

# Challenges for Real Applications

Data Science and Engineering (I)  
Master's Degree in Computer Engineering



UNIVERSIDAD  
DE MÁLAGA





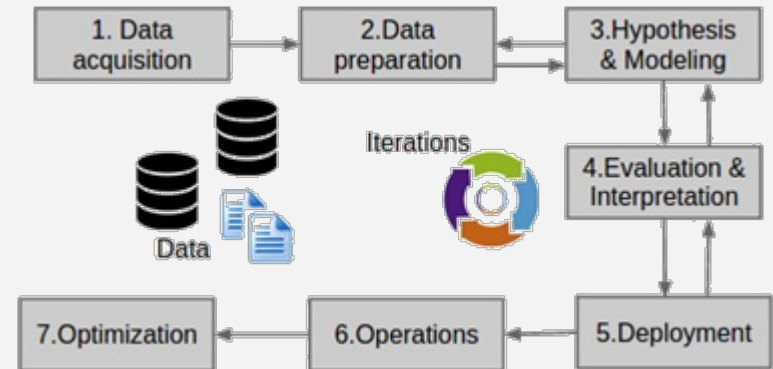
# Challenges for real products

1. **Managing** a data science and engineering project
2. Search, **optimization**, and learning
3. **Needs of real projects**: scalability, dynamism, robustness, multiple objectives, restrictions, and self-control
4. **Examples** of real products and services
5. **Modern techniques** for real applications



# Management of a DS project (I)

- The typical data science project is an **engineering procedure**: start, steps, end
- Full of **informed decisions** on whether to continue based on pre-defined criteria
- **Goal**: optimize resource utilization, get high-quality results and maximize benefits
- **Money** is an issue, but **realistic** hypotheses and ideas are a must
- **The data science life-cycle**:
  1. Data acquisition
  2. Data preparation
  3. Hypothesis and modeling
  4. Evaluation & Interpretation
  5. Deployment
  6. Operations
  7. Optimization



# Management of a DS project (II)

1. **Data acquisition** – acquiring data from internal and external sources
2. **Data preparation** (“data wrangling”) - involves cleaning the data and reshaping it into a readily usable
3. **Hypothesis and modeling** – applying ML techniques to all data (MS: model selection). MS involves to identify training/test sets
4. **Evaluation and interpretation** – comparing model performances
  - *Steps 2-3-4 are repeated; as the understanding of data and business becomes clearer*

# Management of a DS project (III)

5. **Deployment** – the project is run in a production environment. It could include fast-tweaks *after* deployment, based on the continuous deployment model.
6. **Operations** (maintenance) – This phase could also follow a DevOps model which gels well with the continuous deployment model, given the rapid time-to-market requirements in big data projects. Steps 5 and 6 are mixed usually (like agile software in software engineering).
7. **Optimization** – This could be triggered by failing performance, or due to the need to add new data sources and retraining the model, ...

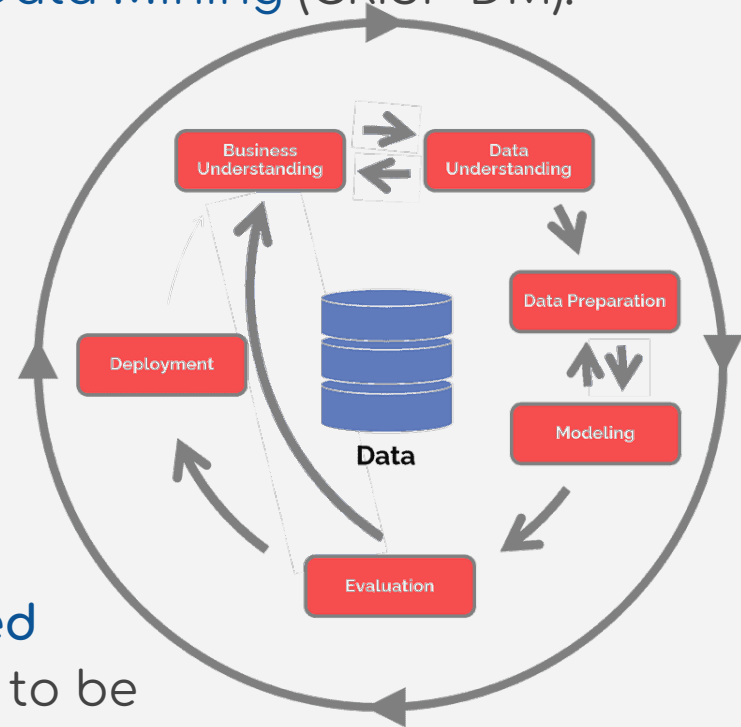
# Examples

In which step is the activity done? (1. Data acquisition, 2. Data preparation, 3. Hypothesis and modeling, 4. Evaluation & Interpretation, 5. Deployment, 6. Operations, and 7. Optimization)

- A.- Removing outliers
- B.- Calculating vehicle speed from its positions
- C.- Running the complete system on a Docker infrastructure for testing
- D.- Splitting the dataset into train and test set
- E.- Deploy improved version of the model
- F.- Rebooting the complete system after an unrecoverable failure
- G.- Applying cross-validation
- H.- Tuning the model parameters
- I.- Examining which models can be applied to the data
- J.- Obtaining values from car's sensors (OBD-II)

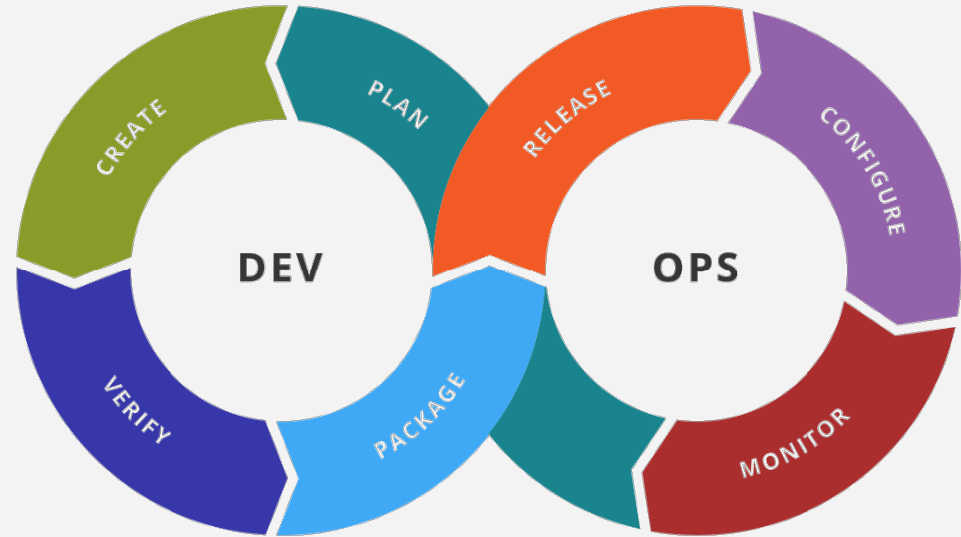
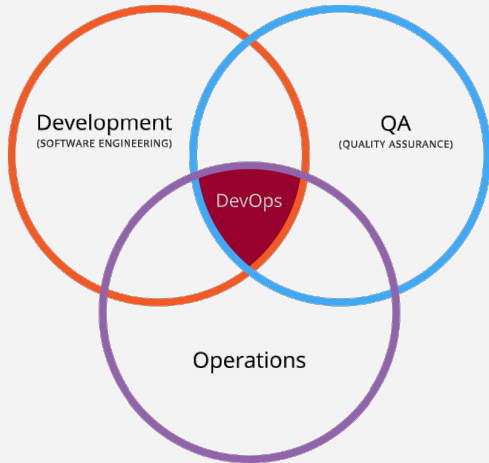
# You should now also on (I) CRISP-DM

- **C**Ross Industry Standard Process for Data Mining (CRISP-DM):
  1. Business understanding
  2. Data understanding
  3. Data preparation
  4. Modeling
  5. Evaluation
  6. Deployment
- **L**ibrary of **a**ssets (expertise/maturity):
  1. Library of business use case
  2. Data requirements
  3. Minimum data quality requirements
  4. ...
- **D**ata scientists are likely to have **limited business domain expertise**. They need to be paired with business people and those with expertise in understanding the data.



# You should now also on (II) DevOps

- Set of practices to **reduce the time** between committing a change to a system and the change being placed into normal production, while ensuring **quality**
- It uses different sets of tools (toolchains) rather than a single one
- **Steps** - Coding + Building + Testing + Packaging + Releasing + Configuring + Monitoring



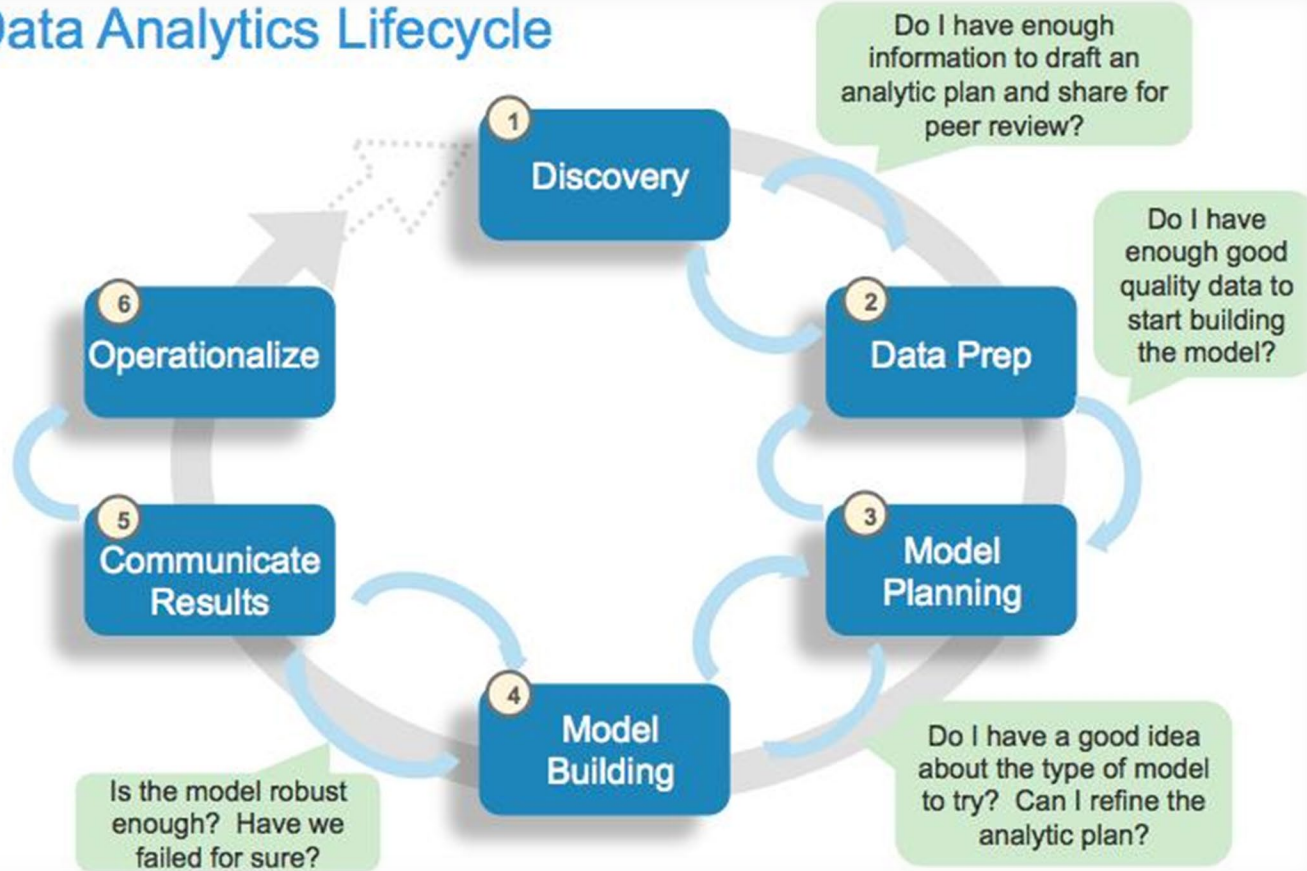


# Other models having seven steps

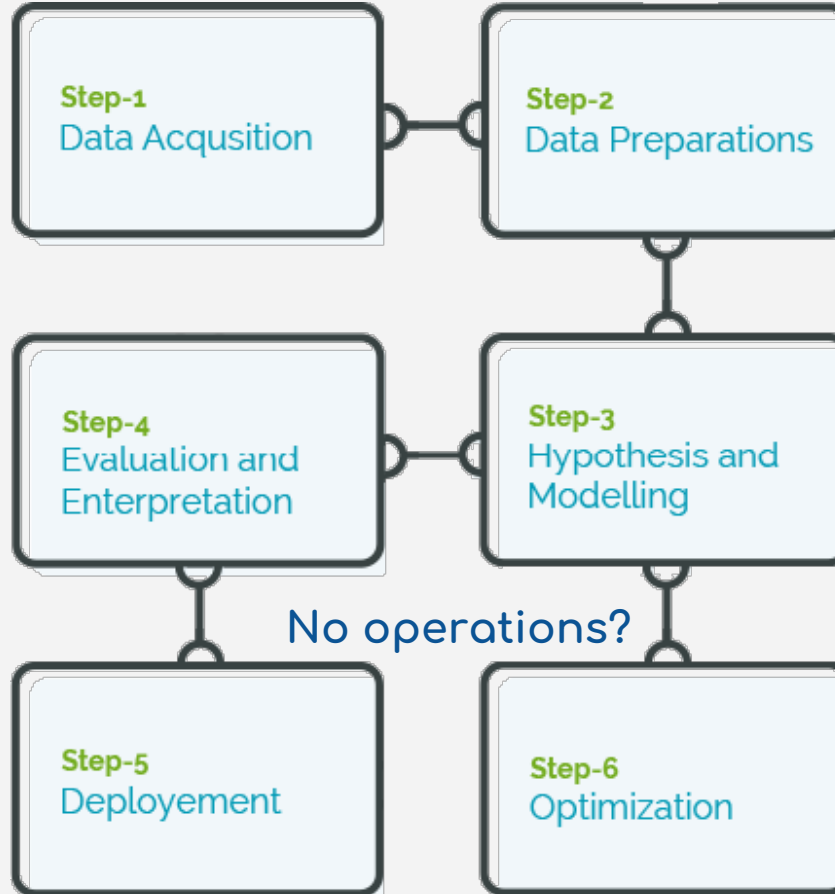


# Other models having six steps (I)

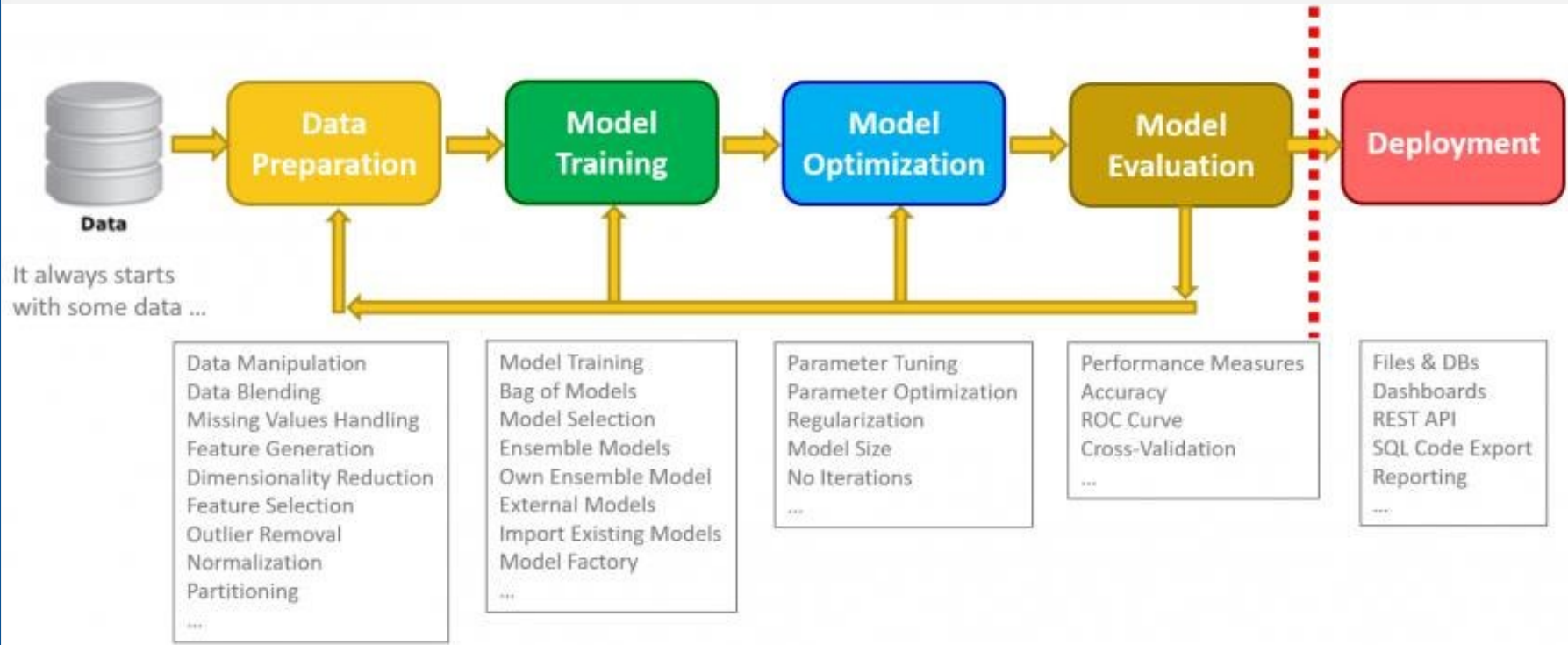
## Data Analytics Lifecycle



# Other models having six steps (II)

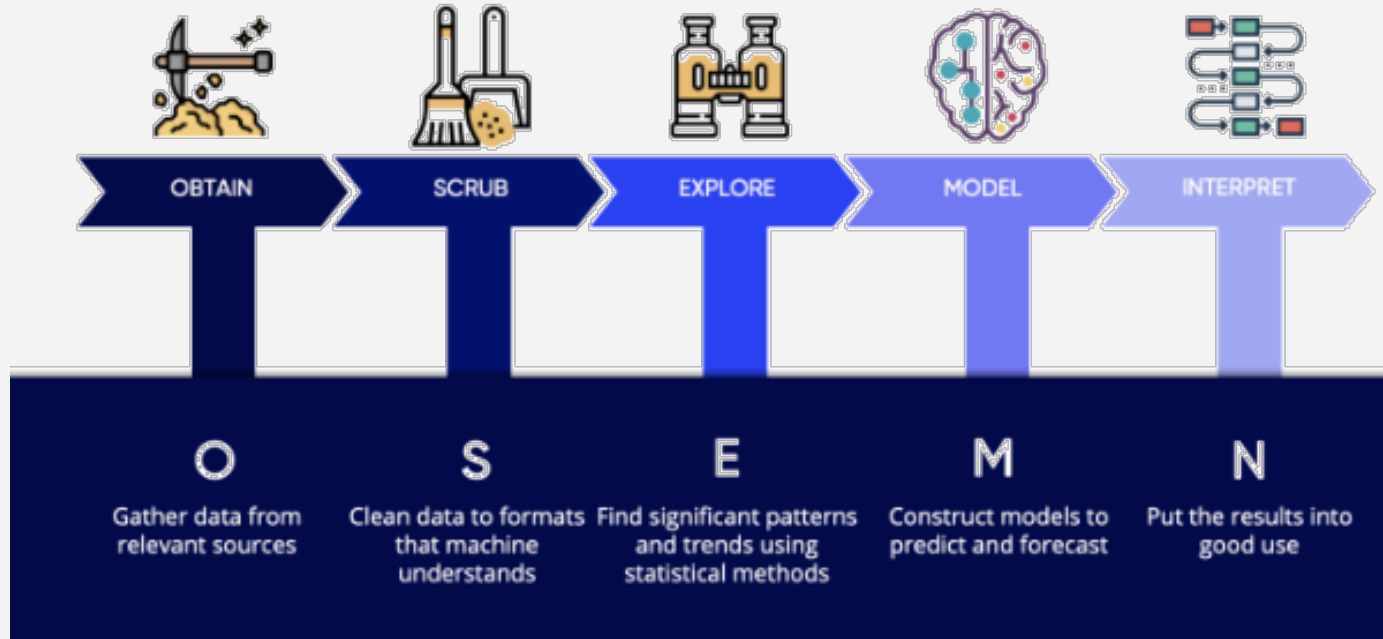


# Other models a smaller number of steps

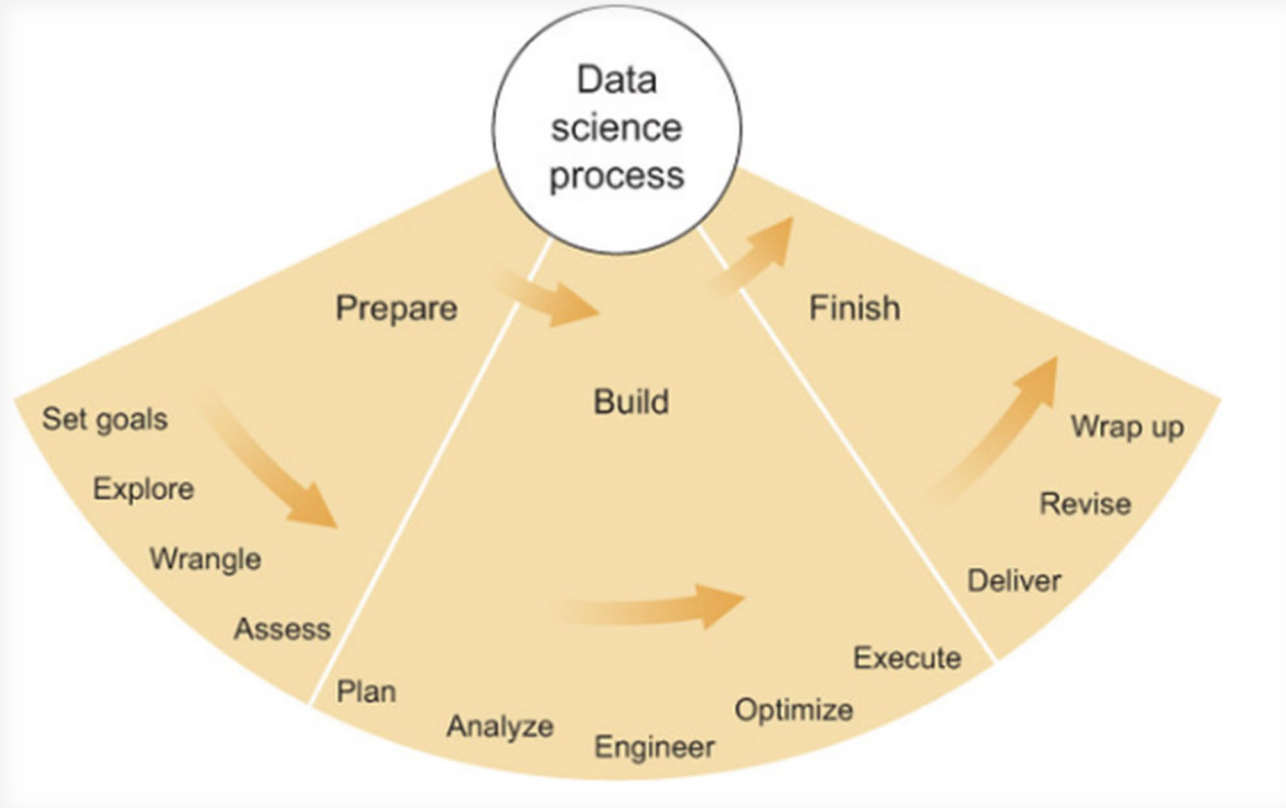


# Other models a smaller number of steps

## Data Science Process



# Models having a larger number of steps!





# ... OK; let's go wild!

Transform, Binning  
Temporal, Text, Image  
Feature Selection

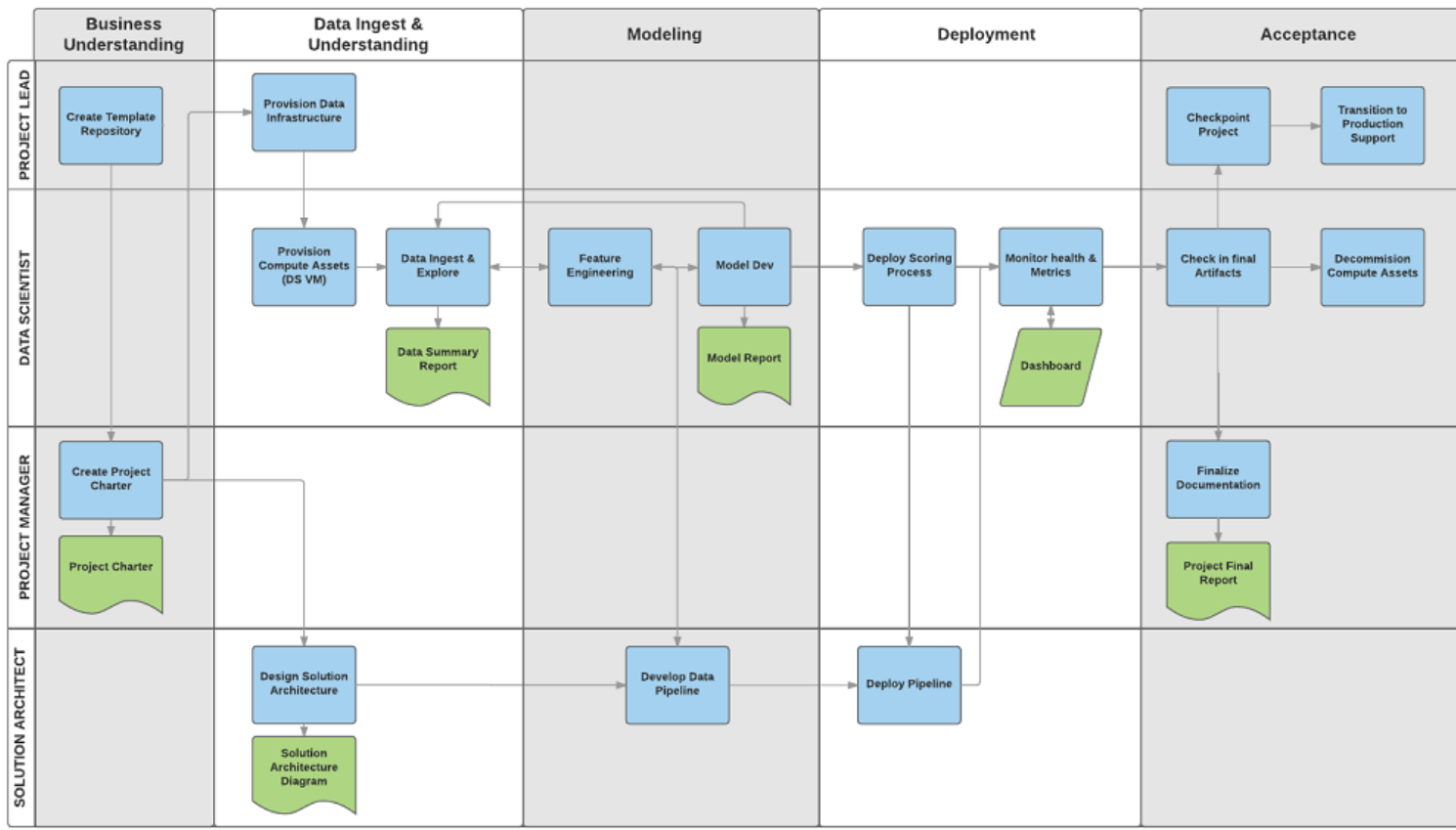
Algorithms, Ensemble  
Parameter Tuning  
Retraining  
Model management

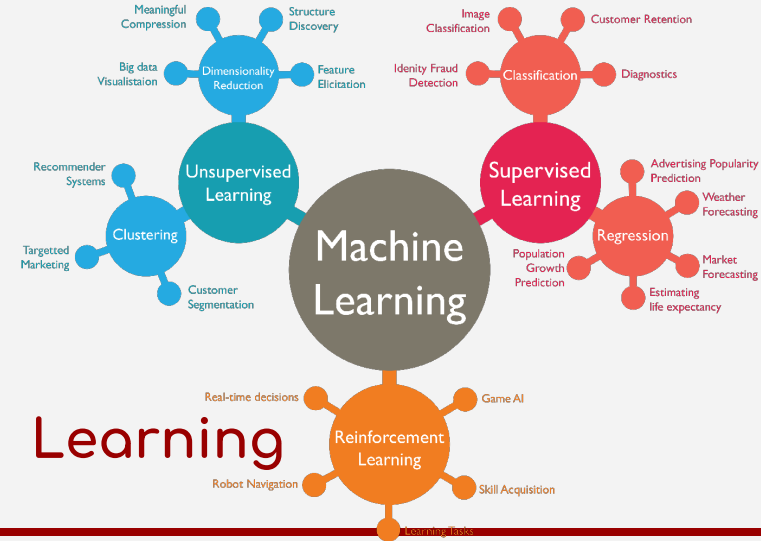
Cross Validation  
Model Reporting  
A/B Testing

**Feature Engineer**

**Model Training**

**Model Evaluation**

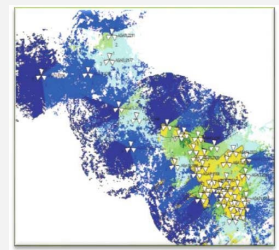
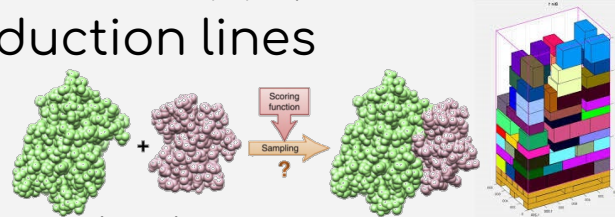






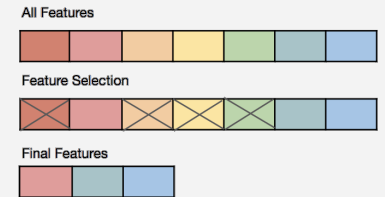
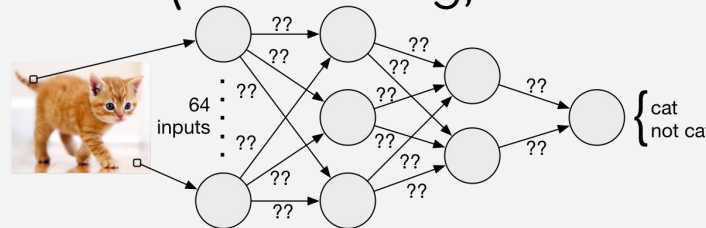
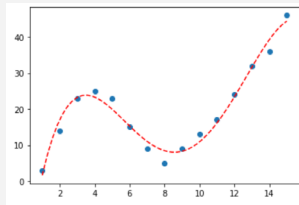
# Optimization problems are everywhere!

- Logistics, transportation, supply change management
- Manufacturing, production lines
- Timetabling
- Cutting & packing
- Computer networks and telecommunications
- Health
- Videogames
- Software (SBSE)



STAFF	MON				
	Period 1	Period 2	Period 3	Period 4	Period 5
JAMESON	ENGLISH 2A 5	FRENCH 2B 4	HISTORY 2C 1	I.T. 1A LAB 2	MATHS 3B 3
HOLDEN	HOME EC 3A LAB 1	HOME EC 4A LAB 1	MATHS 1 3B 12	P.E. 3A GYM	GERMAN HIST 1C 8 3C
BENNETT	MATHS 4B 3	ENGLISH 4A 8	P.E. 3B GYM	HISTORY SC 3	I.T. 4B LAB 2
WHITESIDE	I.T. 2B LAB 2	MATHS 4A 7	ENGLISH 1B LIB	ENGLISH 2C LIB	HOME EC 1C LAB 1

... even in **data science** (data fitting, NN training, feature selection...)



# Optimization problems

- Most general form:

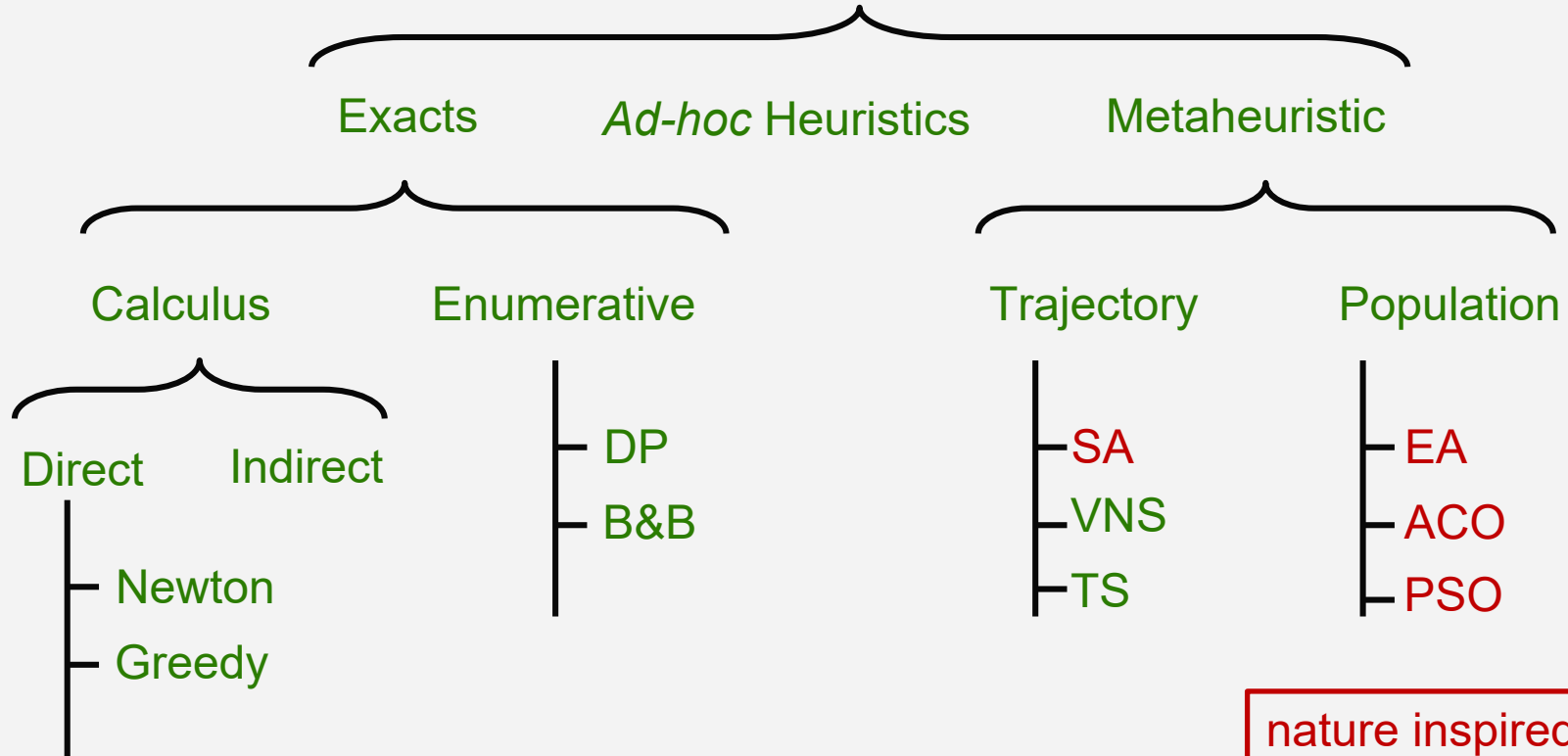
$$\min_{x \in X_{ad}} f(x)$$

Terminology:

- $f: X_{ad} \rightarrow R$ : **fitness function**, objective function, usually real-valued
- $\min \leftrightarrow \max$  by replacement  $f \leftrightarrow -f$
- $x$ : **control** or **optimization parameters**
  - integer/discrete, continuous, or mixed-integer problems
- $X$ : usually vector space or unbound set
- $X_{ad} \subset X$ : **admissible** or **feasible set**
  - $X_{ad} = X$ : **unconstrained problem**
  - $X_{ad} \neq X$ : **constrained problem**

# A taxonomy of modern AI techniques

## Optimization Algorithms

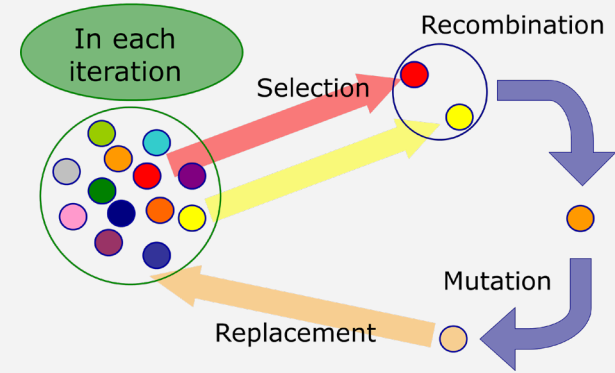


nature inspired in red

# Evolutionary Algorithm

- Based on the ideas of Darwinian Evolution theory

```
t := 0
initialize(P(t))
evaluate(P(t))
while not end condition do
    P'(t) := selection(P(t))
    P'(t) := recombination(P'(t))
    P'(t) := mutation(P'(t))
    evaluate(P'(t))
    P(t+1) := replacement(P(t), P'(t))
    t := t+1
end while
```

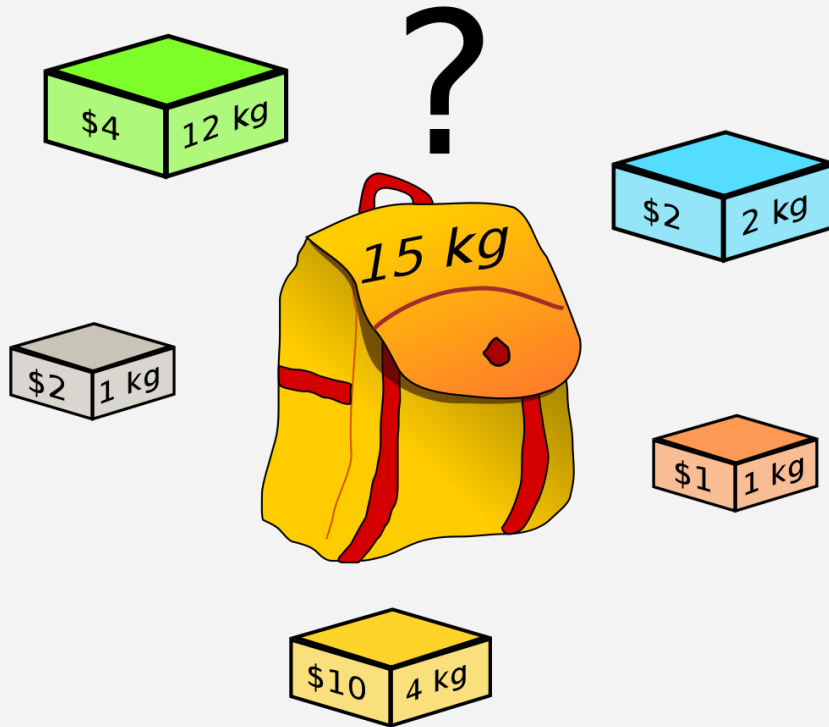


In order to use one EA several steps of instantiation are needed:

- Problem: **genotype** (encoding) and **fitness function**
- Operators** and their parameters
- Stopping criterion

# Evolutionary Algorithm: example (I)

- 0-1 Knapsack problem



Maximize  $\sum_{i=1}^n v_i x_i$

Subject to  $\sum_{i=1}^n w_i x_i \leq W$  and  $x_i \in \{0,1\}$

# Evolutionary Algorithm: example (II)

- **Genotype:** bit string

0	1	1	1	0	0	0	1	1	0	1	0	1	1	1
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

- **Fitness function:**  $\sum_{i=1}^n v_i x_i$
- **Stop condition:** 100000 evaluations

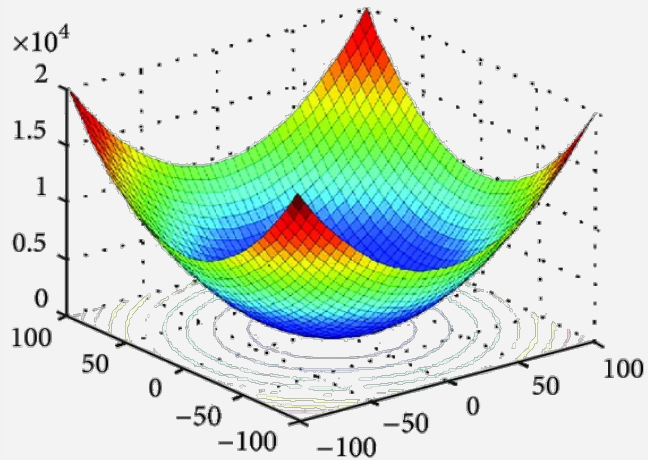
- **Population:**
  - Size: 100
  - Random generated

0	0	1	1	1	0	0	0	1	1	0	1	0	1	1	1
1	1	1	0	0	1	1	1	0	1	0	1	0	1	1	0
2	1	0	1	1	0	1	0	1	0	1	0	1	0	1	1
	...														
99	0	0	0	1	1	0	1	1	1	0	1	1	1	0	0

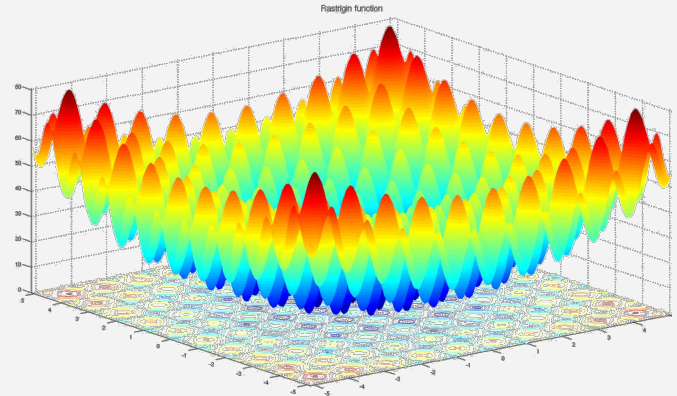
- **Selection:** Random
- **Replacement:** Worst



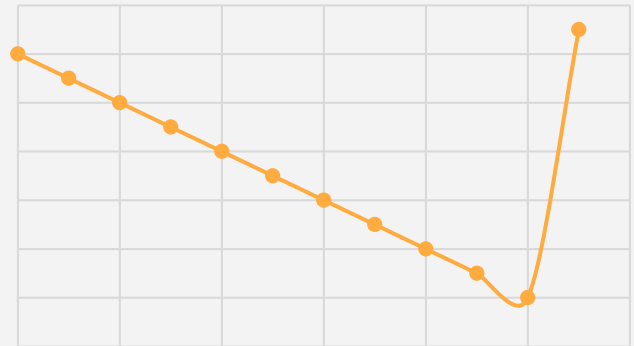
# Search space



**Unimodal**



**Multimodal**



**Deceptive**



Population generation

Selection

Crossover



# Search space and GA operators

25

Population generation

Selection

Crossover

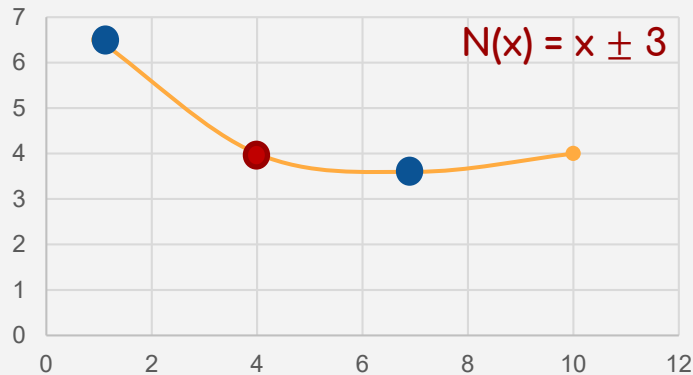
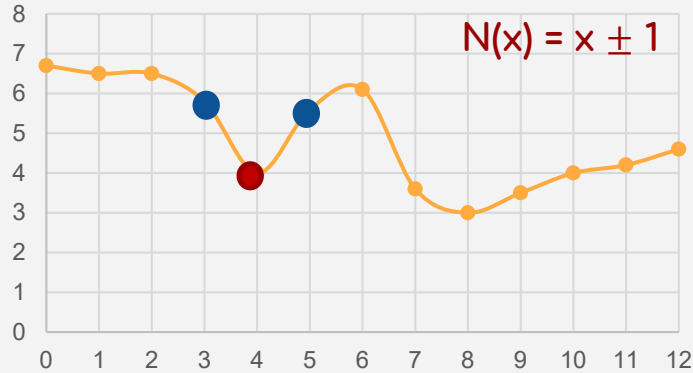
Mutation

Replacement

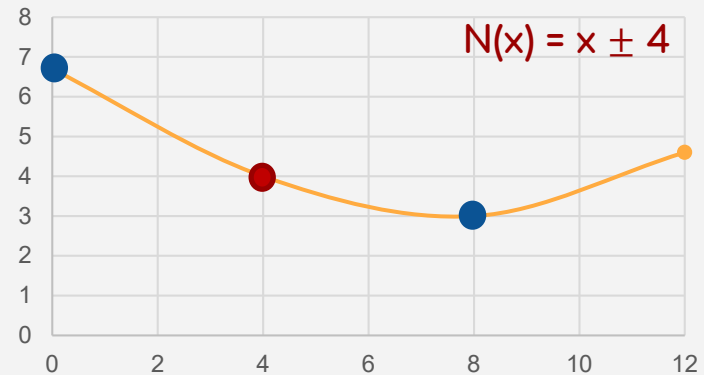
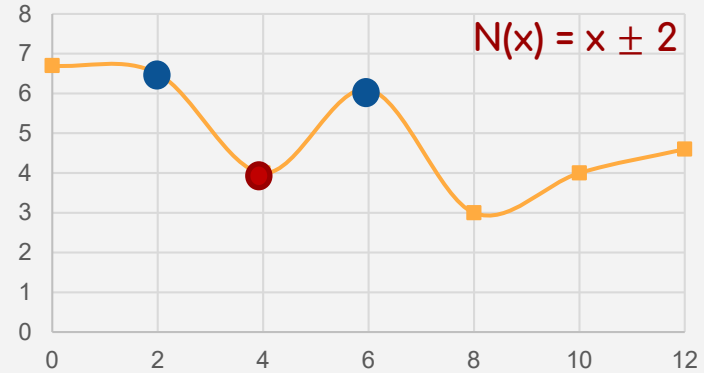


# Search space and Neighbourhood

## Current solution



## Neighbours



# Particle Swarm Optimization (I)

- Particle Swarm Optimization (PSO) is a population based metaheuristic inspired in the social behavior of **birds** within a flock
- It was initially designed for **continuous optimization** problems, but can be used in discrete ones also
- In PSO, each potential solution is called a **particle** and the population of particles is called a swarm
- In this algorithm, each **particle position**  $p_i$  is updated each generation  $k$  by means of this equation ( $v^i$  is its **velocity**):



$$p_i^{k+1} \leftarrow p_i^k + v_i^{k+1}$$

# Particle Swarm Optimization (II)

- The velocity of the particle is given by the expression:

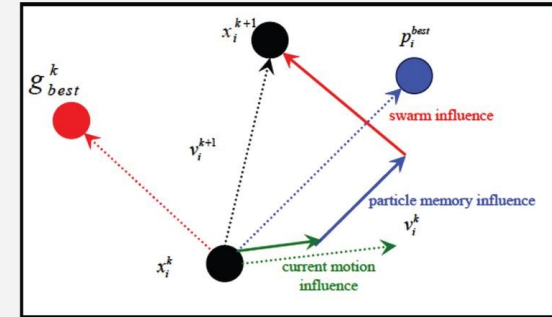
$$v_i^{k+1} \leftarrow w \cdot v_i^k + c_1 \cdot r \cdot g_{best}^k + c_2 \cdot r \cdot p_i^{best}$$

## Algorithm 1 Pseudocode of PSO

```

1: initializeSwarm()
2: locateLeader(b)
3: while !stopCondition() or  $g < maxGenerations$  do
4:   for each particle  $x_g^i$  do
5:     updateVelocity( $v_g^i$ ) // Equation 2
6:     updatePosition( $p_g^i$ ) // Equation 1
7:     evaluate( $p_g^i$ )
8:     update( $bp_g^i$ )
9:   end for
10:  updateLeader( $b_g$ )
11: end while

```



# Simulated Annealing

- It is based on **annealing** in metallurgy
- SA is a **hill-climbing** method
- It **accepts worse solutions** to avoid getting stuck in local optima, according a criterion (y is new solution and x the old one):

$$\text{rand}(0,1) \leq \min \left( 1, e^{\frac{f(x)-f(y)}{T}} \right)$$

**Algorithm 1** Simulated annealing algorithm

```
1: procedure SA( $f, N, \Omega, x^0, T_0$ )
2:    $k \leftarrow 0$ 
3:    $x_{\min} \leftarrow x^k$ 
4:    $f_{\min} \leftarrow f(x_{\min})$ 
5:    $T_k \leftarrow T_0$ 
6:   while stopping criterion is not satisfied do
7:      $z^k \leftarrow \text{rand}(N(x^k, T_k))$ 
8:      $y^k \leftarrow x^k + z^k$ 
9:     if  $\text{rand}(0, 1) \leq \min\{1, \exp\{(f(x^k) - f(y^k))/T_k\}\}$  then
10:       $x^{k+1} \leftarrow y^k$ 
11:     else
12:       $x^{k+1} \leftarrow x^k$ 
13:     if  $f(x^{k+1}) < f_{\min}$  then
14:       $x_{\min} \leftarrow x^{k+1}$ 
15:       $f_{\min} \leftarrow f(x_{\min})$ 
16:      $k \leftarrow k + 1$ 
17:      $T_{k+1} \leftarrow$  temperature is updated
18:   return  $x_{\min}$ 
```



# Variable Neighbourhood Search

- VNS is a stochastic algorithm with a **set of neighbourhood structures** are defined,
- Each iteration: **shaking**, **local search** and **move**
- VNS explores a set of **neighbourhoods** to get different local optima and **escape from local optima**

**Procedure Algorithm** of variable neighborhood search:

**begin**

find the best solution found  $x$ ;

$k := 1$

**while** ( $k \leq k_{max}$ ) **do**

randomly generate a new solution  $y \in N_k(x)$ ;

**if** ( $f(x) > f(y)$ ) **then**

$x := y$ ;

$k := 1$ ;

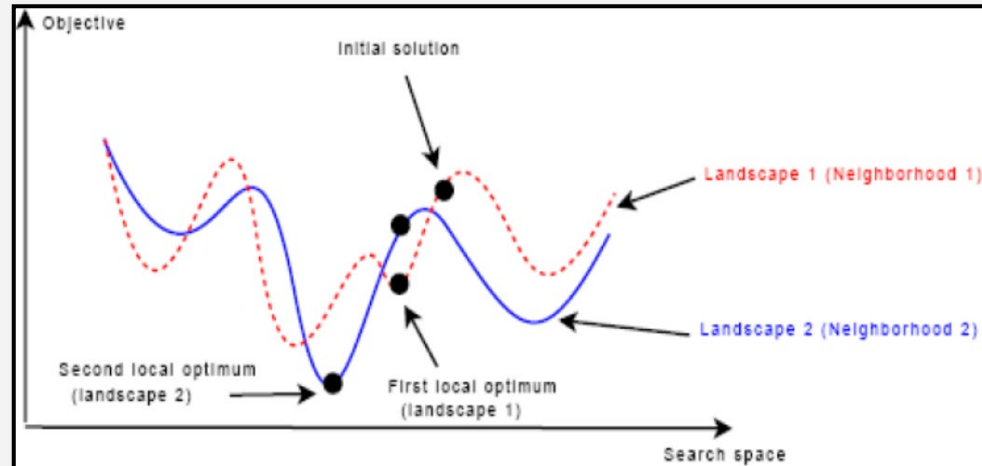
**else**

$k := k + 1$ ;

**endif**

**endwhile**

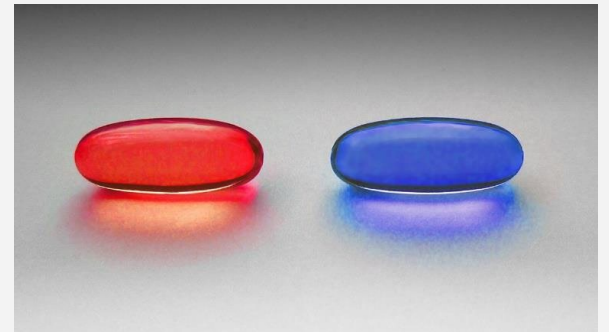
**end**





## Reality is challenging:

- **Large scale**, every is really big
- **Time** consuming and real time
- **Dynamic**, everything changes in time
- **Uncertainty** in all tasks and phases
- **Complex** relations, interdependences
- Several **goals** at the same time
- **Human** preferences and interfaces
- Lots of **restrictions** (legal, technical..)
- **Mobile** plus **desktop** applications







# Scalability

**Scalability** is the property of a system to handle a growing amount of work by adding resources to the system



# SCALABLE

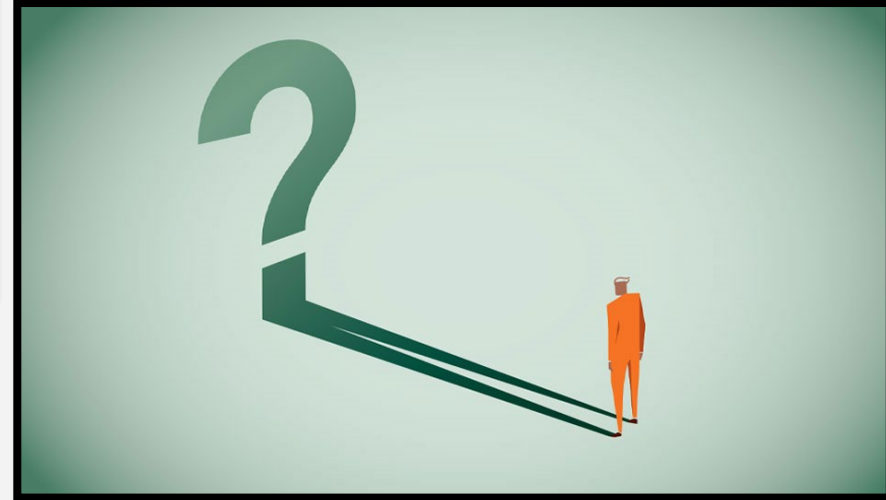
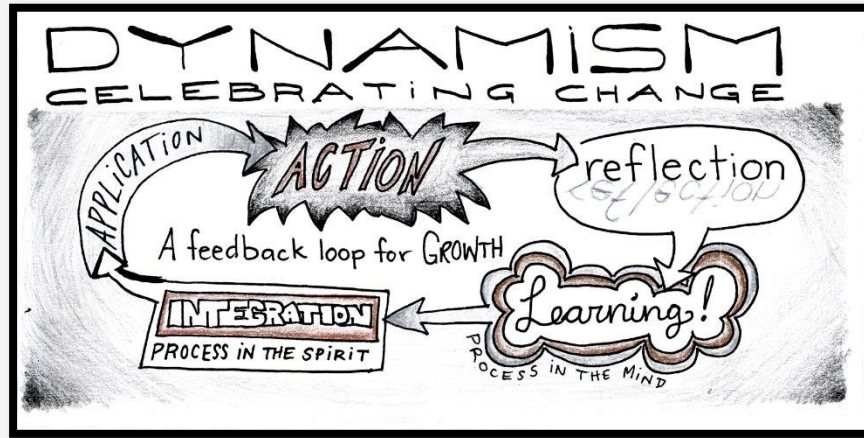




# Dynamism and Uncertainty

**Dynamism:** the problem conditions change over the time in an unpredictable way

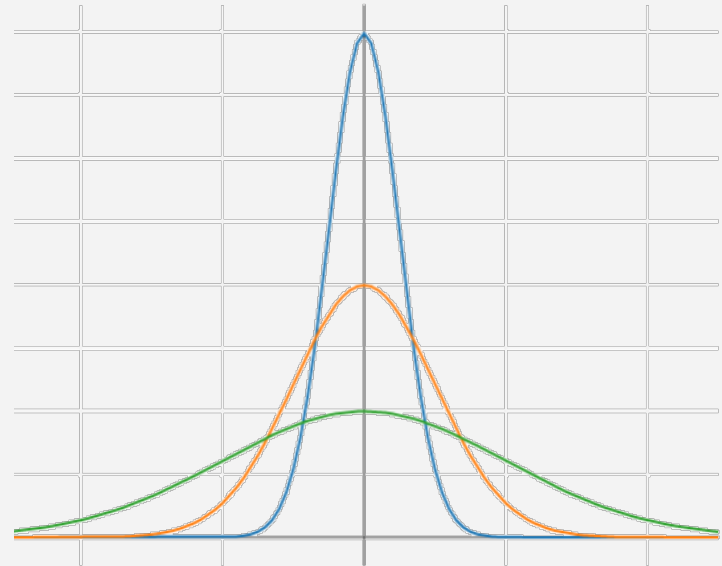
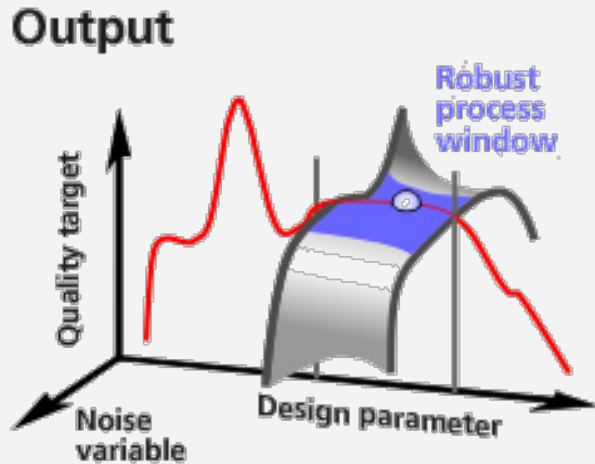
**Uncertainty:** the problem involves imperfect or unknown information





# Robustness

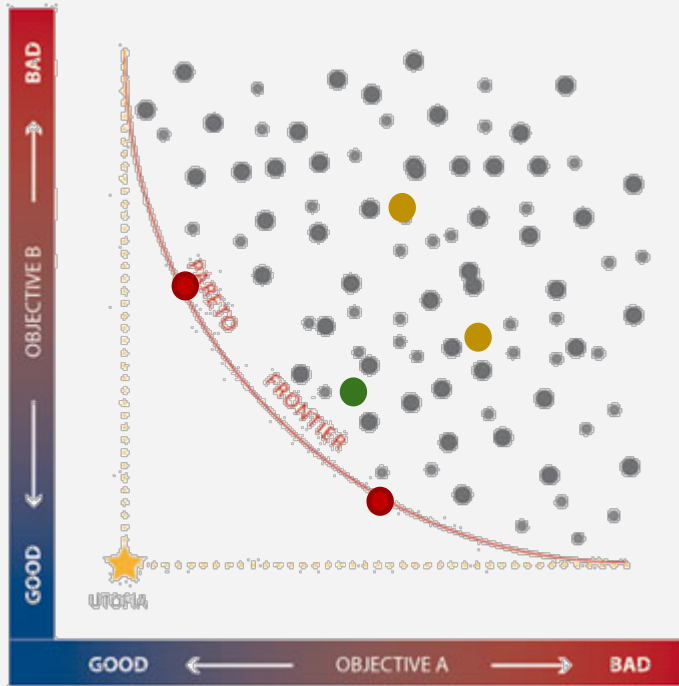
**Robustness:** the performance is stable after adding some noise to the environment





# Multiple Objectives

Green dominates yellow. Red are non-dominated.



Multi-Objective Optimization:  
No single "optimum" solution

The Pareto Front

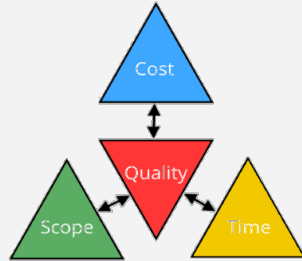
Higher-level Decision Making

The Chosen Solution



# Constraints

... many types of constraints ...

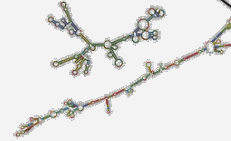


Project Constraints

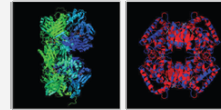


## Types of Data

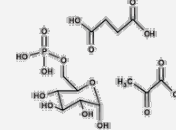
A. Gene Expression



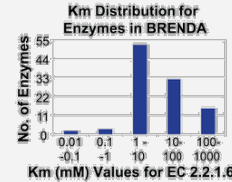
B. Protein Expression



C. Metabolite Concentration



D. Kinetic Parameters



## Types of Constraints

Flux Capacity- Boolean (On/Off)

$$y_j \cdot v_j^{\min} \leq v_j \leq y_j \cdot v_j^{\max}$$

where  $y_j = \{0,1\}$

Flux Capacity- Continuous

$$p_j \cdot v_j^{\min} \leq v_j \leq p_j \cdot v_j^{\max}$$

where  $p_j = [0,1]$

Thermodynamic Constraints

$$\text{if } v_j \geq 0 \text{ then } \Delta G_j \leq 0$$

$$\text{if } v_j \leq 0 \text{ then } \Delta G_j \geq 0$$

$$\Delta G_j = \Delta G_j^0 + RT \sum_i S_{i,j} \ln C_i$$

Molecular Crowding Constraints

$$\sum_j w_j \cdot v_j \leq 1$$

Kinetic Constraints

$$v_j = \frac{k_{cat,j} \cdot C_i}{k_{m,j} + C_i} \quad (\text{Biochemical})$$

$$v_j = k_j \prod_i C_i^{S_{i,j}} \quad (\text{Mass Action})$$



# AutoML

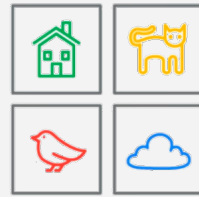
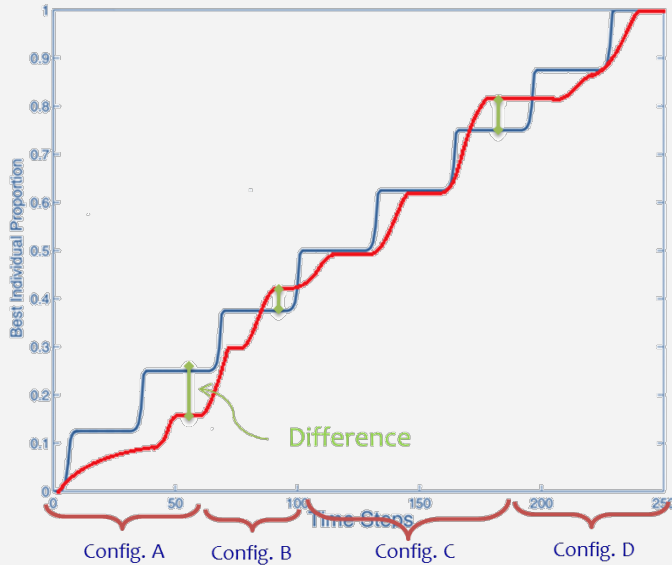


Photo Dataset

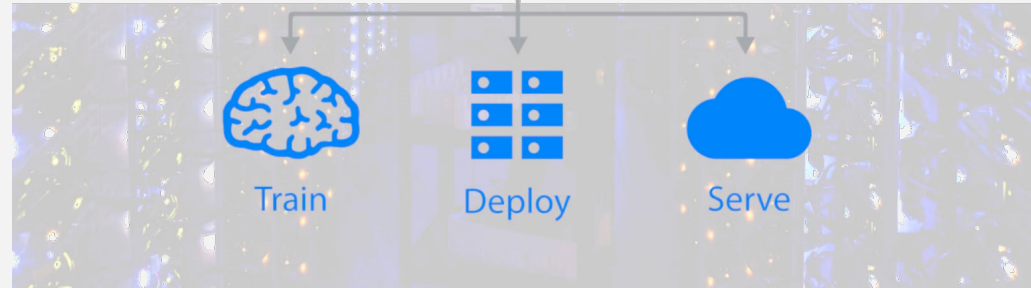


Cloud AutoML Vision



Rest API

Generate predictions with a REST API

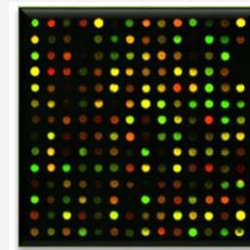




# An example (I)

## Problem:

- Gene selection and cancer classification of DNA
- Microarray, feature selection

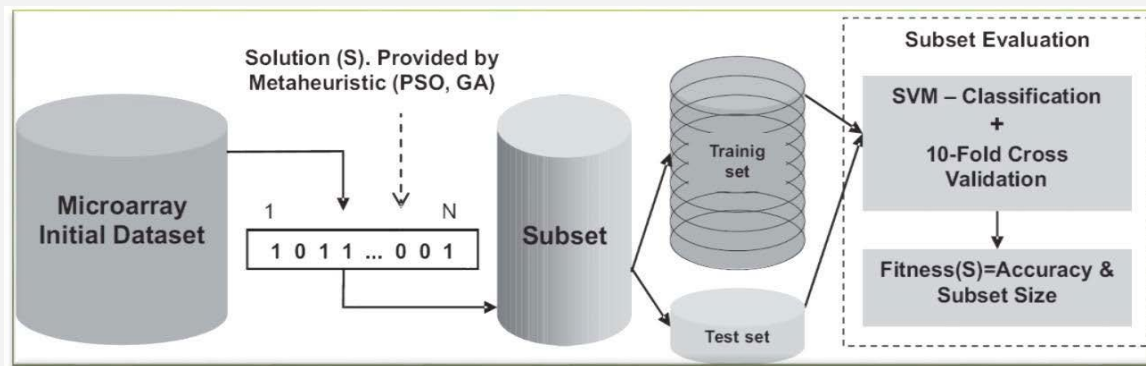


## Objectives:

- Maximize accuracy of prediction
- Minimize the number of selected genes
- Maximize sensibility and specificity ( ROC factors )

## Phases:

- Feature selection
- Training
- Validation
- Fitness calculation





# An example (II)

## Fitness:

- Monobjective: aggregative:  $(\alpha \cdot 100 / \text{accuracy} + \beta \cdot \# \text{features})$
- Multiobjective:  
2 (accuracy, #features) or 3 (sensitivity, specificity, #features)

## Classification:

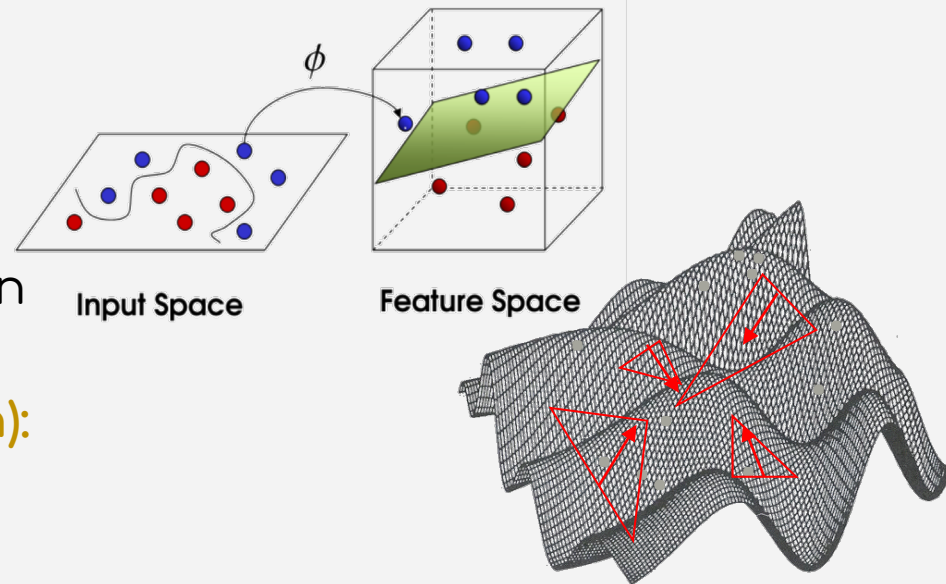
- SVM
- K-means

## Validation:

- Leave one out cross-validation
- 10-fold cross-validation

## Algorithms (for feature selection):

- PSO variant
- GA variant







# An example (III)

## Instances:

- Large scale datasets of well-known cancer DNA Microarrays: Leukemia, Colon, Prostate, Lung, Ovarian, Breast (e.g. breast 24481 genes and 97 patient samples)

**Results:** comparison against other techniques (S.O.T.A.)

Dataset	GPSO	GA	Huerta et al.	Juliusdoti r et al.	Deb et al.	Guyon et al.	Yu et al.	Liu et al.	Shen et al.
<i>Leukemia</i>	97.38(3)	97.27(4)	100(25)	-	100(4)	<b>100(2)</b>	87.44(4)	-	-
<i>Breast</i>	86.35(4)	<b>95.86(4)</b>	-	-	-	-	79.38(67)	-	-
<i>Colon</i>	<b>100(2)</b>	100(3)	99.41(10)	94.12(37)	97(7)	98(4)	93.55(4)	85.48(-)	94(4)
<i>Lung</i>	99.00(4)	<b>99.49(4)</b>	-	-	-	-	98.34(6)	-	-
<i>Ovarian</i>	<b>99.44(4)</b>	98.83(4)	-	-	-	-	-	99.21(75)	-
<i>Prostate</i>	<b>98.66(4)</b>	98.65(4)	-	88.88(20)	-	-	-	-	-

## Leukemia Gene Subset:

PSO: K01383, U03056, J04130 vs GA: L40379, S85963, U83192, Z49099

# Advanced Tools

Data Science and Engineering (I)  
Master's Degree in Computer Engineering



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# Advanced techniques and technologies

1. **Complex** problems need advanced tools
2. **Measuring** efficacy and efficiency
3. **Parallel hardware**, or how new technology helps
4. **Algorithm hybridization**, or how new techniques can help
5. **Practical Examples**





# Real problems need more than you expect / know

3

- **Graduate** students know some tools to deal with engineering apps
- Most graduate programs offer a **small sample** of algorithms and technologies
- Graduate students then only know **very basic concepts**
- **Real** problems seldom admit the **constraints** of basic tools
- A complex real application needs **advanced** algorithms and technologies
- **Research** in algorithms, software, AI, and new technologies is full of them
- Just **few techniques** that can be used as described in books
- To work well, they need to be improved...

How do we improve them?

# Important questions

**What is the computational complexity of your algorithm?**

Measure it as  $O(n)$   $O(\log n)$   $O(n \cdot \log n)$   $O(n^2)$   $O(n^3)$  ...  $O(2^n)$  ...  $O(n!)$  ...  $O(n^n)$  ...

**How much simple is a technique? Occam's razor principle applies**

If more complex than one with similar behaviour, then not interesting

**How measure complexity: computational, software, understanding...?**

In terms of input, branches, length of description, time to learn it, ...

**What is defining the limits of a technique or a technology?**

Its complexity, but also its accuracy in solving a problem, its robustness...

**How a technique could be improved? And a technology?**

New design (operations, concepts), new implementation, latest hardware, ...

**Similarities to other existing tools? Do they inspire to improve?**

See the basics of the tool, similar structure, know on cross-fertilization

**Can we quantify all the decisions? Identify all the needed steps?**

Data driven decision making, always measure ... scientific method

# Always measure: efficacy measures

## MSE – Mean Squared Error:

- Risk measure (quality of estimator)

$$MSE = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$$

## Logarithmic Loss:

- Penalising the false classification

$$LogLoss = \frac{-1}{N} \sum_{i=1}^N \sum_{j=1}^M y_{ij} * \log(p_{ij})$$

Accuracy  $Accuracy = \frac{\# \text{ correct predictions}}{\# \text{ input samples}}$

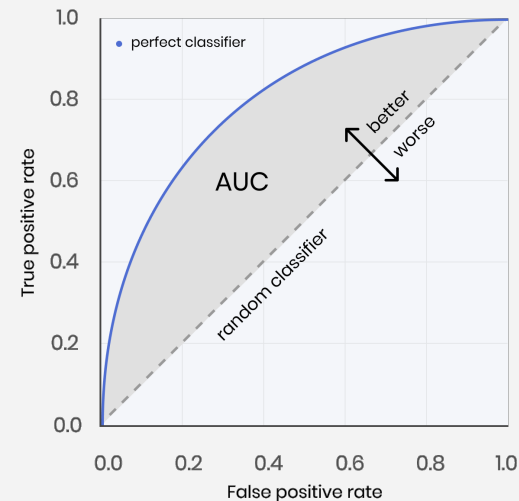
## Confusion Matrix



		True Class	
		Positive	Negative
Predicted Class	Positive	TP	FP
	Negative	FN	TN

## Area under de curve (AUC)

- How well the test separates the group being tested into 2 classes?
- $TPR = TP / (TP + FN)$        $FPR = FP / (FP + TN)$



# Always measure: efficiency measures

## Wall Clock Time

- $T = t_{\text{end}} - t_{\text{start}}$



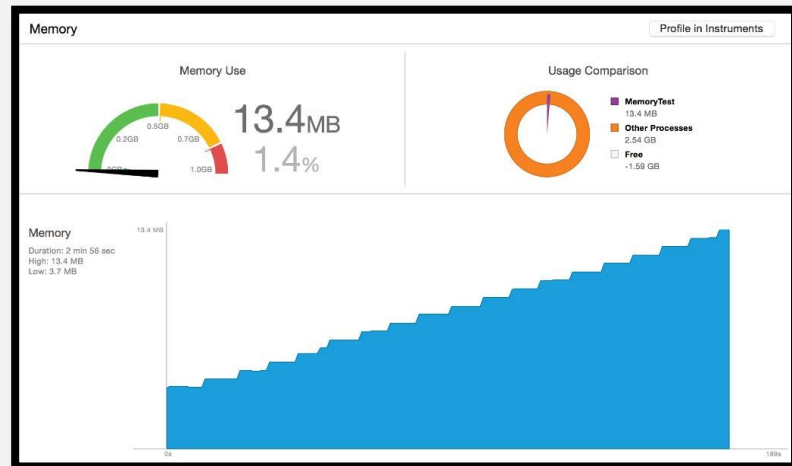
User time  
 CPU time  
 Communication time  
 ...

## Speedup

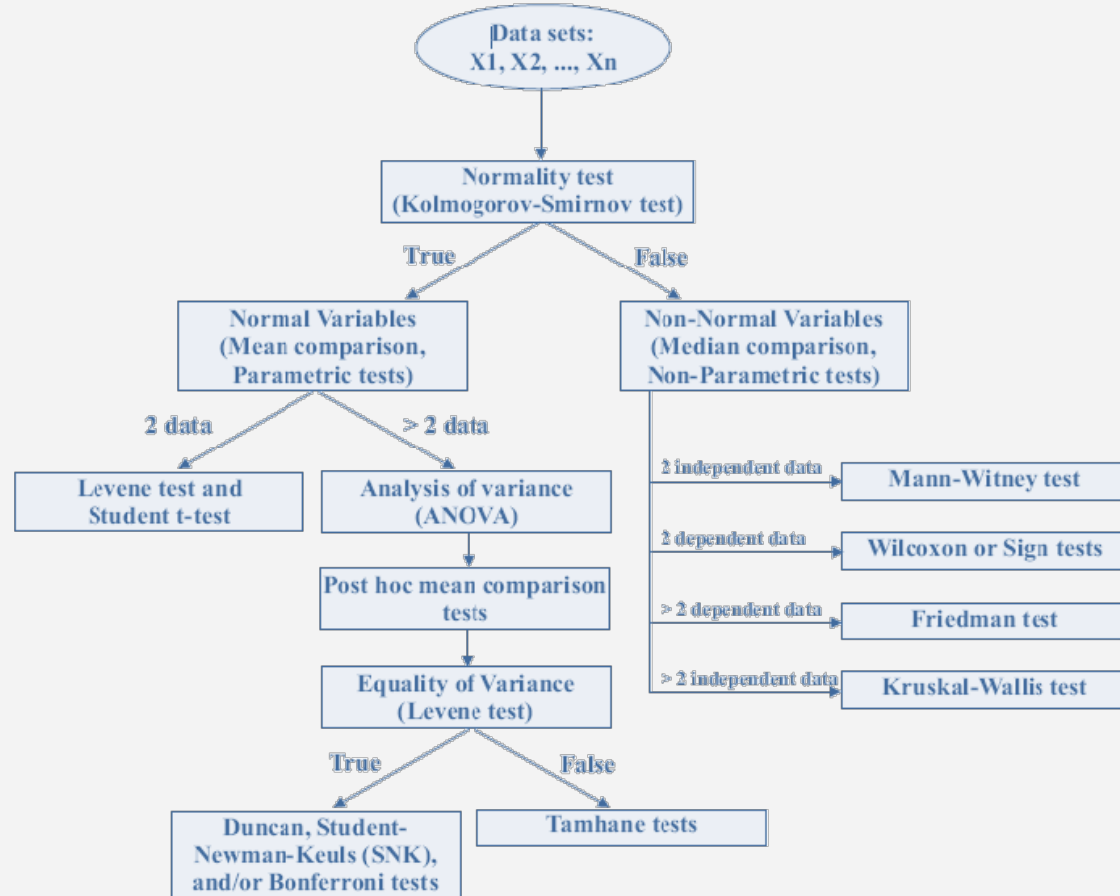
$$S_m = \frac{\bar{T}_1}{\bar{T}_m}$$

Memory usage  
 Size of data files

Battery consumption (phone)  
 Kwh consumption (data center)



# Statistical analysis mandatory





# Parallelism: parallel algorithms plus HW

- Even very advanced algorithms reach a **maximum efficiency**. This happens in large problem instances, or when using simulators, or in real time scenarios, or in web services for clients, ...
- Advances in **parallel hardware** like clusters, multicores, GPUs, cloud, etc. allow to make more than one step per unit time in the used techniques
- Sometimes you are not only looking for **reduced times**, but for **new types** of techniques that search for different solutions at the same time collaborating
- Sometimes you have a multicore or a lab full of cores: **explode them !!!**
- Thus, you can make new techniques and also run them faster, **both !!!**



Problems not solved before,  
now become solvable by  
using parallel tools

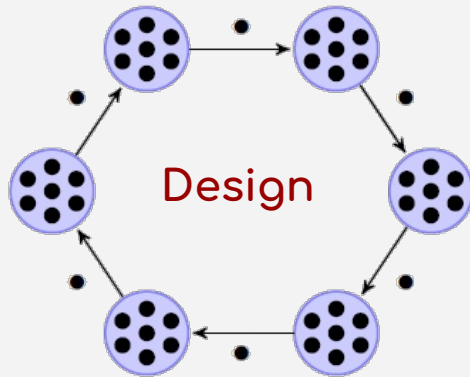
# Parallelism: parallel algorithms plus HW

## Parallelism and Metaheuristics:

The increasing availability of new kinds of CPUs and the parallel nature of metaheuristics have allowed the fast development of parallel metaheuristics

### Advantages:

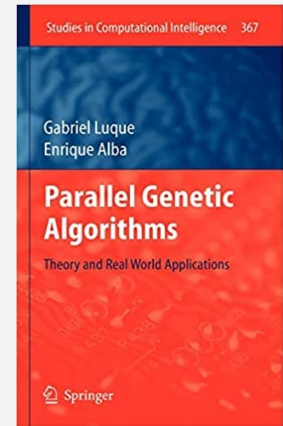
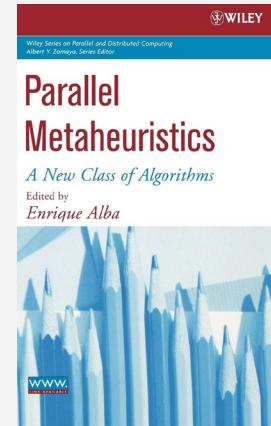
- Allow to tackle more complex problems/instances
- Allow to reduce the execution time
- Allow to improve quality of the found solutions



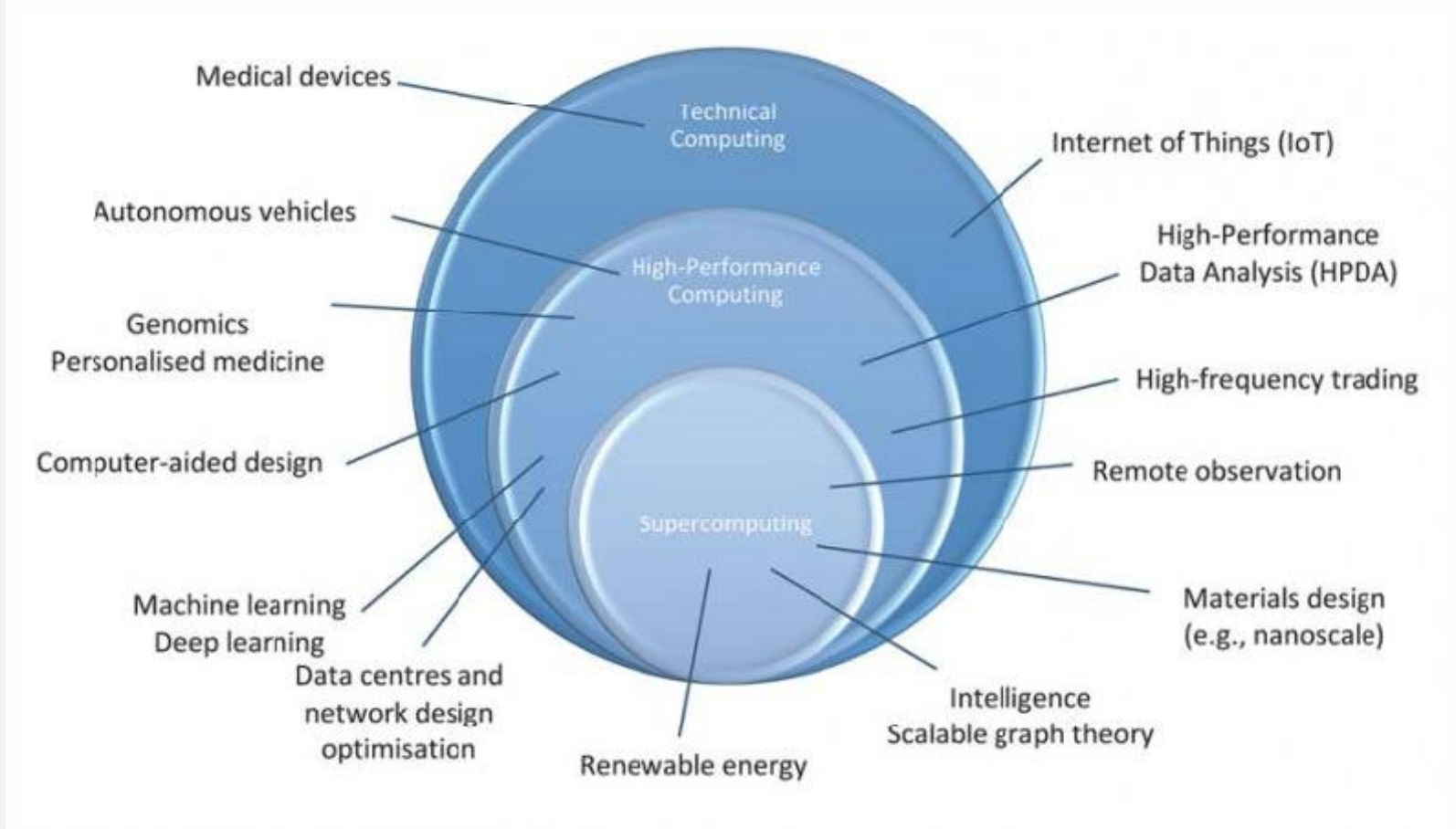
Design



Implementations



# High performance computing and folks



# Hardware is important

## Grid and cloud computing



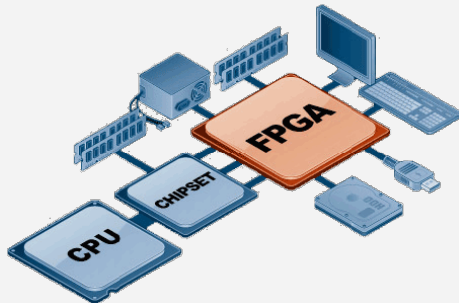
## Cluster computing



## GPU



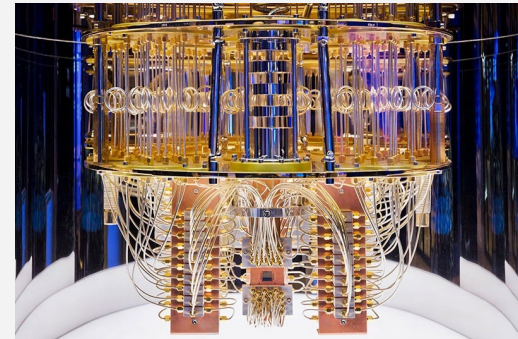
## FPGA



## Manycores



## Quantum Computers



# Design vs implementation, not the same

- Node in a distributed EA

$t := 0$

`initialize`( $P(t)$ )

`evaluate`( $P(t)$ )

**while** not end condition **do**

$P'(t) :=$  `selection`( $P(t)$ )

$P'(t) :=$  `recombination`( $P'(t)$ )

$P'(t) :=$  `mutation`( $P'(t)$ )

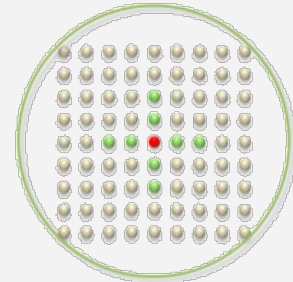
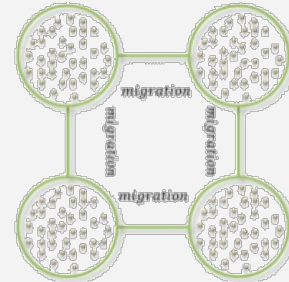
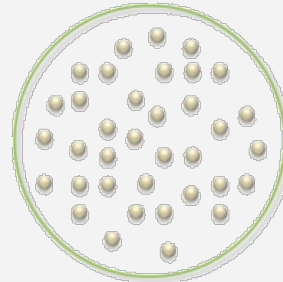
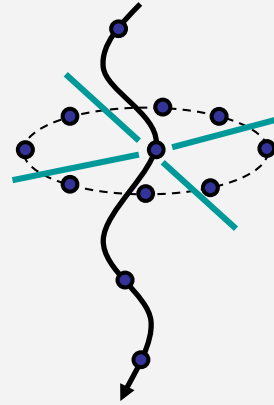
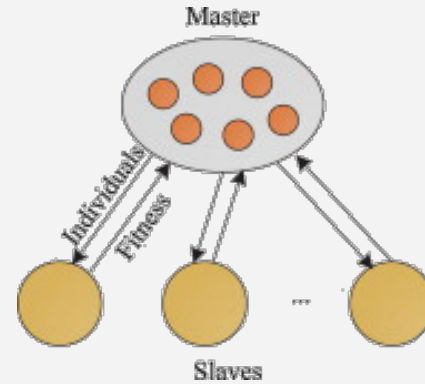
`evaluate`( $P'(t)$ )

$P(t+1) :=$  `replacement`( $P(t)$ ,  $P'(t)$ )

**<<Communication with neighbours >>**

$t := t+1$

**end while**



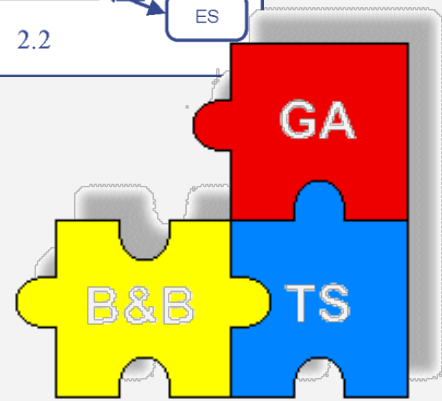
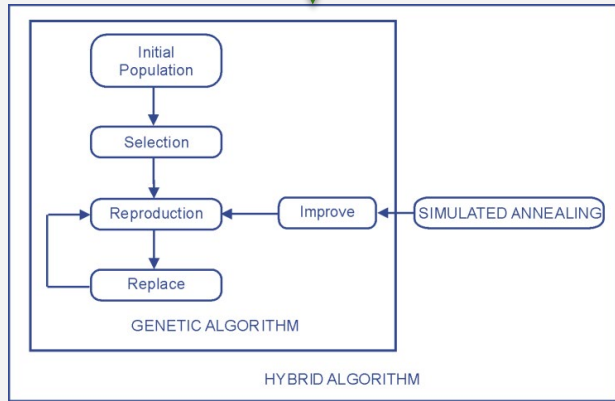
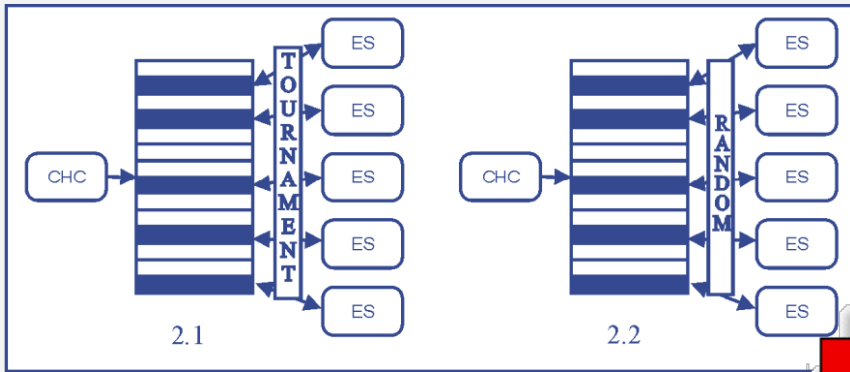
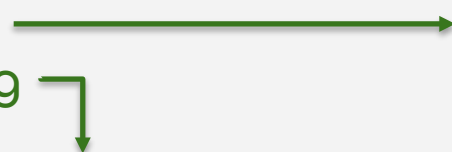


# Hybridization: a good way to build techniques

**Hybridization** is the inclusion of problem-dependent information in the algorithm, but also combining fields, operations, data, technologies, frameworks ...

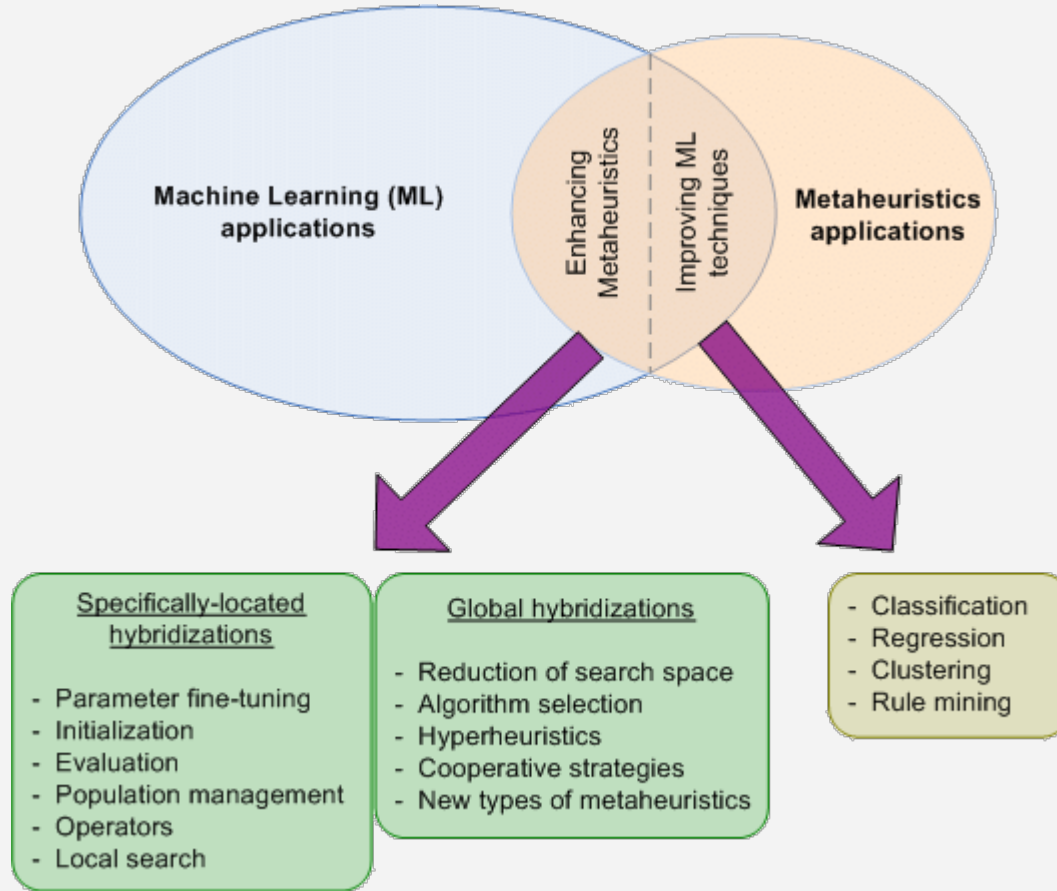
## Types

- Weak
- Strong





# Hybridizing ML with metaheuristics



Optimization + Learning

Hybrids = ML + MetaH

Tuning ML tools

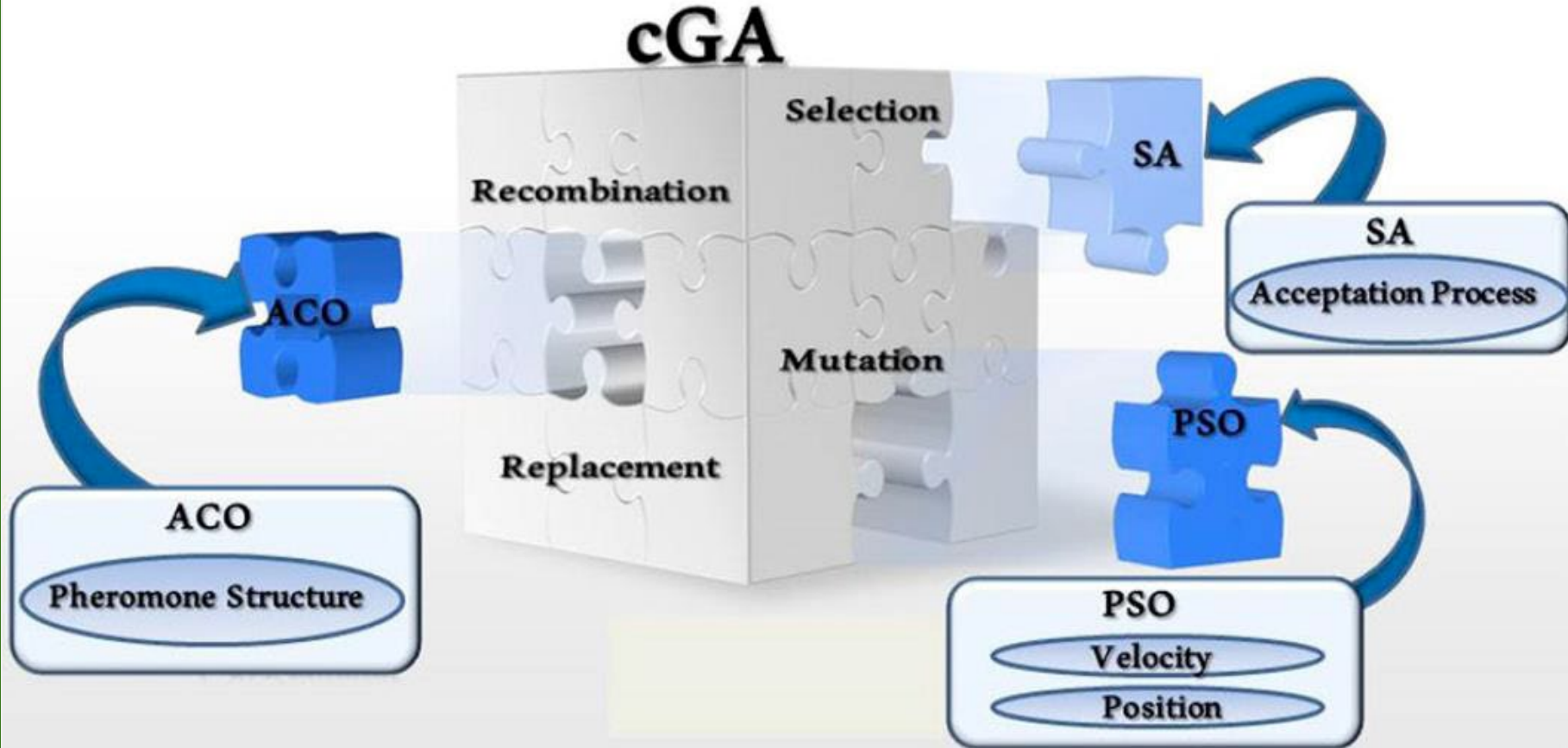
Surrogate systems

Collaboration processes





# Building Blocks



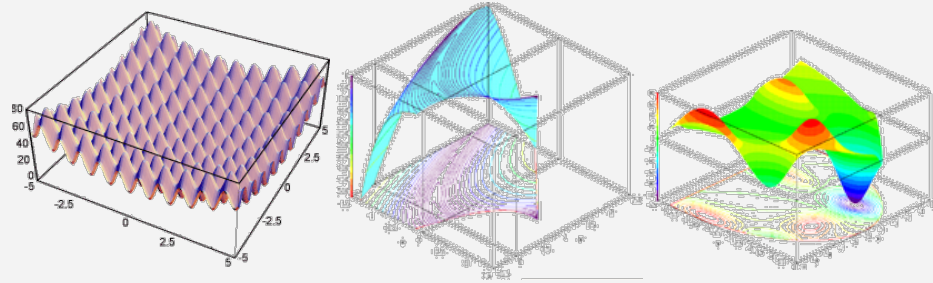




# Academic problem domains

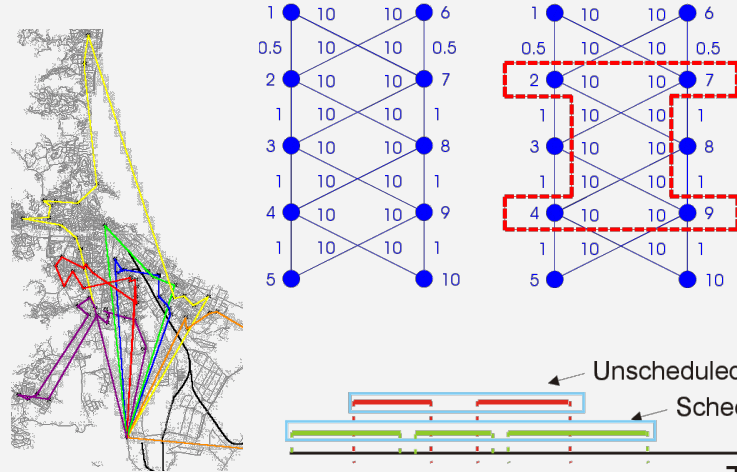
## Mathematical Optimization:

- Rastrigin, Rosenbrock, Mishra's Bird...



## Combinatorial optimization:

- Routes, scheduling, graphs...



## Domain dependent benchmarks:

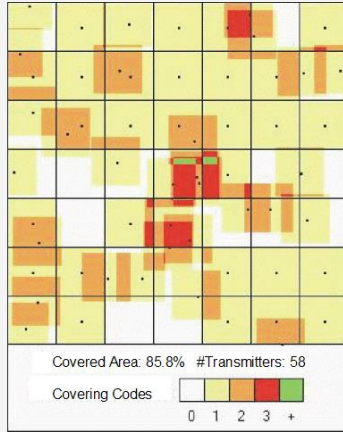
- Multiobjective
- Temporal series
- Data mining
- Neuronal network training

Know on standard benchmarking!!!

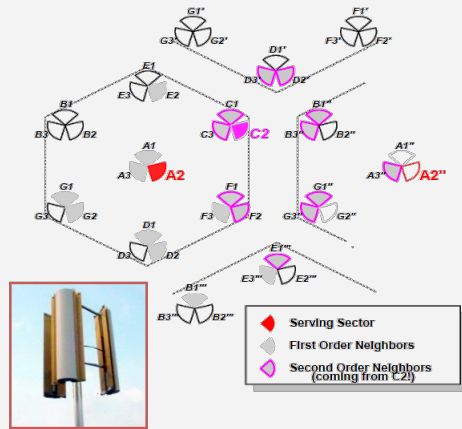


# Sectoral domains: Telecoms in this case

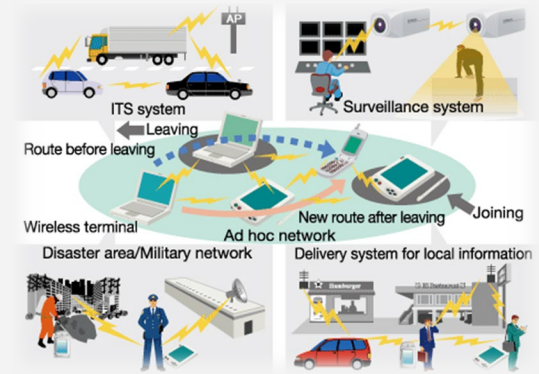
## Radio Network Design



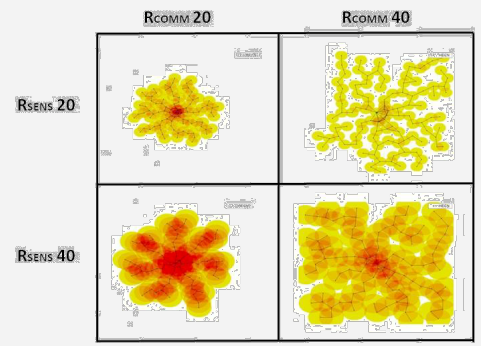
## GSM Frequency Assignment



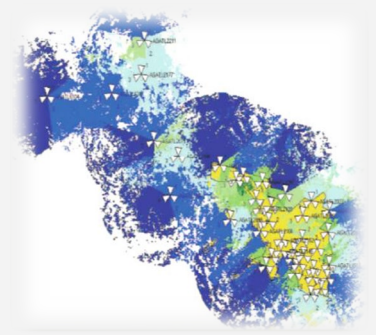
## MANETs



## Sensor Network Layout



## Location Area in 4G/5G



## VANETS





# Every single domain is a good target

Designing Quantum Circuits

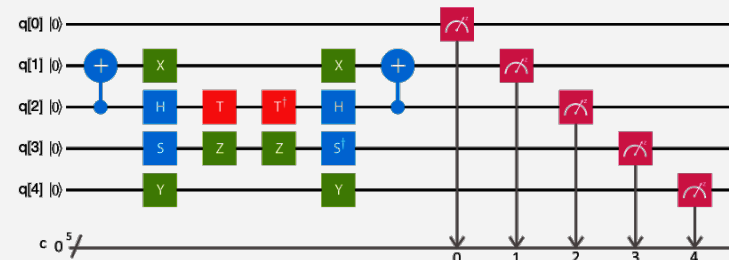
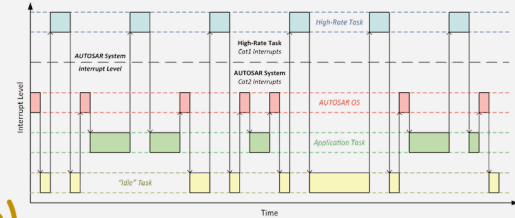
Data Based (Data Mining, Query Optimization)

Dynamic Optimization Problems (DOPs)

Tasks Scheduling in Operating Systems

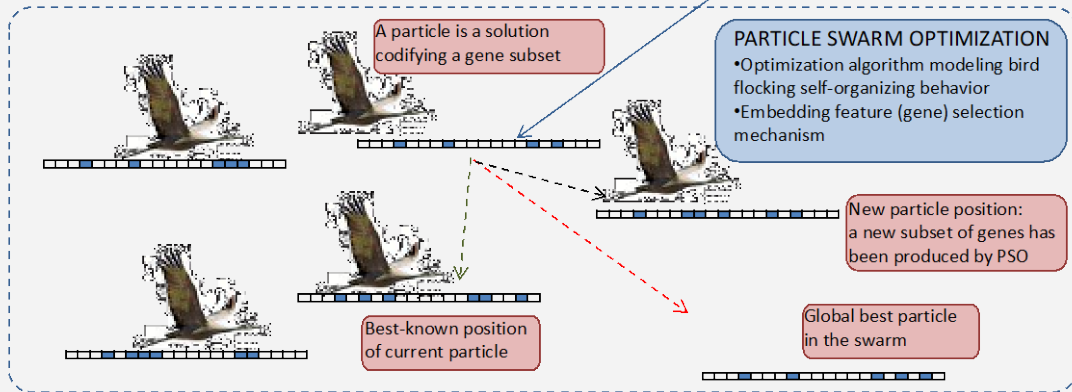
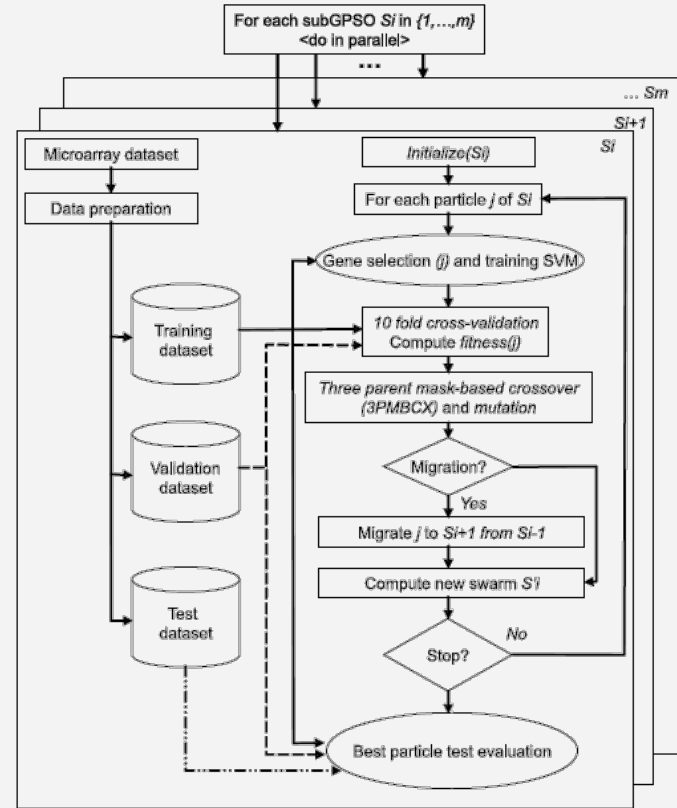
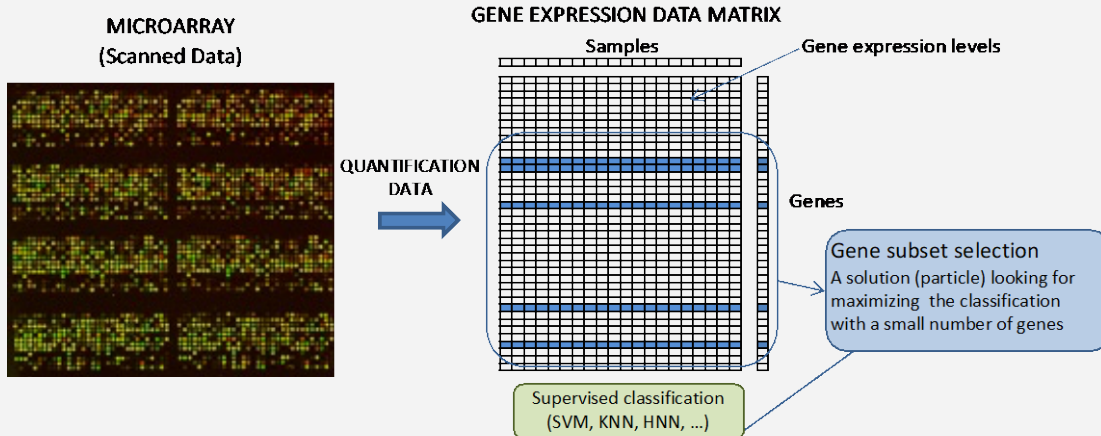
Genomics (Fragment assembly, protein structure)

Games





# Parallelism, Hybridization, and a real application



# Real Use Cases

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# Learn more in going for real applications

1. Feature selection
2. Neuroevolution
3. Surrogate models
4. Real applications



# Feature selection

- The computational ability of machine learning models **depends** a lot on the **feature set**.
- Retaining the significant features vastly **improves** the learning **time**, and also improves **accuracy**.
- In **feature selection**, we find the **optimal feature subset** that contributes most to our predicted variable.
- **Advantages:**
  - **Improve generalization** of models by reducing overfitting of data.
  - **Remove** unnecessary/redundant data.
  - Curtail the **Curse Of Dimensionality**
  - **Optimize** training time

## Feature Selection

Full Feature Set



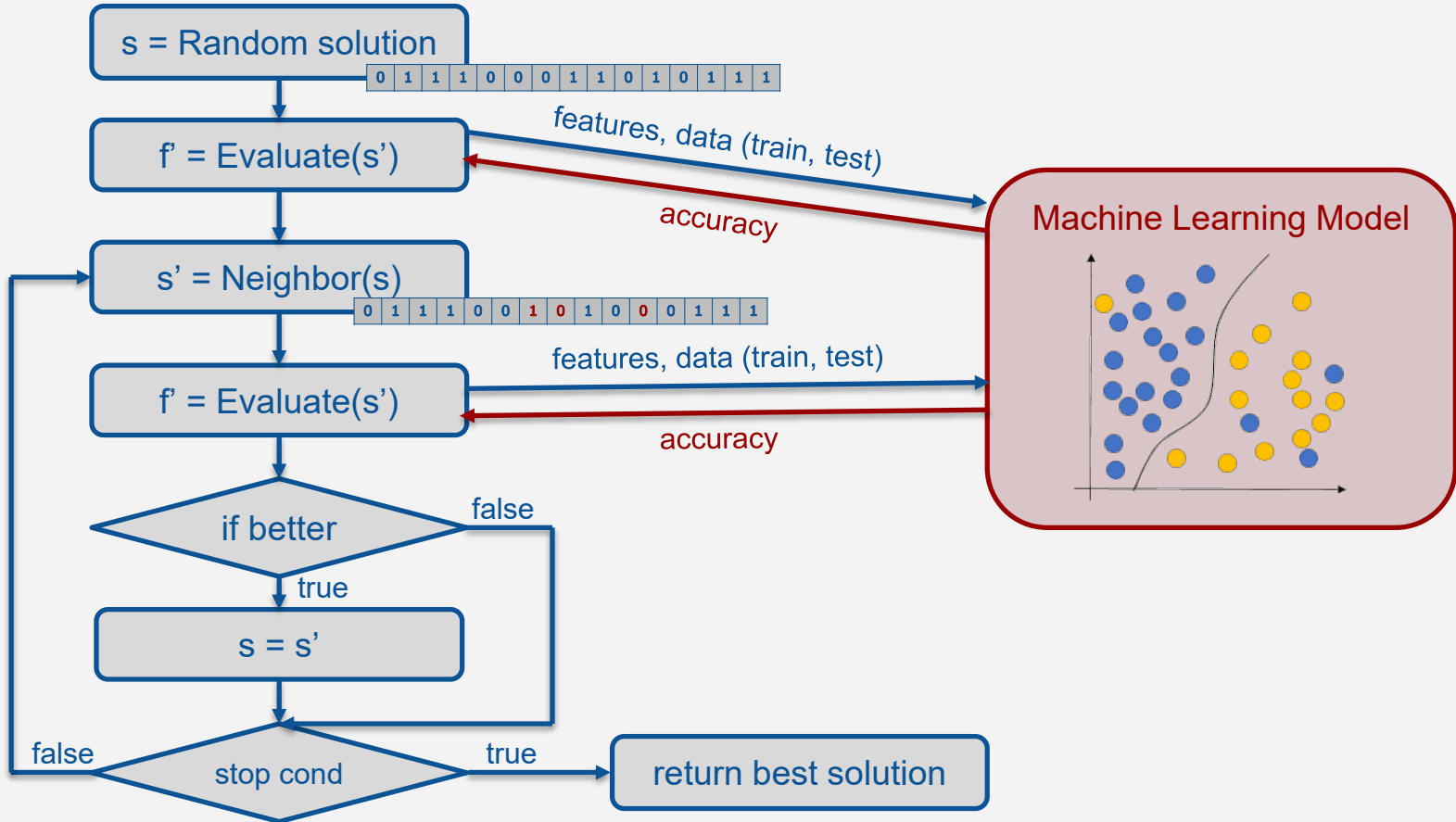
Identify Useful Features



Selected Feature Set



# Feature selection as optimization problem 4





# Feature selection as optimization problem 5

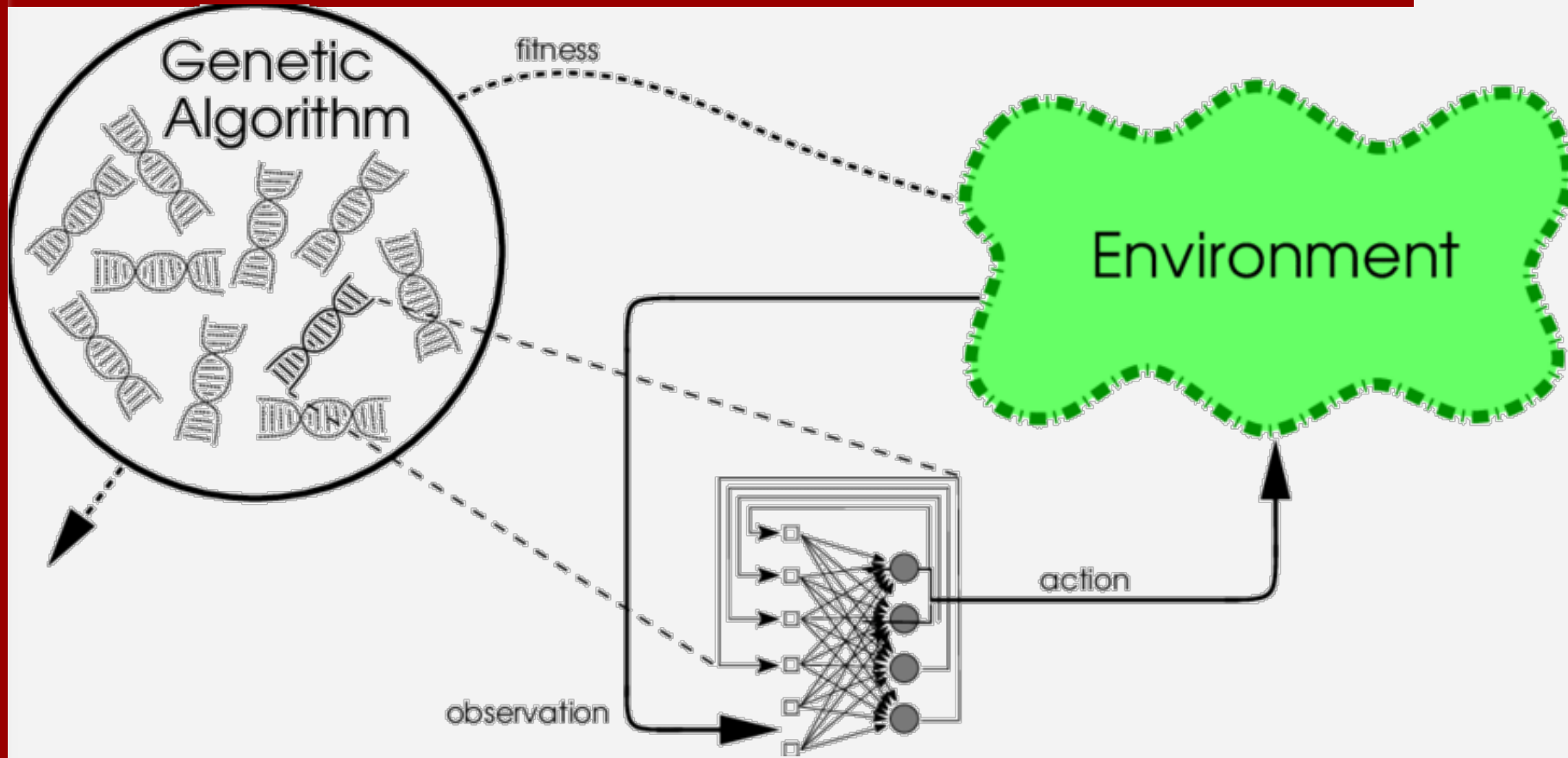
- **Solution encoding:**
  - The solution can be implemented as a **bit string**.
  - The **solution's length** is taken as the **number of features** in the dataset.
  - **0/1** indicates the **presence/absence** of the *i*th **feature** in the solution.

0	1	1	1	0	0	0	1	1	0	1	0	1	1	1
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

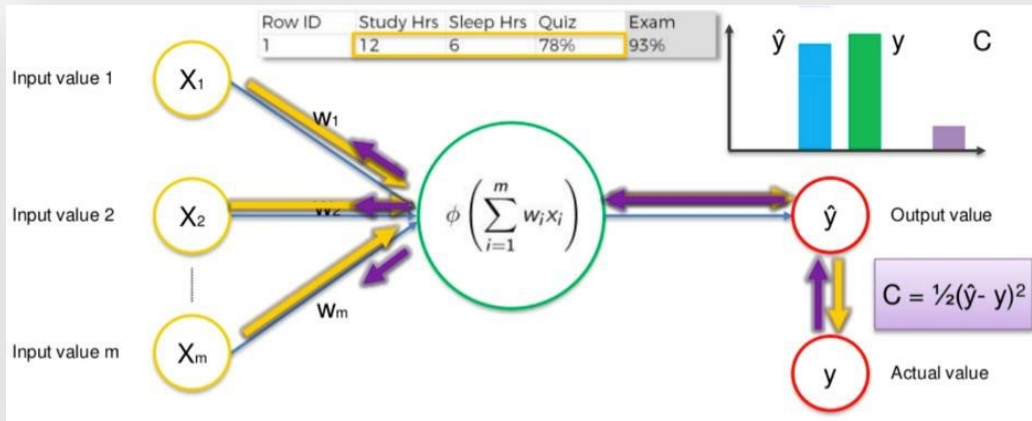
- **Fitness function:**
  - Number of features selected (*nof*)
  - Model accuracy (*acc*)
- **Approaches:**
  - Multiobjective
  - Aggregate function:

$$\max f = \alpha \cdot \frac{\text{MaxFeatures} - \text{nof}}{\text{MaxFeatures}} + (1 - \alpha) \cdot \text{acc}$$

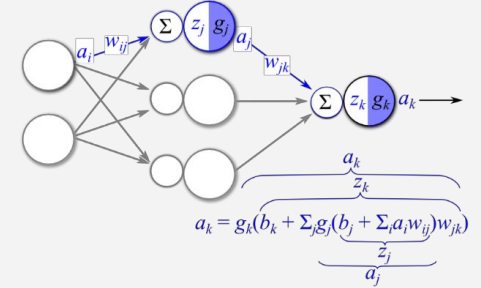
# Neuroevolution



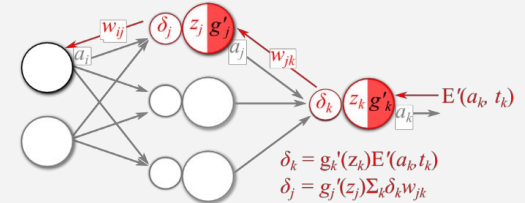
# Forward propagation of inputs



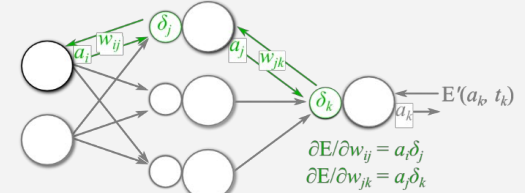
## I. Forward-propagate Input Signal



## II. Back-propagate Error Signals



## III. Calculate Parameter Gradients



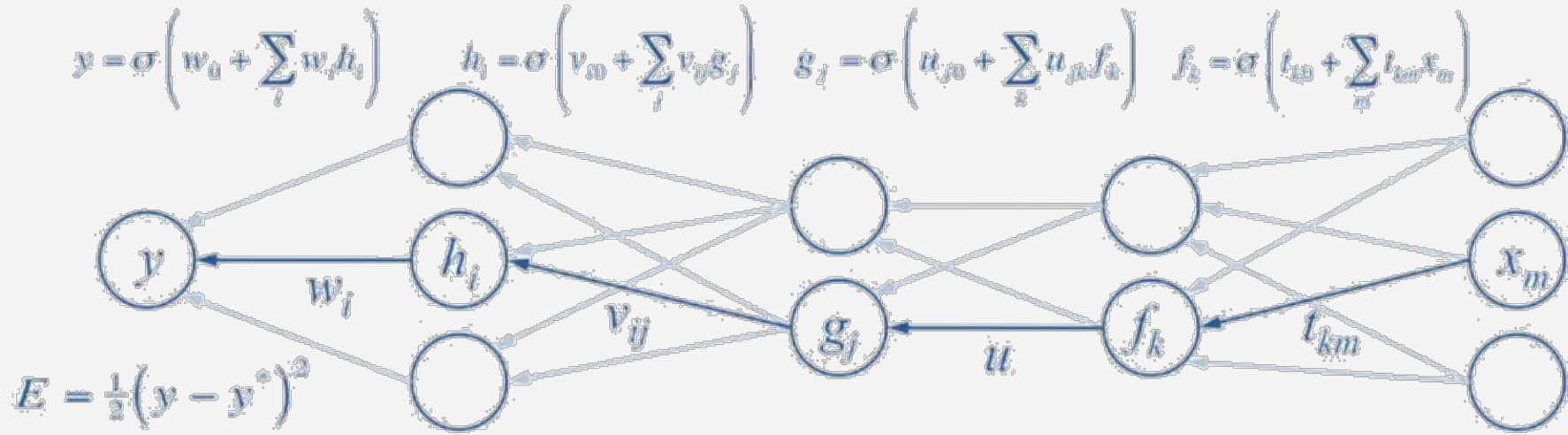
## IV. Update Parameters

$$w_{ij} = w_{ij} - \eta (\frac{\partial E}{\partial w_{ij}})$$

$$w_{jk} = w_{jk} - \eta (\frac{\partial E}{\partial w_{jk}})$$

for learning rate  $\eta$

# Backpropagation of errors

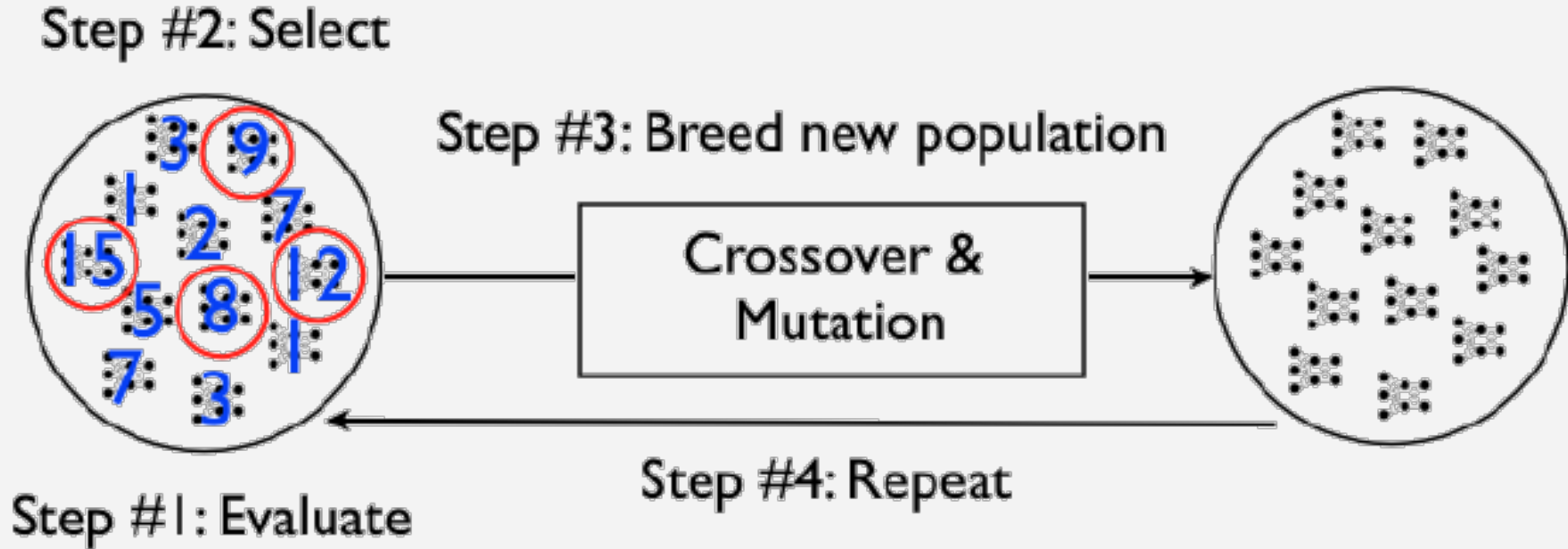


$$\frac{\partial E}{\partial h_i} = (y - y^*) y (1 - y) w_i$$

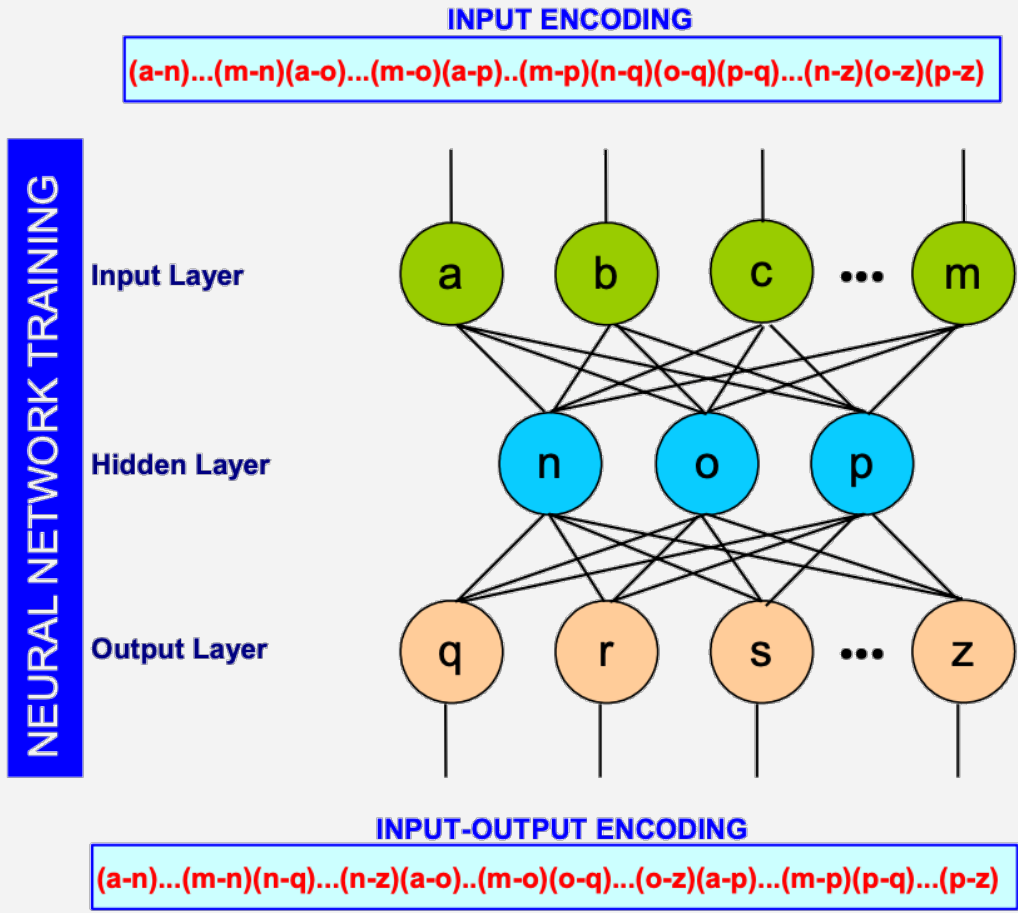
$$\frac{\partial E}{\partial g_j} = (y - y^*) y (1 - y) \sum_i w_i h_i (1 - h_i) v_{ij}$$

- Prone to local optima
- Not appropriate for complex NN
- Oscillations
- Depends on structural functions
- Need unfolding in deep learning

# Neuroevolution

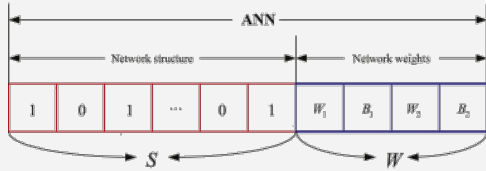


# Encoding weights vs. backpropagation



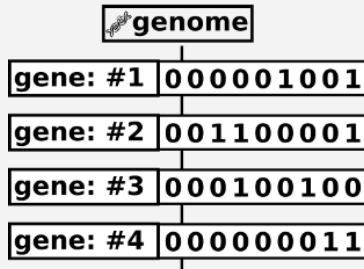
- **Solution encoding:**
  - List of float numbers
  - Mapping between position in list and weight in NN
  
- **Fitness function:**
  - Model accuracy

# Evolving NN structures!!!

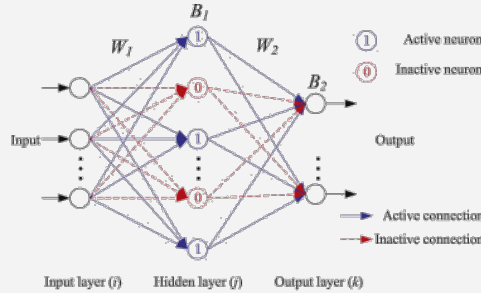


1: represents active neuron  
0: represents inactive neuron

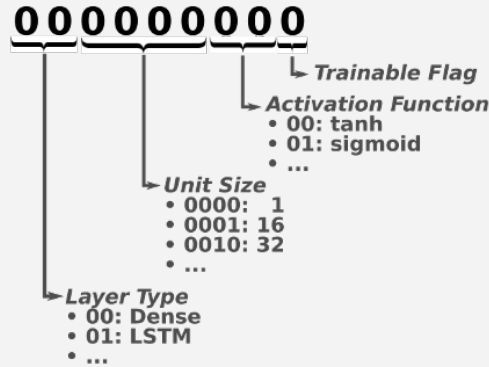
(i) Mixed-coding scheme



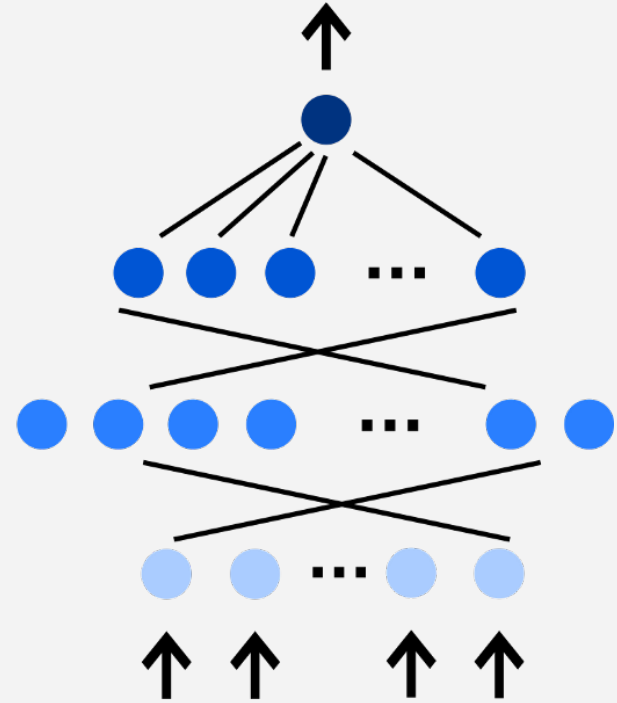
Genotype



(ii) The configurations of three-layer feedforward ANN



Translation Faculty



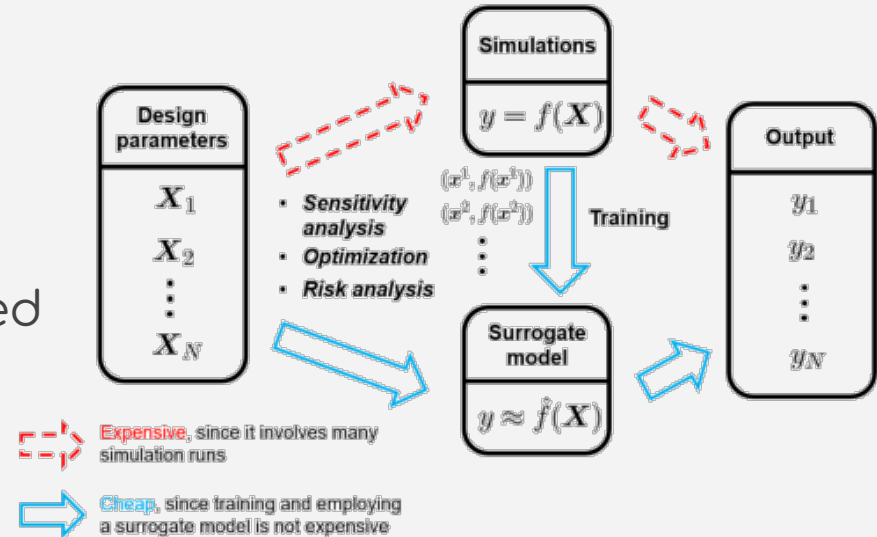
Phenotype



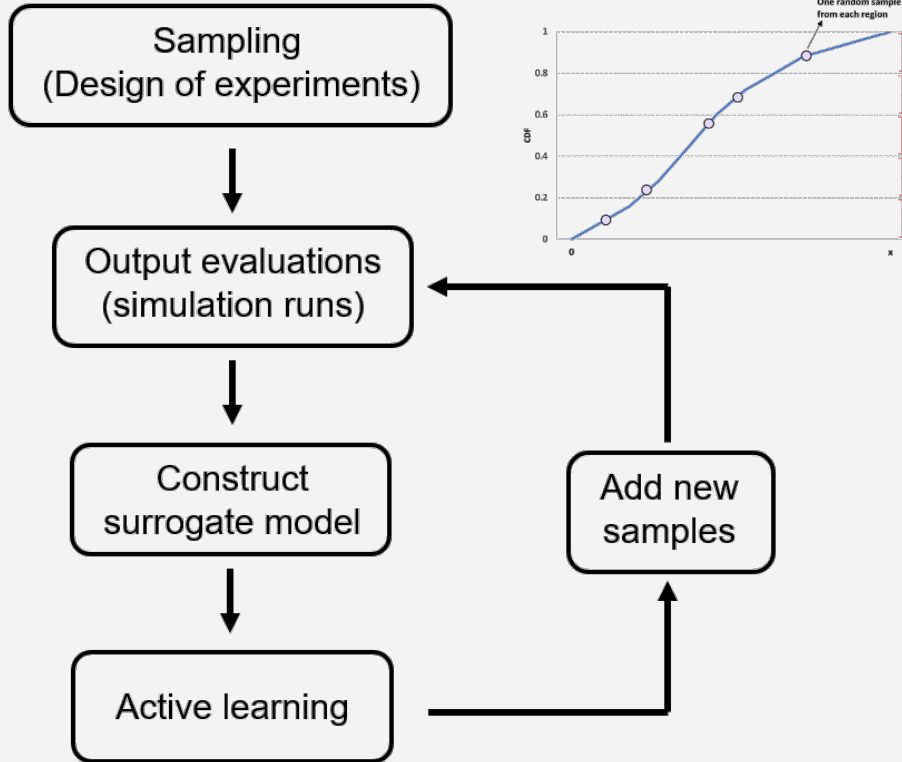
- A lot of engineering **problems** require experiments and/or **simulations** to evaluate design objective and constraint functions as a function of design variables.
- A single **simulation** can take many **minutes, hours, or even days** to complete, thus rendering them infeasible in practice.

**Surrogate models** are a statistical model to **accurately approximate** the simulation output.

This **trained model** can be deployed to **replace** the original computer simulation.







## Sampling:

- Random
- Latin hypercube

## Construct model:

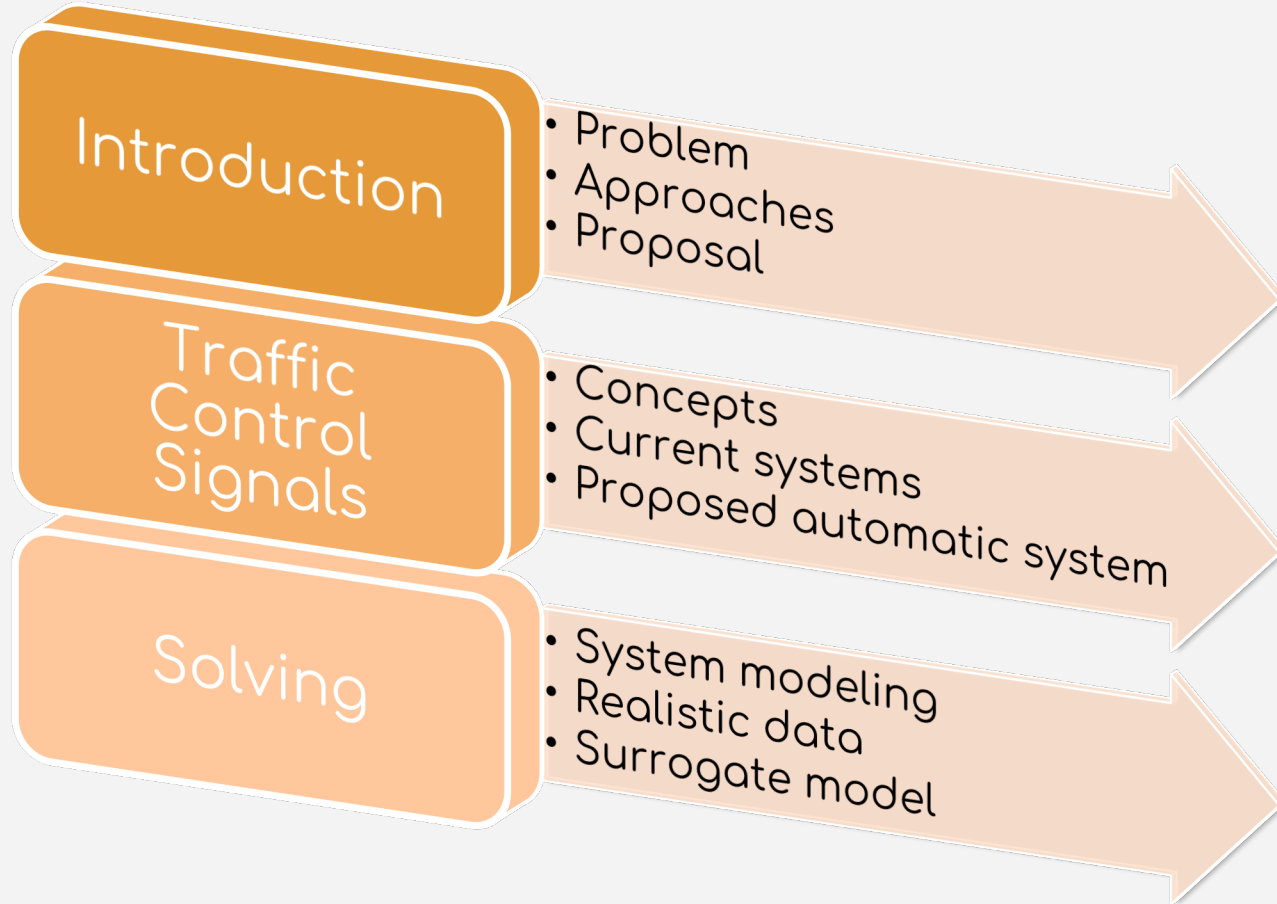
- Model selection
- Tuning parameters
- Feature selection?

## Utilization:

- Only surrogate model
- Mixed model:  
surrogate + simulation
- New samples?



# Real Applications: An example





# Problem

- **City evolution:**
  - Nowadays, cities are **growing** in the number of **inhabitants**, many of whom are arriving at the city for the first time
  - By 2050 the human population will reach 9 billion with **75%** of the world's inhabitants **living in towns and cities**
- As consequence, the **number of vehicles** in streets is continuously **increasing**, affecting all aspects of daily life:
  - Traffic jams
  - Pollution
  - Security
  - Stress
  - Economic losses
  - ...





# Potential Solutions



- “Classic” solutions:
  - Infrastructures
  - Promote the use of **public transportation** or green vehicles (bikes)
  - Promote the use of **car-sharing** (VAO lanes)
  - **Limiting car** access to city centers
- “Intelligent” solutions:
  - Provide **real-time and accurate data** to citizens to make **informed decisions** (traffic intensity, free park slots, ...)
  - Automatic assistance tools: **adaptative and/or customized routes**
  - Better **tuning** of **existing elements**: routes and frequencies of public transportation, traffic light timing...



## Automatic Traffic Control Signals

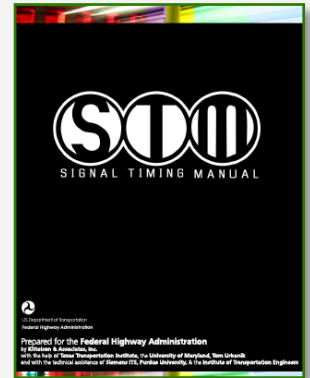
- Reduce the traffic jams
- Minimize the waiting times in red lights
- Faster routes
- Reduce the gas emissions





# Traffic Control Signals

- First, we need to **study** the elements, constraints, and regulations in **the problem domain**
- Multiple sources of information:
  - **International regulations.** (I.e., U.S. Transport Department):
    - Manual on Uniform Traffic Control Devices (862 pages)
    - Traffic Signal Timing Manual (274 pages)
  - **National regulations.** (I.e., DGT):
    - Regulación semafórica (32 pages)
    - Cruces semafóricos y sincronismo (32 pages)
  - **Specialized personnel** (city traffic managers)
  - **Scientific literature**
- Information filtering

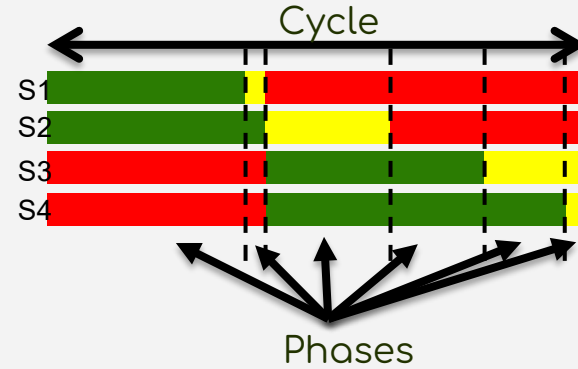




# Traffic Control Signals

- **Important concepts:**

- Intersections
- Cycle
- Phases
- Traffic light schedule or plan

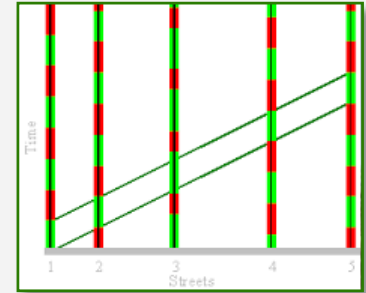


Intersection



# Traffic Control Signals

- More information:
  - The **duration of phases and cycles** can be modified
  - The **phases CANNOT** be modified
  - Recommended **duration of a cycle**: 60-120 seconds
  - **Yellow phases** (before red light): 4 seconds
  - **Minimum duration** of some phases (i.e., red phases at crosswalks should allow to safely cross the road => minimum duration =  $1 \text{ m/s} * 4 \text{ m/lane} * \#\text{lanes}$ )
  - Promote **green waves** in important avenues
  - **Traffic-dependent planes** (time, weekday, season,... )
  - ...



Green wave





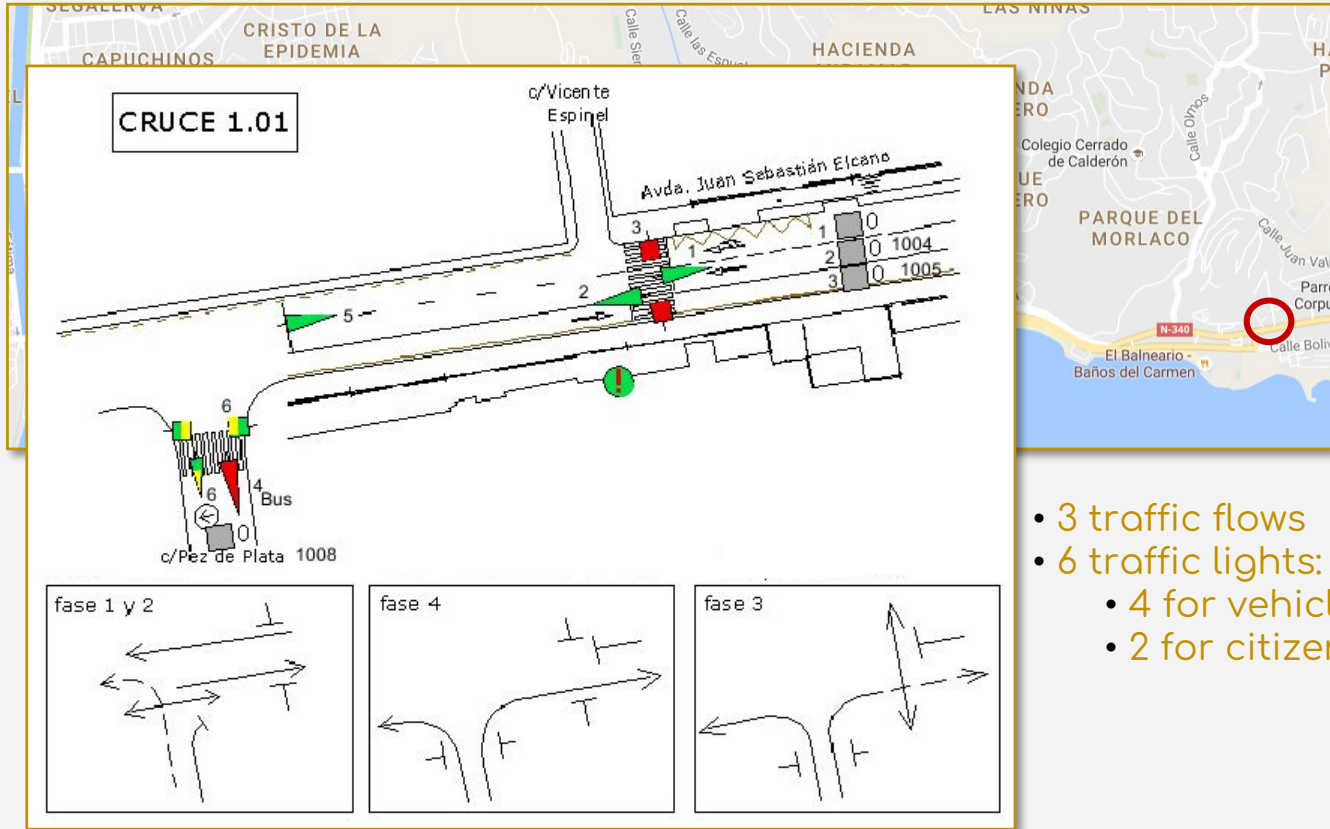
# How are traffic lights configured?

- **Location/type:**
  - Some locations are mandatory according to **regulations**
  - Other locations are recommended but not mandatory
- **Phases of traffic lights:**
  - **Regulations** establish a procedure to set the phases
- **Duration of phases/cycles:**
  - It is defined by **city traffic managers** according to some constraints
  - Usually, it is **manually** done in **each intersection**
  - Based on **experience** and accumulated **knowledge**
  - There are **dynamic systems** (they react to current traffic). Problem: Quick changes that don't improve traffic





# How are traffic lights configured?



- 3 traffic flows
- 6 traffic lights:
  - 4 for vehicles (1 for bus)
  - 2 for citizens



# How are traffic lights configured?

Cruce: 01010

PLAN:

Actual: 003

Descripción: Juan Sebastián Elcano - c/ Vicente Espinel

Comentario:



06-jun-2016 14:31:43

ns that are chosen

SELECCIÓN HORARIA - VERANO 2015			
SUB 1 LABORABLE			
Hora	Plan	Ciclo	Sentido
0:00	12	80	Oeste
2:00	13	70	Oeste
5:00	12	80	Oeste
6:30	20	115	Oeste-Simultáneo (118 a 115)
11:00	5	110	Oeste
16:00	2	115	Oeste
20:30	5	110	Oeste
22:30	7	100	Oeste
SUB 1 SABADO			
Hora	Plan	Ciclo	Sentido
0:00	7	100	Oeste
3:00	12	80	Oeste
10:00	5	110	Oeste
14:00	7	100	Oeste
17:30	5	110	Oeste
22:30	7	100	Oeste
SUB 1 DOMINGO			
Hora	Plan	Ciclo	Sentido
0:00	7	100	Oeste
3:00	12	80	Oeste
10:00	11	90	Oeste
11:30	10	95	Oeste
16:00	7	100	Oeste
17:00	20	115	Oeste
22:30	7	100	Oeste



# Proposed system

- **Automatically generated cycle and phase times:**
  - Those times must respect the constraints
- Simultaneously consider **all traffic lights in the city** or the area defined by the traffic control center
- Obtain **different plans** (offline) according to traffic intensity
- The final goal is to obtain **more fluid traffic** that reduces the pollution



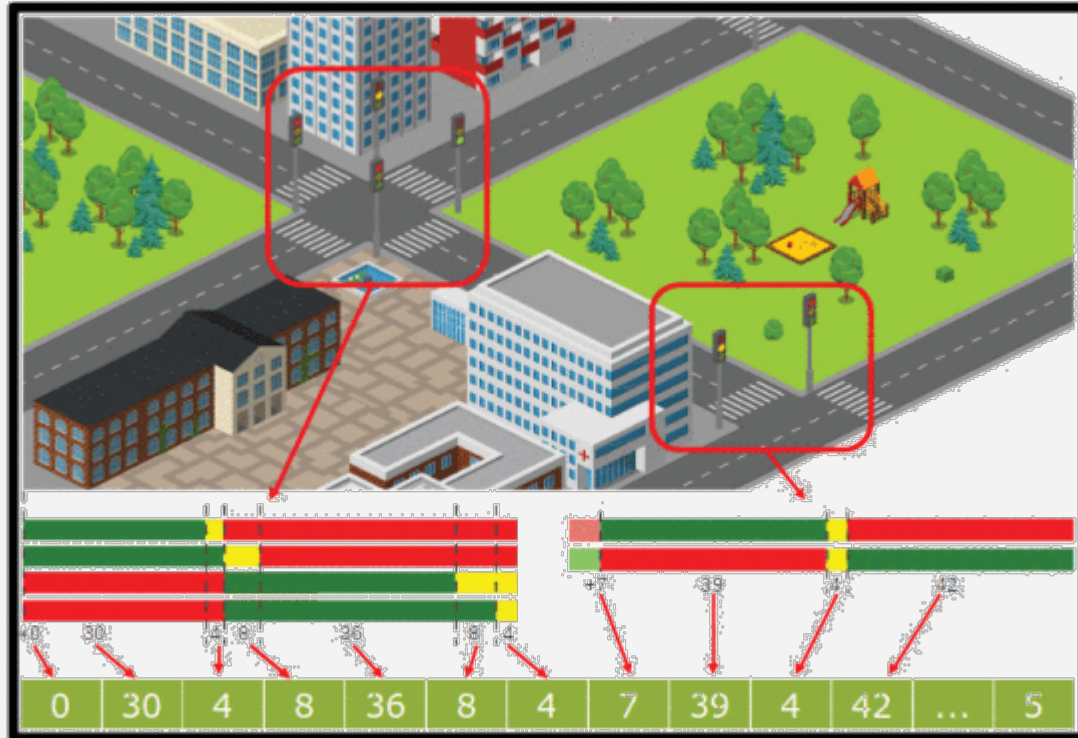
# Modeling the problem

- Given the following **input data**:
  - **Intersections** to improve (location, phases)
  - And the **traffic flows**
- **Objective**: to find the configuration (duration for the phases) that outperforms the rest of the existing configurations
- **Questions**:
  - What is computationally a solution (**representation**)?
  - When is a configuration **better** than another one (from a numerical point of view)?
  - Where do we get the **information** from?
  - How do we **find the best**?



# Solution encoding

- List of numbers (duration of phases):





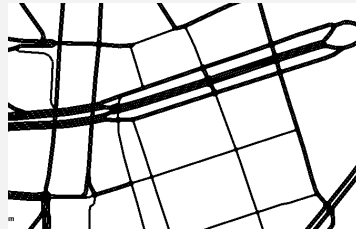
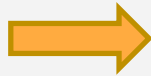
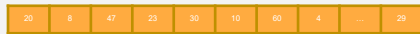
# Solution encoding

- **Restrictions** not met by default:
  - Yellow phases to 4
  - Cycles  $> 60$  and  $< 120$
  - Green Wave Promotion
- Other **alternative representations**:
  - Each intersection: cycle time + percentage that each phase occupies
  - Reduce the number of traffic lights:
    - Cluster the intersections into groups
    - Only one in the group is optimized
    - The rest are small variants of the optimized
  - Others?

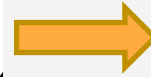


# Solution fitness

- To compare solutions, we need quantitative values (fitness)
- The traffic system is very complex
  - No (realistic) mathematical models
  - Utilization of simulators
- SUMO (Simulator of Urban Mobility)
  - Input: Roadmap, traffic flows, traffic light plans
  - Output: statistics of the simulation



SUMO



Vehicles reaching destination: 30  
Average trip time: 120  
CO2: 543452  
Average waiting time: 10  
...





# Solution fitness

## Statistics about simulation:

- Number of vehicles that reach their destination during a given simulation time
- Average trip time
- Emissions (CO<sub>2</sub>, CO, NO<sub>x</sub>, PM<sub>10</sub>, HC, ...)
- W...

## Fitness

- O...
- C...
- Multi-objective approach
- Derivate values (green waves?)

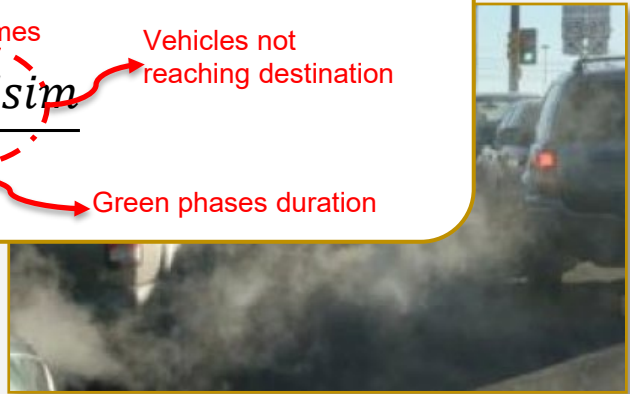
$$f_{obj} = \frac{T_{trip} + T_{sw} + VNRT_{sim}}{V_R^2 + P}$$

Diagram illustrating the components of the fitness function  $f_{obj}$ :

- $T_{trip}$ : Trip duration
- $T_{sw}$ : Waiting times
- $VNRT_{sim}$ : Vehicles not reaching destination
- $V_R^2$ : Vehicles reaching destination
- $P$ : Green phases duration

## Additional challenge:

- SUMO only calculates statistics for vehicles that reach their destination





# Realistic data

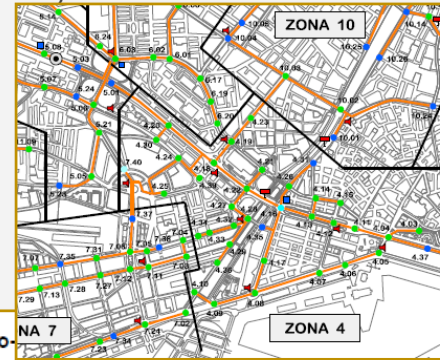
- **Input for our system:**
  - City map
  - Location of traffic lights
  - Vehicle flow according to several factors (time, weekday, or season)
  - Constraints in phase duration
- **Source of the data:**
  - Maps: OpenStreetMap
  - Traffic lights: traffic control center of the city
  - Routes: Mobility department





# Realistic data

- Challenges: Maps and traffic lights
  - Incomplete maps: missing road, road directions, traffic lights, ...
  - Errors in conversion (OSM => SUMO)
  - Manual correction of the maps. Labour intensive process



- Challenges: Routes

- Not enough details
- Non-automatable format
- Conversion of traffic intensity to traffic flows

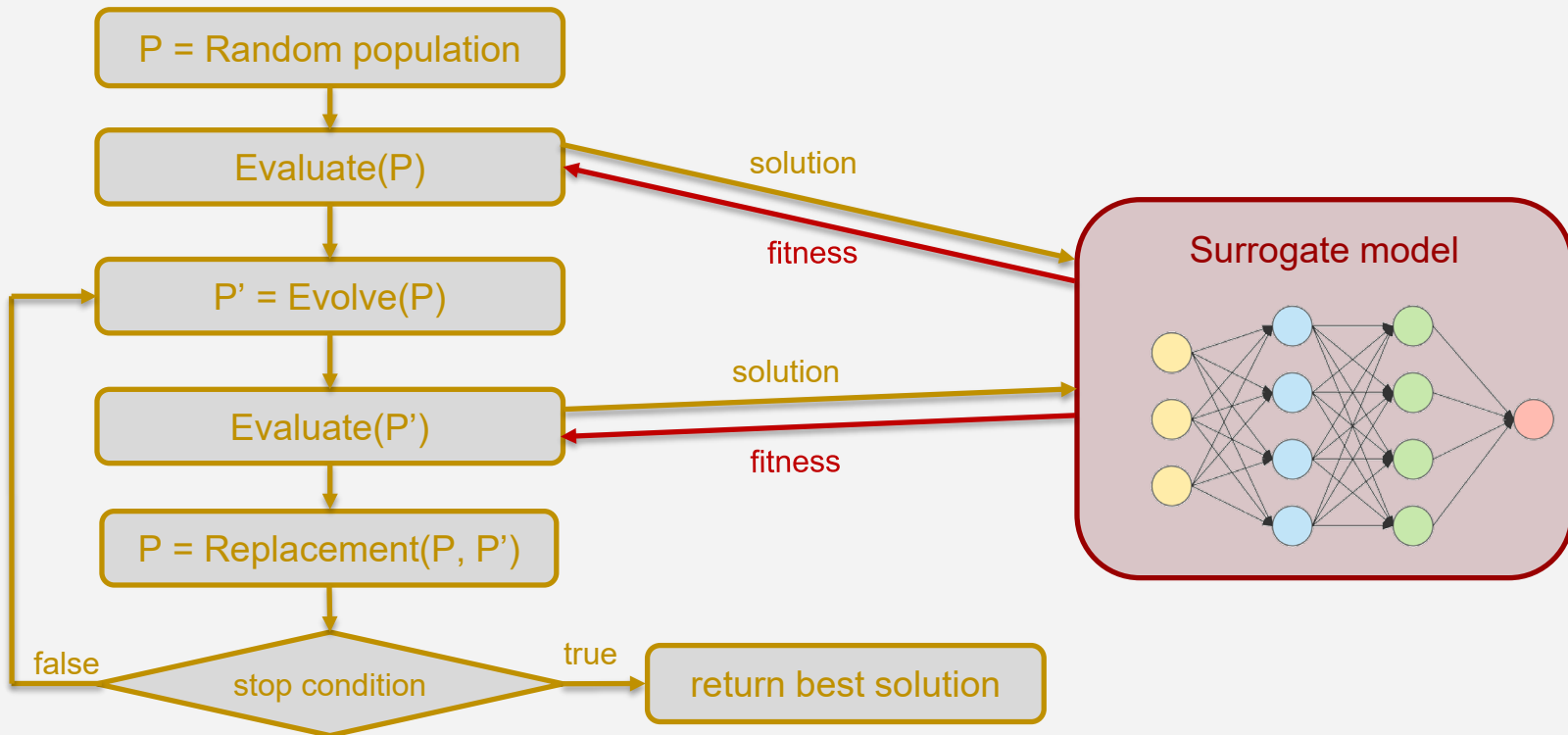
Intensidad de vehiculos Mayo

PM	Ubicación	I.M.D.L	I.M.D.S	I.M.D.D	I.M.H.P.L	H.P.L.M	I.M.H.P.S	H.P.S.M	I.M.H.P.D	H.P.D.M
1	Avda. Juan Sebastián Elcano - Este	2.004	1.636	1.388	189	12:00	149	12:00	138	13:00
2	Avda. Juan Sebastián Elcano - Oeste	20.383	17.890	15.188	1.465	8:00	1.278	21:00	1.238	21:00
3	Bolivia - Este	16.775	15.174	12.898	1.413	14:00	1.250	14:00	1.091	13:00
4	P.M. Pablo Ruiz Picasso - Este	19.376	15.574	12.631	1.908	14:00	1.337	14:00	1.044	13:00
5	P.M. Pablo Ruiz Picasso - Oeste	28.829	23.675	20.368	2.192	8:00	1.632	21:00	1.582	21:00
6	Pso. Reding - Este	8.528	6.767	5.298	687	14:00	554	14:00	418	13:00
7	Pso. Reding - Oeste	6.987	5.930	4.655	546	9:00	445	12:00	342	21:00
8	Victoria - Sur *	5.874	5.255	4.285	419	8:00	443	22:00	319	22:00
9	Victoria - Norte *	6.474	5.888	4.923	483	14:00	454	22:00	360	22:00
10	Túnel Alcazaba - Este	15.870	14.744	12.561	973	8:00	849	14:00	701	1:00



# Algorithms

- GA + ANN as surrogate model



# Summary

