	2	5.08
0	0	0	0	0	0	0	1	3	5.12
1	1	1	1	1	1	0	0	252	14.88
1	1	1	1	1	1	1	0	254	14.96
1	1	1	1	1	1	1	1	255	15.00

APLICATION EXAMPLE

GRAY CODE

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

Gray codes have the property that adjacent integers only differ in one bit position.

APLICATION EXAMPLE

Chromosome Fitness Evaluation

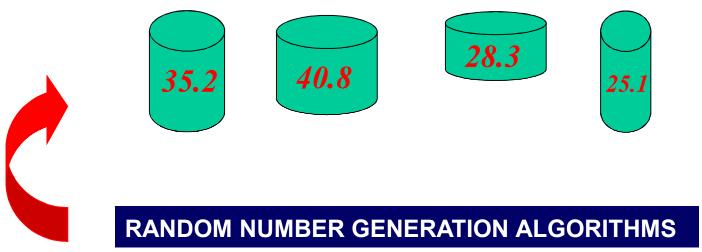
- Calculate the value of the superficial area of the can and multiply it by cost/area.
- If the condition concerning the volume limit is not satisfied penalise fitness (or eliminate the solution).

APLICATION EXAMPLE

Calculation of objective function

$$f(d,h) = 1 * \left(\frac{\pi 8^2}{2} + \pi * 8 * 10 \right) = 35.2$$

Initialization of the population (randomly)



APLICATION EXAMPLE

Choosing Parents to Reproduce

- To choose one parent:
  - Choose two chromosomes randomly from the population.
  - Whichever has the highest fitness is the parent.

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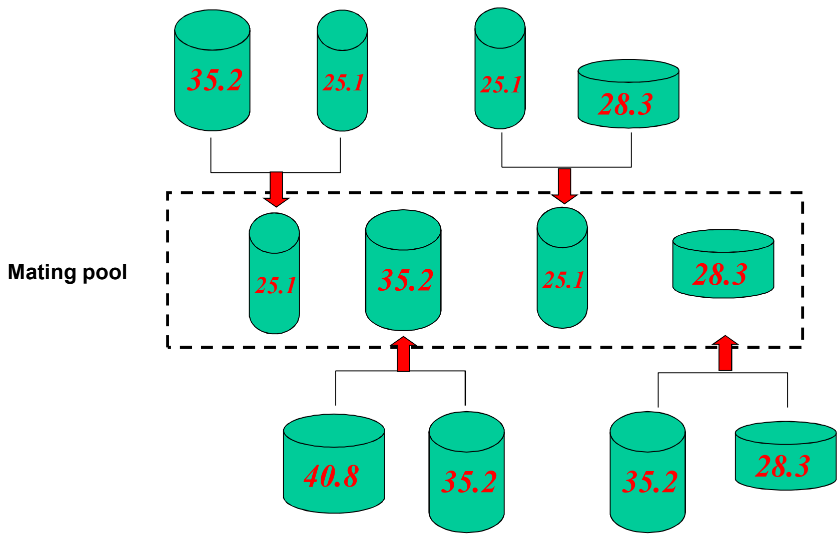
APLICATION EXAMPLE

Recombination operator (selection of solutions for reproduction)



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Producing a child by *Recombination*

- Random selection of a each gene from one of the Parents:

Parents

0	1	1	0	0	0	1	1
1	1	0	0	1	1	1	0

→

Offspring

0	1	0	0	1	1	1	1

Mutation

- Only a small chance of flipping is allowed for each gene, such as for example: 1/(length of string)

0	1	0	0	1	1	1	1

→

0	1	0	0	0	1	1	1

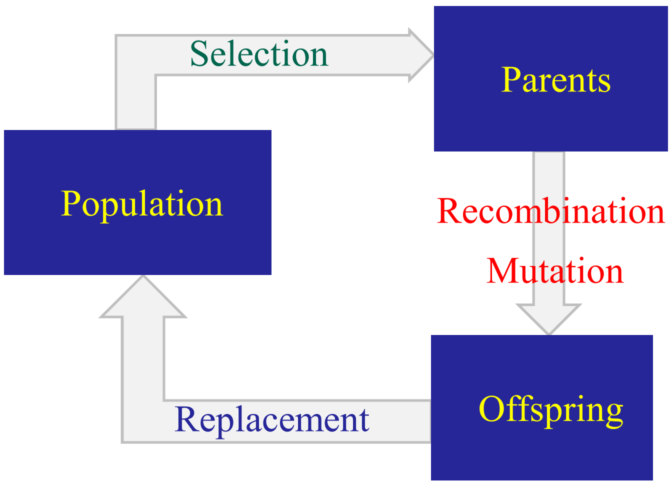
APLICATION EXAMPLE

Replacement

- The insertion of a new child into the population requires, necessarily, the elimination (replacement) of an existing member:
  - Random selection from the population.
  - Selection of the less fittest.

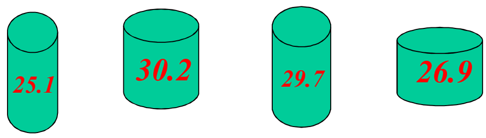
APLICATION EXAMPLE

The evolution cycle



APLICATION EXAMPLE

New Population



Fitness average of initial population = 32.4

Fitness average of new population = 28.0

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CONCLUSIONS

The Evolution Mechanism

- Increasing diversity using genetic operators:
  - mutation
  - recombination

- The diversity decreases by the process of selection of parents.

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CONCLUSIONS

Real World EC

Tends to include:

- More complex representations and operators
- Use of problem specific knowledge for seeding the initial population and creating heuristic operators
- Hybridisation with other methods

CONCLUSIONS

Advantages

- Can handles huge search spaces
- Good balance between exploration and exploitation
- Easy to implement, without the need of intensive knowledge
- Easy to combine with other methods
- Can provides many alternative solutions (MOEAs).

Disadvantages

- Is not possible to guarantee the founding of an optimal solution within finite time
- Weak theoretical basis
- May need extensive parameter tuning
- Often computationally expensive, mainly in the case of real optimization problems