Machine Learning

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Formation INRA, Niveau 3

Outline

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Y can be:

- a numeric variable ($Y \in \mathbb{R}$) $\Rightarrow$ **(supervised) regression** *régression*;
- a factor $\Rightarrow$ **(supervised) classification** *discrimination*.

Basics

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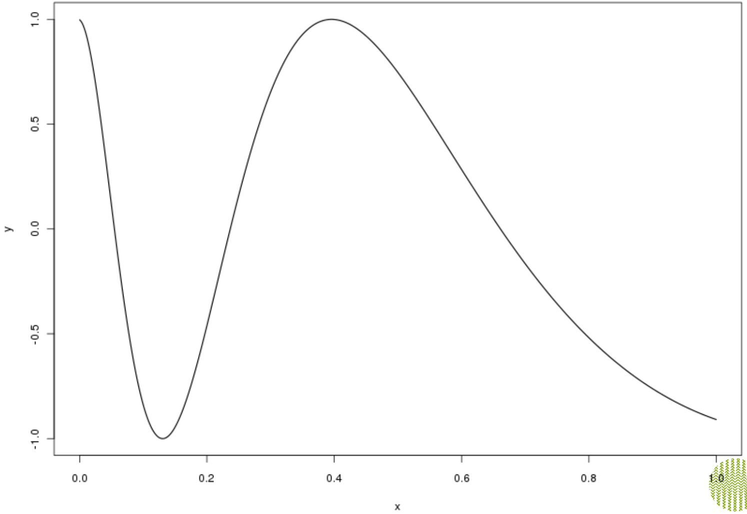
Conflicting objectives!!

Underfitting/Overfitting *sous/sur - apprentissage*

Function $x \to y$ to be estimated



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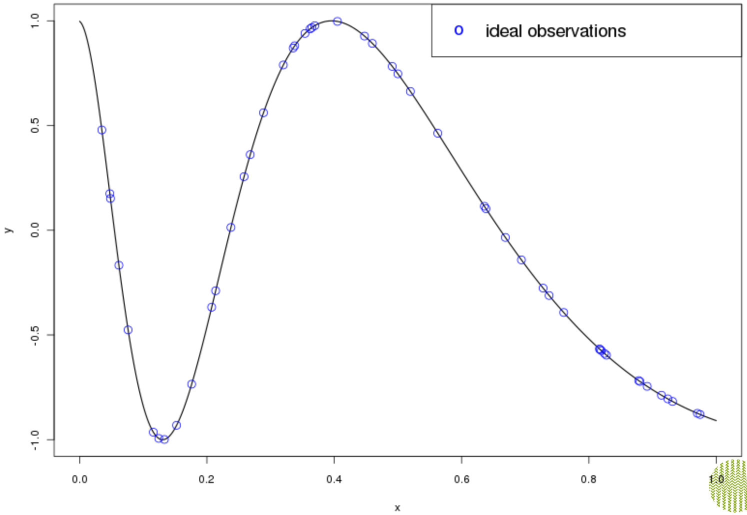
Observations we might have



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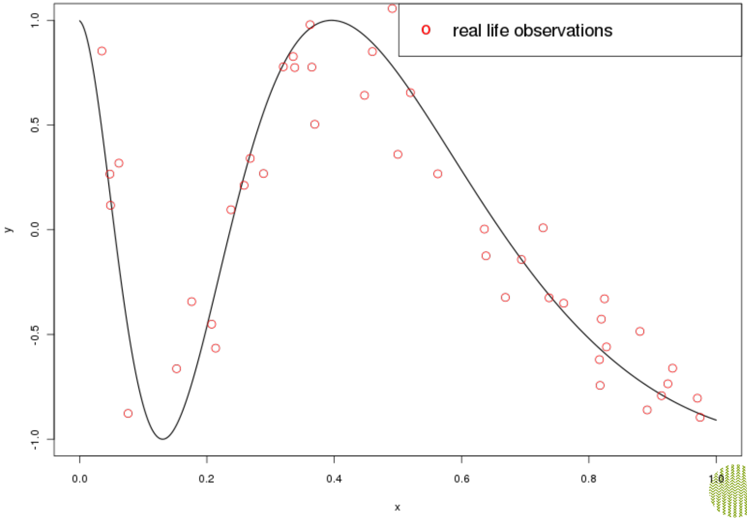
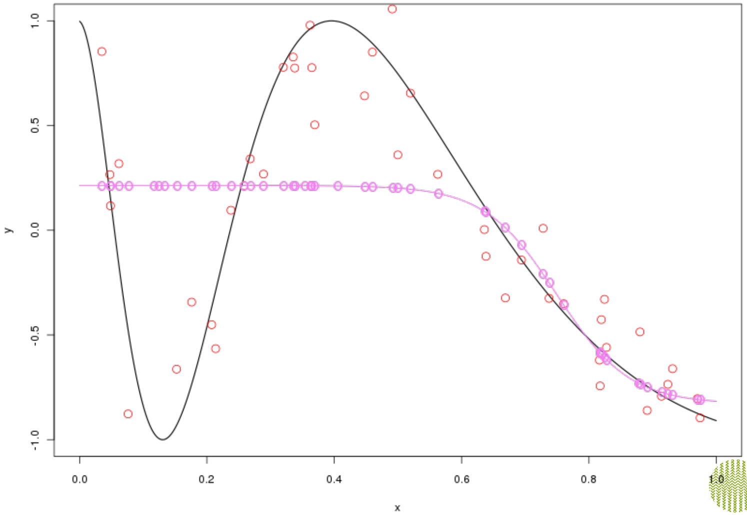
Observations we do have



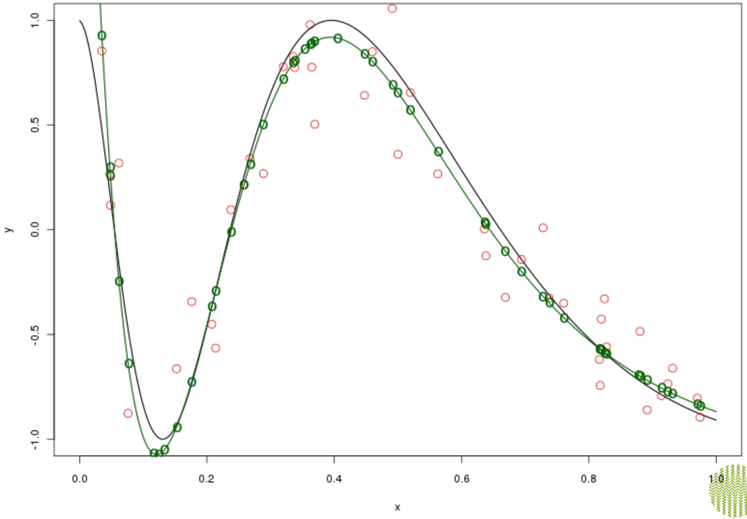
Underfitting/Overfitting *sous/sur - apprentissage*

First estimation from the observations: **underfitting**



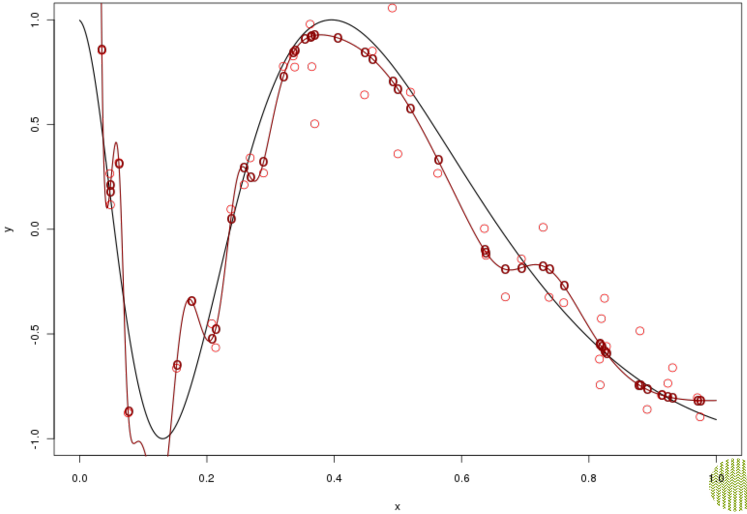
Underfitting/Overfitting *sous/sur - apprentissage*

Second estimation from the observations: accurate estimation



Underfitting/Overfitting *sous/sur - apprentissage*

Third estimation from the observations: **overfitting**



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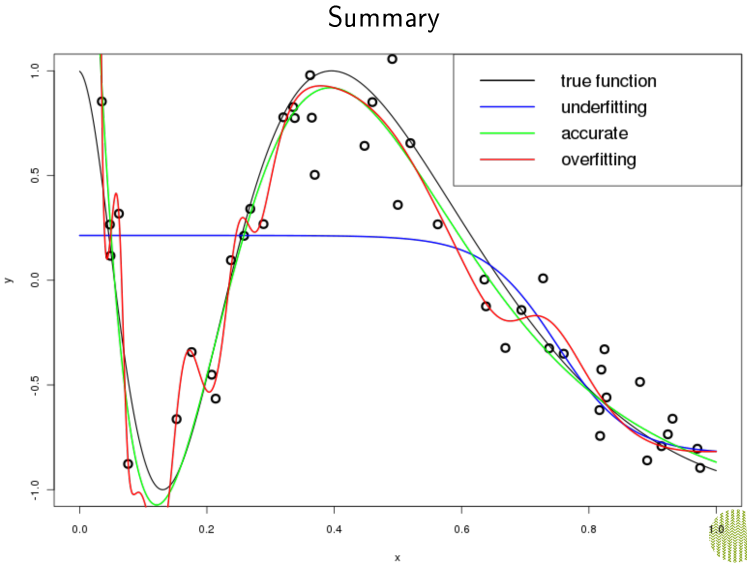

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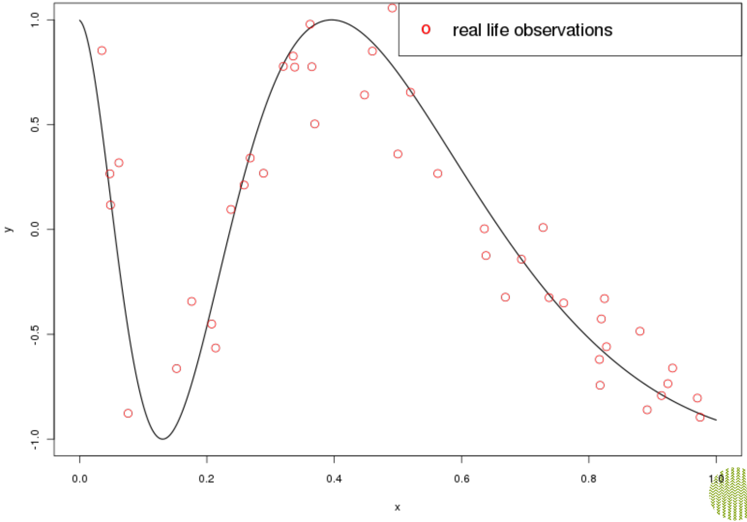
- **test error**: a way to prevent overfitting (estimates the generalization error)
  1. split the data into training/test sets (usually 80%/20%)
  2. train Φ^n from the training dataset
  3. calculate the test error from the remaining data

simple validation

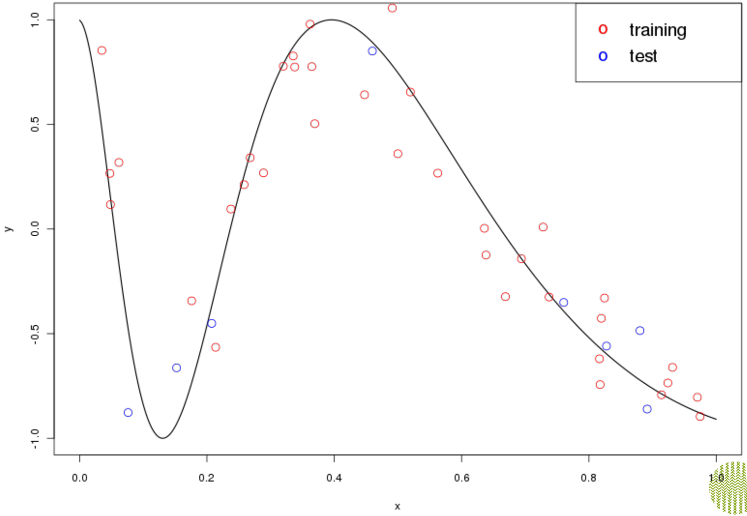
Example

Observations



Example

Training/Test datasets



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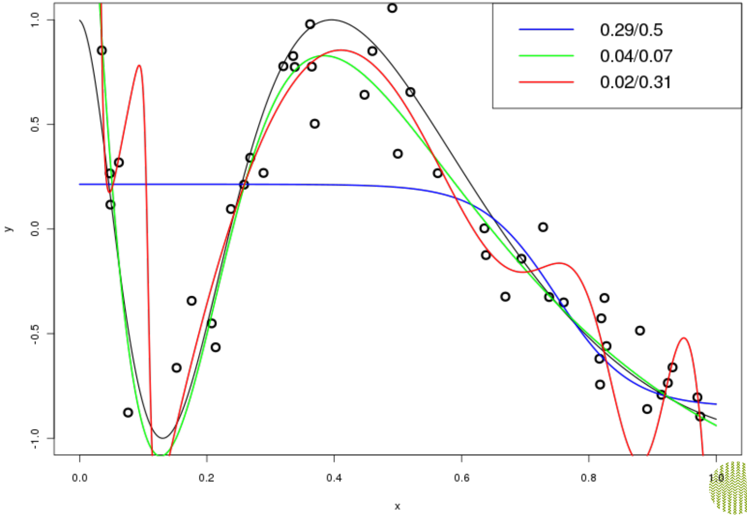
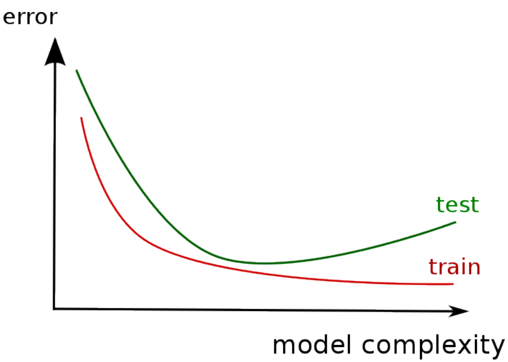
Training/Test errors



Example

Summary



Linear vs Nonparametric

Linear methods:

$$Y = \beta^T X + \epsilon$$

(a priori on the type of link between X and Y)

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(ML) Objective: Build Φ^n from the observations such that its generalization error $\mathbb{E}L\Phi^n$ is (asymptotically) optimal.

Example (regression framework)

$$\mathbb{E}L\Phi^n := \mathbb{E}\left[(\Phi^n(X) - Y)^2\right] \xrightarrow{n\rightarrow+\infty} \inf_{\Phi} EL\Phi$$

whatever (X, Y) distribution.

Use case description

Data kindly provided by Laurence Liaubet described in [Liaubet et al., 2011]:

- microarray data: expression of 272 selected genes over 56 individuals (pigs);
- a phenotype of interest (muscle pH) measured over the 56 invididuals (numerical variable).

file 1: genes expressions
file 2: muscle pH

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Basics [Bishop, 1995]

Common properties

- (artificial) **"Neural networks"**: general name for supervised and unsupervised methods developed in analogy to the brain;

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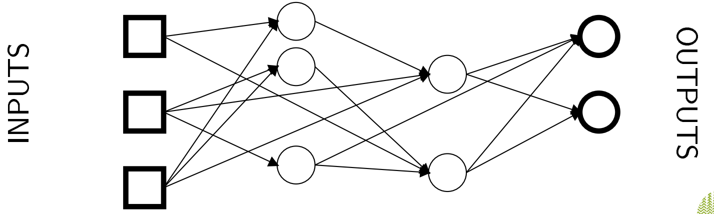
Example of graphical representation:



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- **Self-organizing maps** (SOM): dedicated to unsupervised problems (clustering), self-organized;
- ...

MLP: Advantages/Drawbacks

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- **classification OR regression** (i.e., Y can be a numeric variable or a factor);
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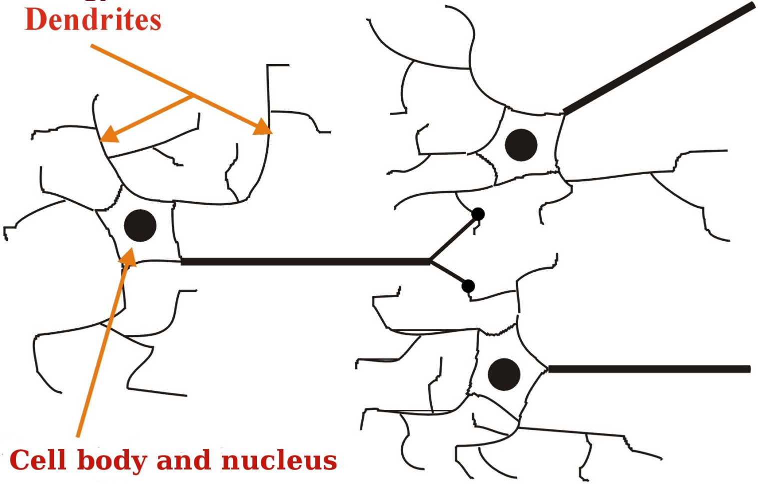
Drawbacks

- **hard to train** (high computational cost, especially when d is large);
- **overfit easily**;
- **"black box"** models (hard to interpret)

Analogy to the brain



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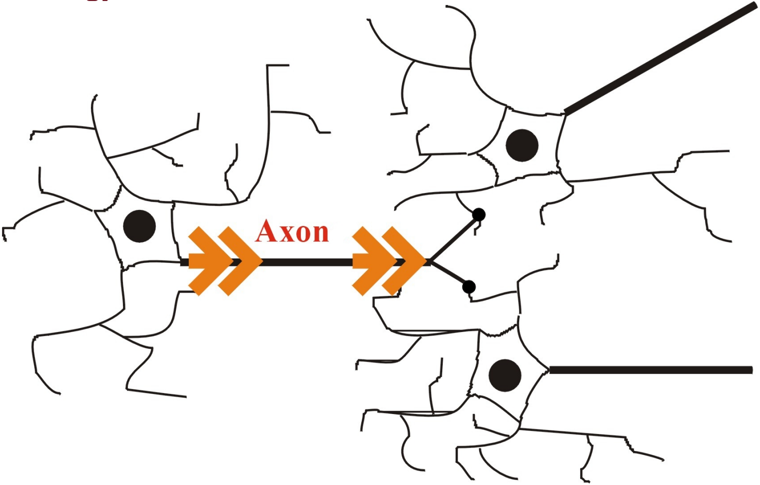

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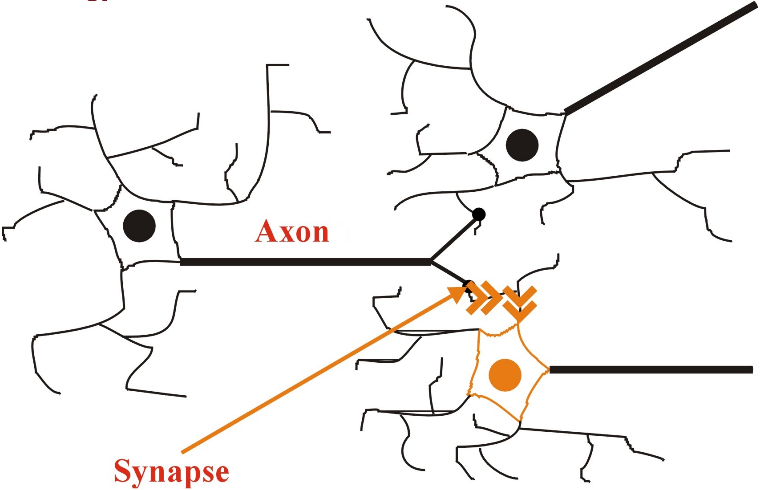

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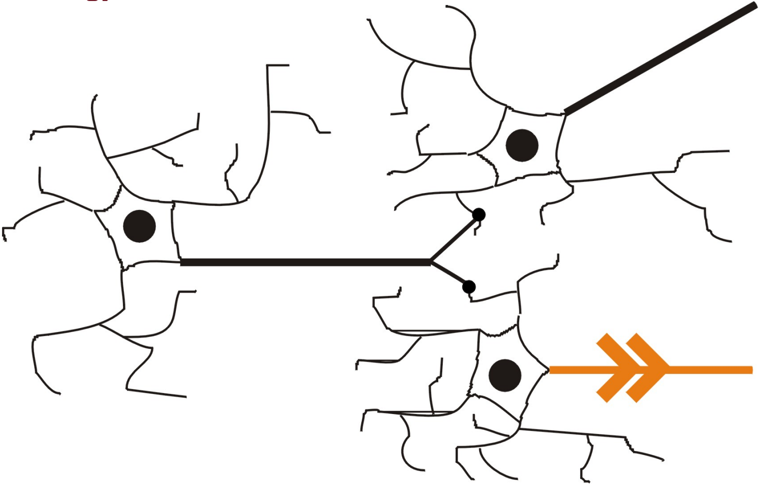

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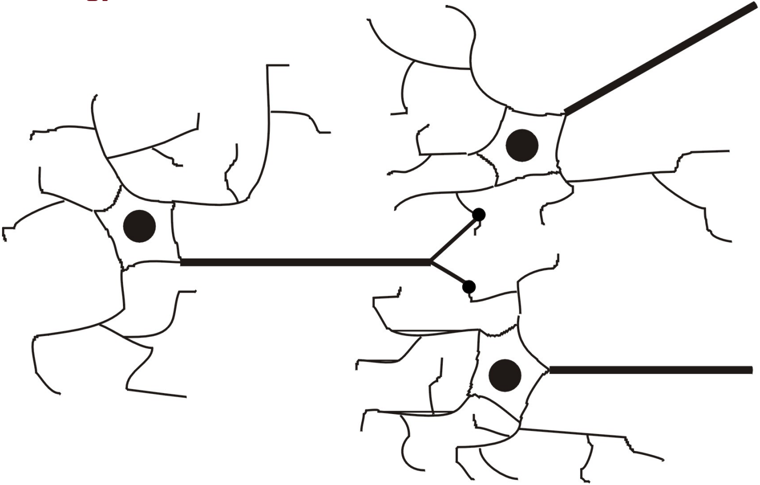

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(artificial) Perceptron

Layers

- MLP have one input layer (X values), one output layer (Y values) and several **hidden layers** (only 1 is necessary);
- no connections within a layer;
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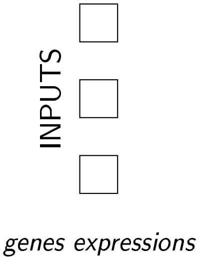

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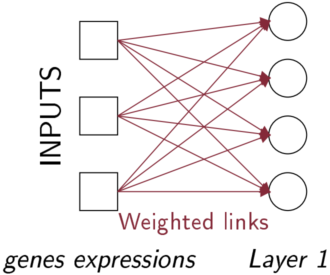

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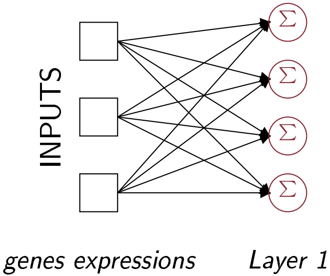

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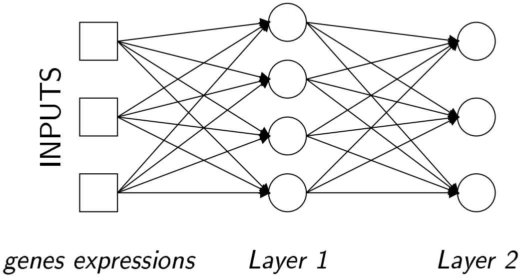

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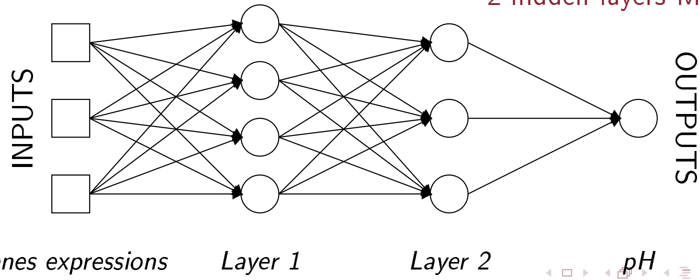
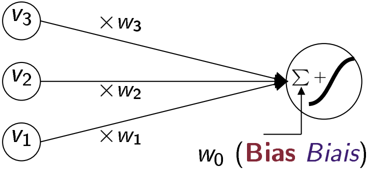
Example:

2 hidden layers MLP



A neuron



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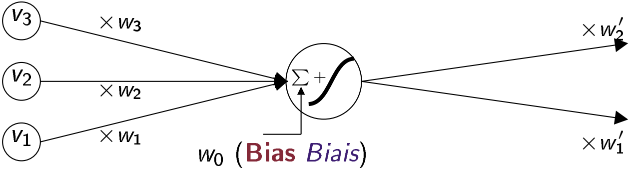
v_3
v_2
v_1
$\times w_3$
$\times w_2$
$\times w_1$
$\Sigma +$
w_0 (**Bias** *Biais*)
$\times w'_2$
$\times w'_1$

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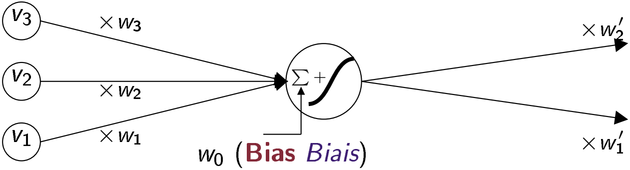
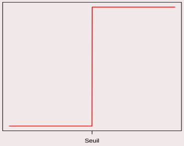


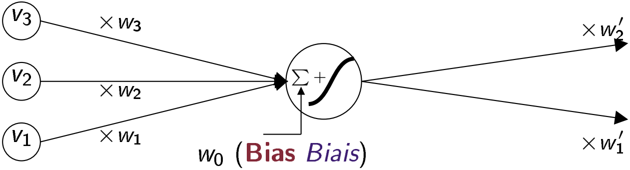
Standard activation functions *fonctions de lien / d'activation*

Biologically inspired: **Heaviside function**



$$S(t) = \begin{cases} 0 & \text{if } t < \text{threshold;} \\ 1 & \text{if not.} \end{cases}$$

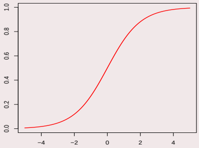
A neuron



Standard activation functions

Main issue with the Heaviside function: not continuous!

Logistic function

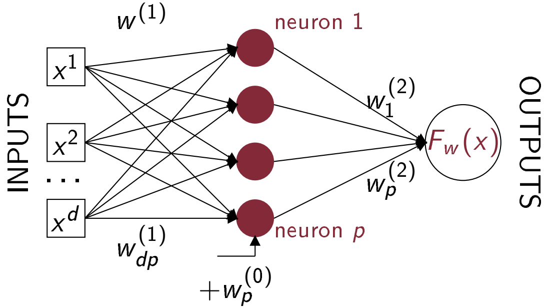


$$S(t) = \frac{1}{1+e^{-t}}$$

Summary

If Y is numeric, **linear output**:

$$\forall x \in \mathbb{R}^d,\ F_w(x) = \sum_{j=1}^{p} w_j^{(2)} \mathcal{S}\left(\sum_{k=1}^{d} w_{kj}^{(1)} x^k + w_j^{(0)}\right).$$



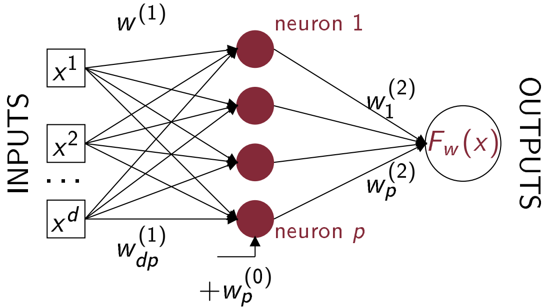
No analytical expression!!

Summary

If Y is a factor, **logistic output**:

$$\forall\, x \in \mathbb{R}^d,\ \mathbb{P}(X = C|x = x) \simeq F_w(x) = \mathcal{S}\left[\sum_{j=1}^{p} w_j^{(2)} \mathcal{S}\left(\sum_{k=1}^{d} w_{kj}^{(1)} x^k + w_j^{(0)}\right)\right]$$

(with a maximum probability rule for the final classification)



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Universal approximation

[Hornik et al., 1989] (among others)

For any given Φ, smooth enough and any precision ϵ, there exists a **one-hidden layer** perceptron (with sigmoïd activation functions) that approximates Φ with a precision at most ϵ.

Learning weights

p is given

Chose w s.t.:

$$w^n = \arg\min_w \frac{1}{n}\sum_{i=1}^n (y_i - F_w(x_i))^2 .$$

(MSE minimization)

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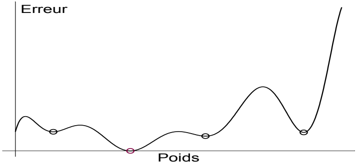

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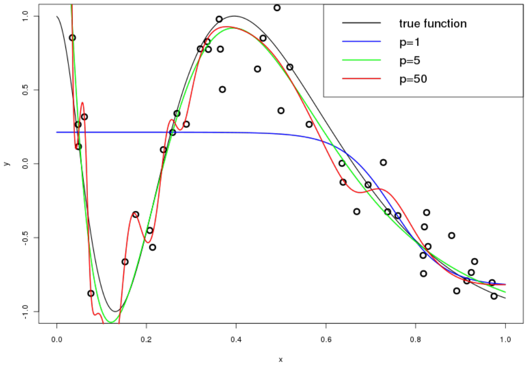
1. no exact solution ($\Rightarrow$ approximation algorithms, e.g., Newton's method + backpropagation principle): **local minima**;
2. **overfitting**: the larger p is, the more flexible the perceptron is and the more it can overfit the data.

Overfitting



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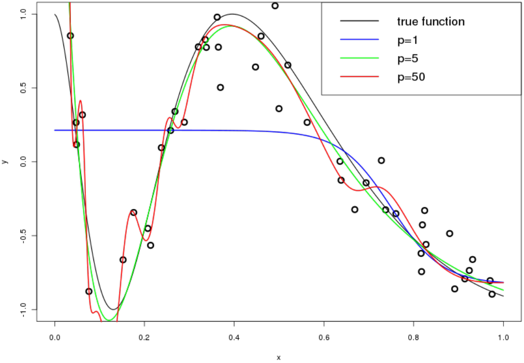

Weight decay can help improve the generalization ability:

$$w^n = \arg\min_w \frac{1}{n}\sum_{i=1}^{n}(y_i - F_w(x_i))^2 + \lambda\|w\|^2$$

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- **grid search** using a **simple validation**;
- **grid search** using a (K-fold) **cross validation** (better but computationally expensive when K is large).

Cross validation

Algorithm

1: Set the grid search for p, $\mathcal{G}_p$, and λ, $\mathcal{G}_\lambda$
2: Split the data into K groups
3: **for** $p \in \mathcal{G}_p$ and $\lambda \in \mathcal{G}_\lambda$ **do**
4:     **for** group $= 1..K$ **do**
5:         Train model$_{p,\lambda,\mathrm{group}}$ without observations in "group"
6:         Test error, $\mathrm{MSE}_{p,\lambda,\mathrm{group}}$ for observations in "group"
7:     **end for**
8:     Average $\mathrm{MSE}_{p,\lambda,\mathrm{group}}$ over "group" $\Rightarrow \mathrm{MSE}_{p,\lambda}$
9: **end for**
10: Select p and λ with minimum $\mathrm{MSE}_{p,\lambda}$

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n-fold cross validation is called **Leave-One-Out** (LOO).
Standard choice for K: LOO or 10-fold CV.

Outline

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- **non parametric** method: no prior assumption needed;
- can deal with a **large number of input variables**, either numeric variables or factors (a variable selection is included in the method);
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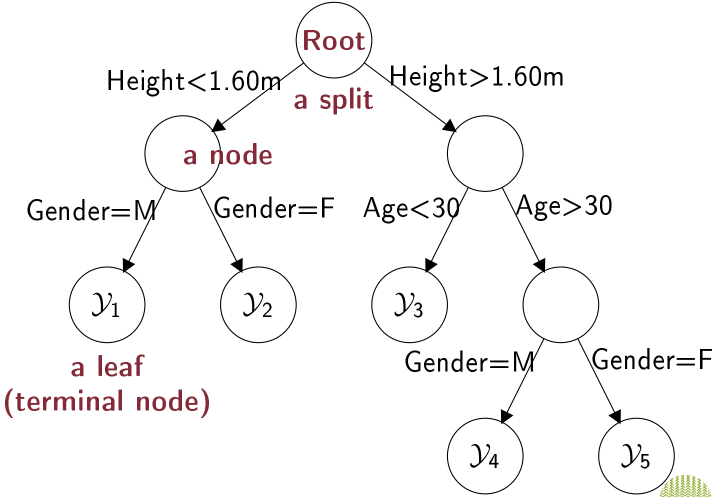
- provide an **intuitive interpretation**.

Drawbacks

- require a **large training dataset** to be efficient;
- as a consequence, are often **too simple** to provide accurate predictions.

Example

$X = (\text{Gender}, \text{Age}, \text{Height})$ and $Y = \text{Weight}$



CART learning process

Algorithm

1: Start from root
2: **repeat**
3: move to a "new" node
4: **if** the node is **homogeneous** or **small** enough **then**
5: STOP
6: **else**
7: split the node into two child nodes with **maximal "homogeneity"**
8: **end if**
9: **until** all nodes are processed

Further details

Homogeneity?

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- Minimum size node (generally 1 or 5)
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Hyperparameters can be **tuned by cross-validation** using a grid search.
An alternative approach is **pruning**...

Choosing an optimal subtree

Algorithm

1: Train the maximal tree, $\mathcal{T}$

2: *Pruning:* Find an "optimal" subtrees sequence $(\mathcal{T}_k)_{k=1,\ldots,K}$

3: **By cross validation, find the errors** $L(\mathcal{T}_k) + \lambda\mathcal{C}(\mathcal{T}_k)$ for $k = 1, \ldots, K$ where L is the error and $\mathcal{C}$ is a complexity measure (number of leafs)

4: Select the subtree s.t. $L(\mathcal{T}_k) + \lambda\mathcal{C}(\mathcal{T}_k)$ is minimum

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Drawbacks

- **black box** model;
- is **not supported by strong mathematical results** (consistency...) until now.

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- **Random forest** $\simeq$ CART bagging.

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General (and robust) approach to solve several problems:

- Estimating **confidence intervals** (of $\overline{X}$ with no prior assumption on the distribution of X)
  1. Build P bootstrap samples from $(x_i)_i$
  2. Use them to estimate $\overline{X}$ P times
  3. The confidence interval is based on the percentiles of the empirical distribution of $\overline{X}$

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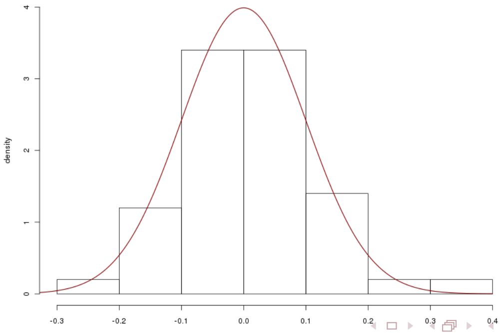

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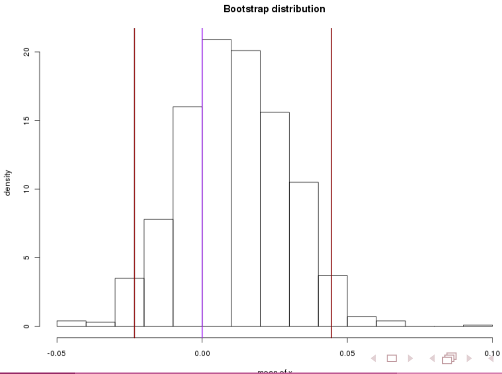

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- Also useful to estimate p-values, residuals, ...

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Average the estimates of the regression (or the classification) function obtained from B bootstrap samples.

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Bagging with regression trees

1: **for** $b = 1, \dots, B$ **do**
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4: **end for**
5: Estimate the regression function by

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For **classification**, the predicted class is the majority vote class.

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CART bagging with **additional disturbances**

1. each node is **based on a random (and different) subset of q variables** (an advisable choice for q is $\sqrt{p}$ for classification and $p/3$ for regression).

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- those of the CART algorithm;
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Random forest **are not very sensitive** to hyper-parameters setting: default values for q and bootstrap sample size ($2n/3$) should work in most cases.

Additional tools

- **OOB (Out-Of Bags) error**: error based on the observations not included in the "bag"

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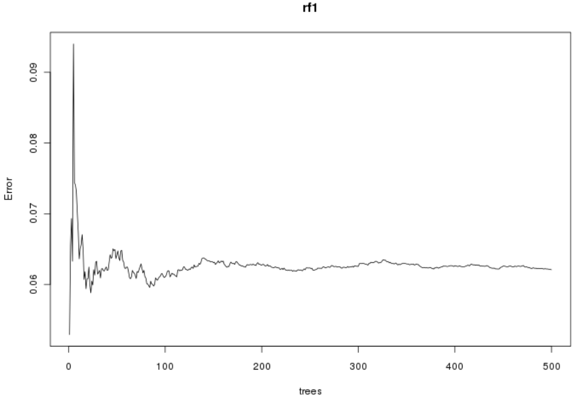
  Stabilization of OOB error is a good indication that there is enough trees in the forest



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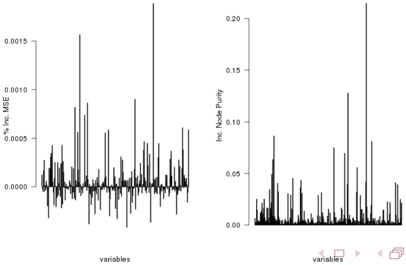
- **OOB (Out-Of Bags) error**: error based on the observations not included in the "bag"
- **Importance of a variable** to help interpretation: for a given variable X^j
  1. randomize the values of the variable
  2. make predictions from this new dataset
  3. the importance is the mean decrease in accuracy (MSE or misclassification rate)



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