



# An overview of Machine Learning

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Thanks to Pierre Gaillard for the slides!

February 4, 2021

# Overview

Introduction

Supervised learning

Empirical risk minimization: OLS, Logistic regression, Ridge, Lasso, Quantile regression

Calibration of the parameters: cross-validation

Local averages

Deep learning

Unsupervised learning

Clustering

Dimensionality Reduction Algorithms

Planning of the class

## Introduction

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## General information

Teachers: Alessandro Rudi and Francis Bach.

Practical sessions: Raphal Berthier.

Website: <https://www.di.ens.fr/appstat/>

The class will last 52 hours (30 hours of class + 22 hours of practical sessions) and can be validated for 9 ECTS. Final grade: 50% final exam, 50% homework.

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**Special online format: inverted classroom!**

- Read lecture notes before
- Short review of material
- ≈ One mandatory question per student per session
- Have video feeds open

# Prerequisites

**Linear algebra** (matrix operations, linear systems)

**Probability** (e.g. notion of random variables, conditional expectation)

**Basic coding skills in Python:** Jupyter notebooks, Anaconda

- If you do not know the language Python, please read (and code the examples of) this 10-minutes introduction to Python:

<https://www.stavros.io/tutorials/python/>.

- For next week: run

[https://www.di.ens.fr/appstat/spring-2020/TP/TD0-prerequisites/crash\\_test.ipynb](https://www.di.ens.fr/appstat/spring-2020/TP/TD0-prerequisites/crash_test.ipynb)

questions if something is unclear (we like them especially if you think they are stupid).

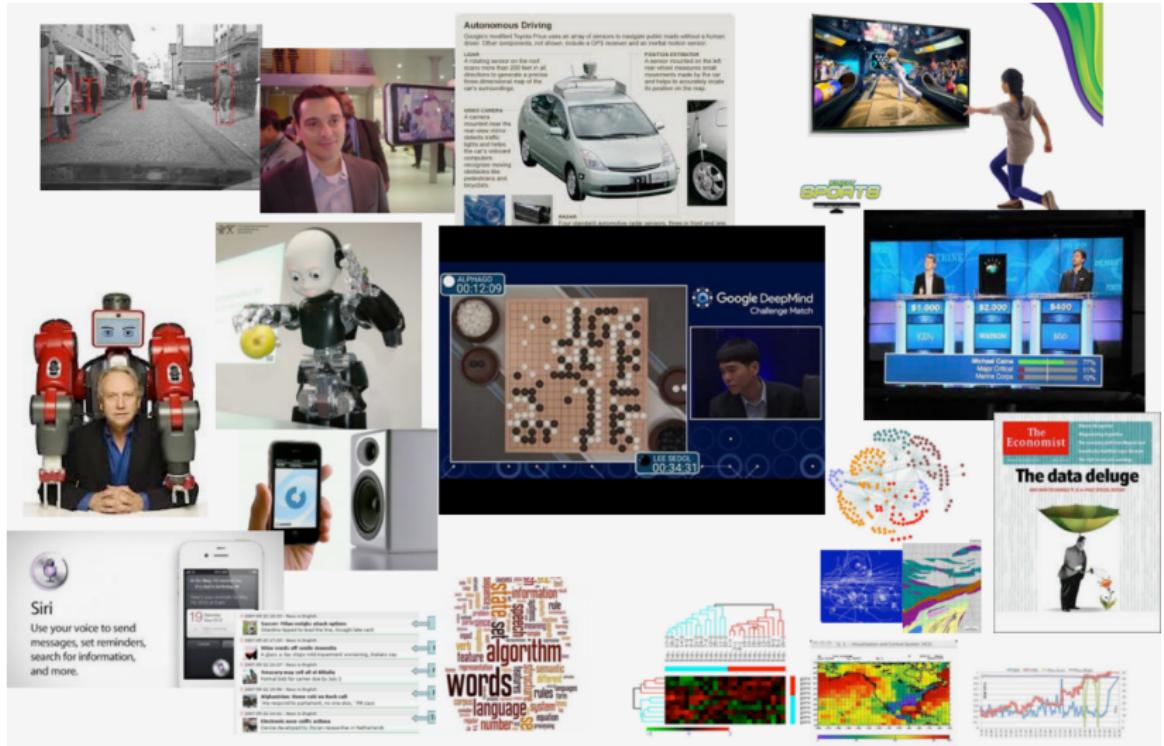
# What is ML?

artificial intelligence which can learn and model some phenomena without being explicitly programmed

**Examples of “success stories”:**

- Spam classification
- Machine translation
- Speech recognition
- Self-driving cars

# What is ML? Examples



# Search engines

Google

machine learning

Tous Actualités Images Vidéos Livres Plus Paramètres Outils

Environ 2210 000 000 résultats (0,54 secondes)

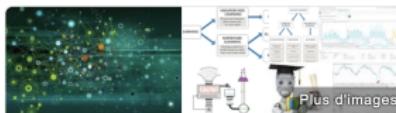
**Apprentissage automatique — Wikipédia**  
[https://fr.wikipedia.org/wiki/Apprentissage\\_automatique](https://fr.wikipedia.org/wiki/Apprentissage_automatique) ▾  
L'apprentissage automatique (en anglais machine learning, littéralement « l'apprentissage machine ») ou apprentissage statistique est un champ d'étude de ...  
Machine à vecteurs de support · Intelligence artificielle · Apprentissage supervisé

**Machine Learning et Big Data : définition et exlications de la ...**  
<https://www.lebigdata.fr/Analytics/Data%20Analytics> ▾  
6 juil. 2018 - Le Machine Learning est une technologie d'intelligence artificielle permettant aux ordinateurs d'apprendre sans avoir été programmés ...

**Qu'est-ce que le machine learning ? - Initiez-vous au machine ...**  
<https://openclassrooms.com/Accueil/Cours/Initiez-vous%20au%20machine%20learning> ▾  
14 mai 2018 - Dans ce chapitre, nous allons étudier l'ensemble des éléments qui entrent en jeu dans la formulation d'un problème de machine learning. ...

**Machine Learning Stanford University Cours - Coursera**  
<https://fr.coursera.org/learn/machine-learning> ▾  
Apprentissage automatique from Université de Stanford. Machine learning is the science of getting computers to act without being explicitly programmed.

Vidéos



**Apprentissage automatique**

Champ d'étude

L'apprentissage automatique ou apprentissage statistique est un champ d'étude de l'intelligence artificielle qui se fonde sur des approches statistiques pour donner aux ordinateurs la capacité d'... [Wikipédia](#)

Commentaires

Afficher les résultats pour

**Apprentissage profond (Domaine d'étude)**  
L'apprentissage profond est un ensemble de méthodes d'apprentissage automatique tentant de ...



# Search engines

Google machine learning

Tous Actualités **Images** Vidéos Livres Plus Paramètres Outils Collections

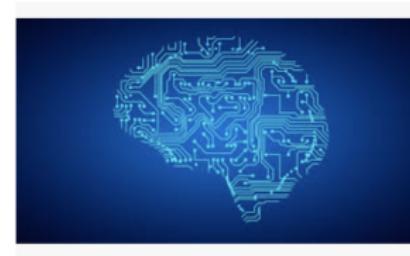
png algorithms marketing intelligence artificielle healthcare artificial intelligence apprentissage ai



Le machine learning en E-commerce : u...  
blog.casaneo.fr



Le machine learning : un engouement t...  
alain-bensoussan.com



Machine learning et lutte contre la fraude - Netheos  
netheos.com



The Machine Learning Revolution...  
forbes.com



An Introduction to Machine Learning | DigitalOcean  
digitalocean.com



Machine Learning with Python: from Linear M...  
edx.org

# Search engines

Google  fbach...\_small.jpg X

Tous **Images** Maps Shopping Plus Paramètres Outils

Environ 25 270 000 000 résultats (0,81 secondes)

 Taille de l'image :  
1702 x 1733

Trouver d'autres tailles de l'image :  
[Toutes les tailles](#) - [Grandes](#)

Recherche associée possible : [francis bach](#)

**Francis Bach - INRIA - ENS - DI ENS**  
<https://www.di.ens.fr/~fbach/> • Traduire cette page  
Francis Bach, INRIA - SIERRA project-team, Département d'Informatique de l'Ecole Normale Supérieure, Centre de Recherche INRIA de Paris 2 rue Simone Iff.

**Francis Bach — Wikipédia**  
[https://fr.wikipedia.org/wiki/Francis\\_Bach](https://fr.wikipedia.org/wiki/Francis_Bach) •  
Francis Bach est un chercheur français spécialiste de l'apprentissage statistique. Sommaire, 1 Biographie, 2 Travaux, 3 Liens externes, 4 Références ...

**Images similaires**



**Francis Bach**  
Chercheur 

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Livres

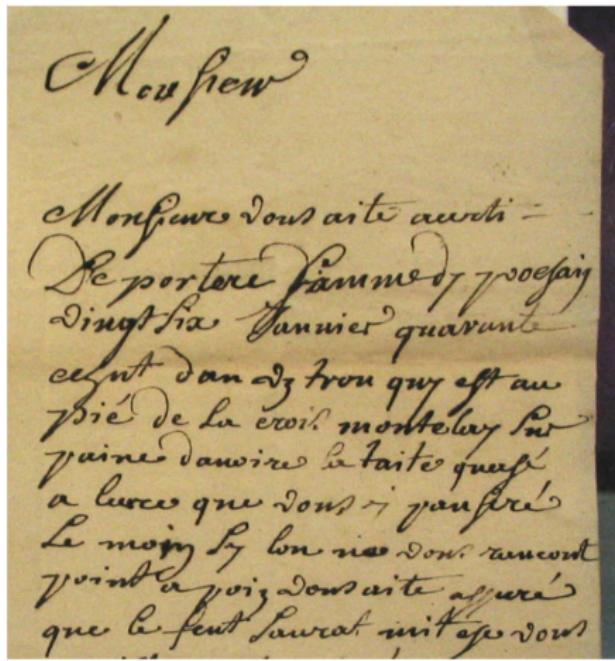


Learning with Submodular Functions 2013  
Sparse Modeling for Image Processing 2014  
Optimization with Sparsity-Inducing Norms 2011

Recherches associées



Julien Jean Ponce



Monsieur,  
Vous êtes averti de porter samedi prochain 26 janvier quarante écus dans un trou qui est au pied de la croix Montelay sous peine d'avoir la tête cassée à l'heure que vous y penserez le moins. Si l'on ne vous rencontre point vous êtes assuré que le feu sera mis chez vous. S'il en est parlé à qui que ce soit la tête cassée vous aurez.

Archives du Val d'Oise - 1737

September 1651. may, during which  
I have been in England, to give you an account of my  
journey & travels, and of the various scenes I have witnessed,  
as well as the many difficulties I have experienced.  
Especially I will speak of the difficulties I have experienced  
and the sufferings I have undergone in my search for truth & justice, as  
also of the trials and tribulations I have suffered in my efforts to  
persuade people to do what is right and just. I will also  
mention the various difficulties I have experienced in my efforts to  
convince people of the truth of my beliefs. I will also  
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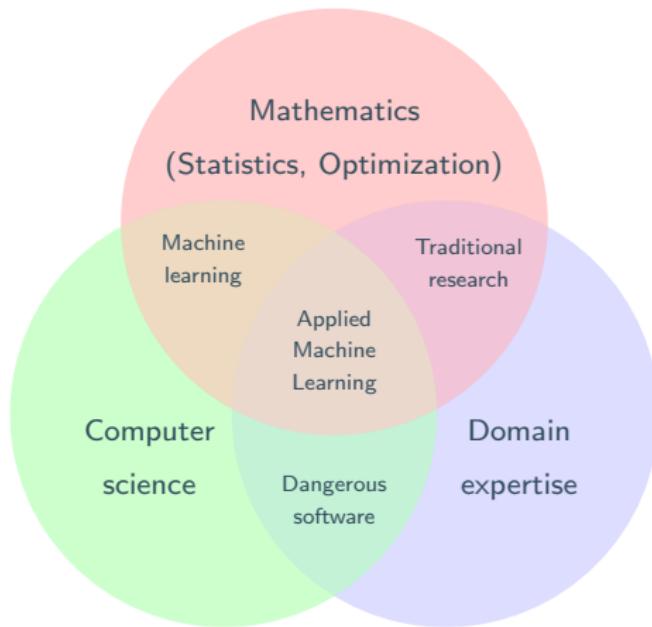
## Large data – Complex data



# What is ML?

**Machine Learning** : artificial intelligence which can learn and model some phenomena without being explicitly programmed

Machine Learning  $\subset$  Statistics + Computer Sciences

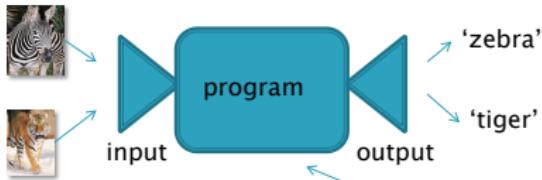


# What is ML?

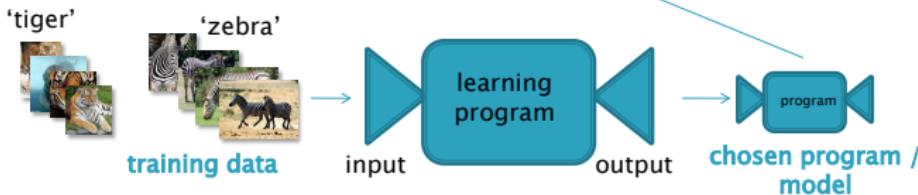
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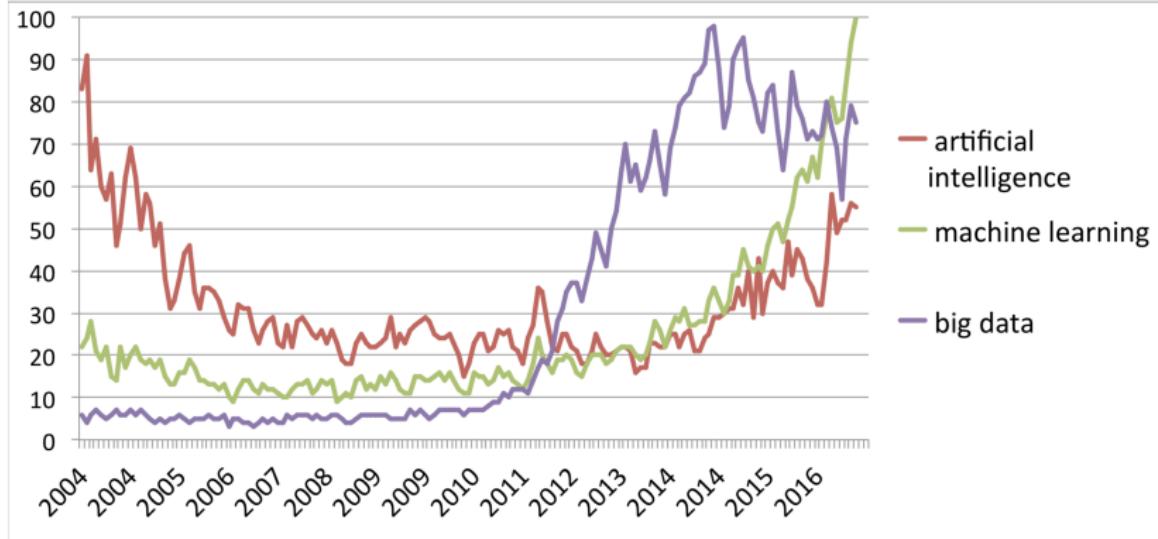
- ▶ Traditional programming:



- ▶ Machine learning:



## Why is ML successful?



# Sexiest job of the century

“Data scientist is  
the sexiest job,  
of the 21st century.”

Harvard Business Review

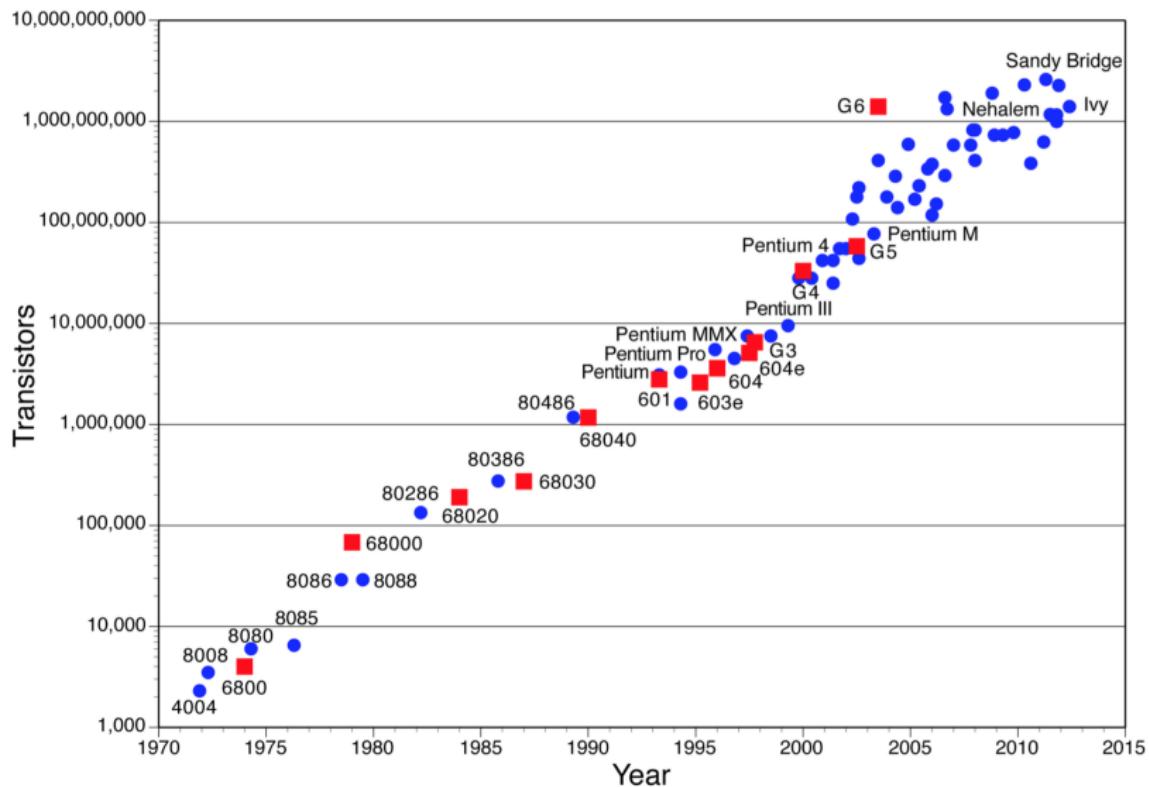


# The machine learning revolution

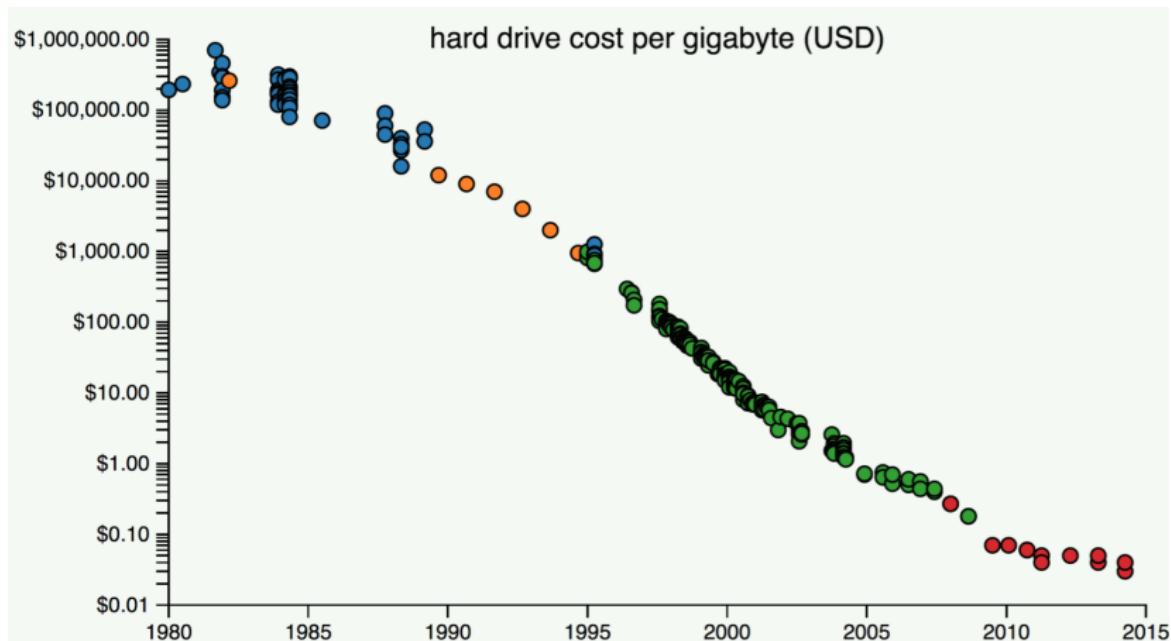
Big data / machine learning / data science / artificial intelligence / deep learning, a revolution?

- **Technical progress:** increase in computing power and storage capacity, lower costs

## Moore's law: more computing power



## Moore's Law: reduced costs



Limits : – debits do not follow

– miniaturization → reach the limits of classical physics → quantum mechanics

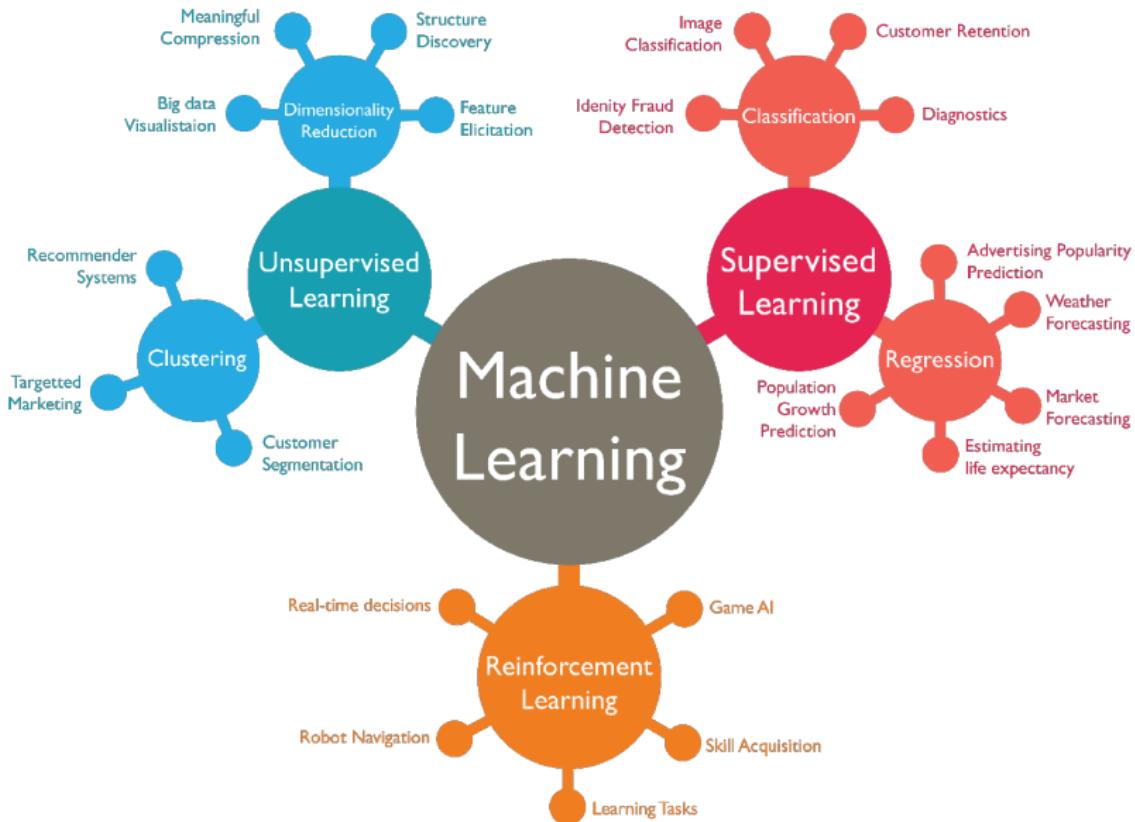
Big data / machine learning / data science / artificial intelligence / deep learning, a revolution?

- **Technical progress:** increase in computing power and storage capacity, lower costs
- **Exponential increase in amount of data:** Volume, Variability, Velocity, Veracity
  - IBM:  $10^{18}$  bytes created each day — 90% of the data  $\leq 2$  years
  - In all area: sciences, industries, personal life
  - In all forms: video, text, clicks, numbers

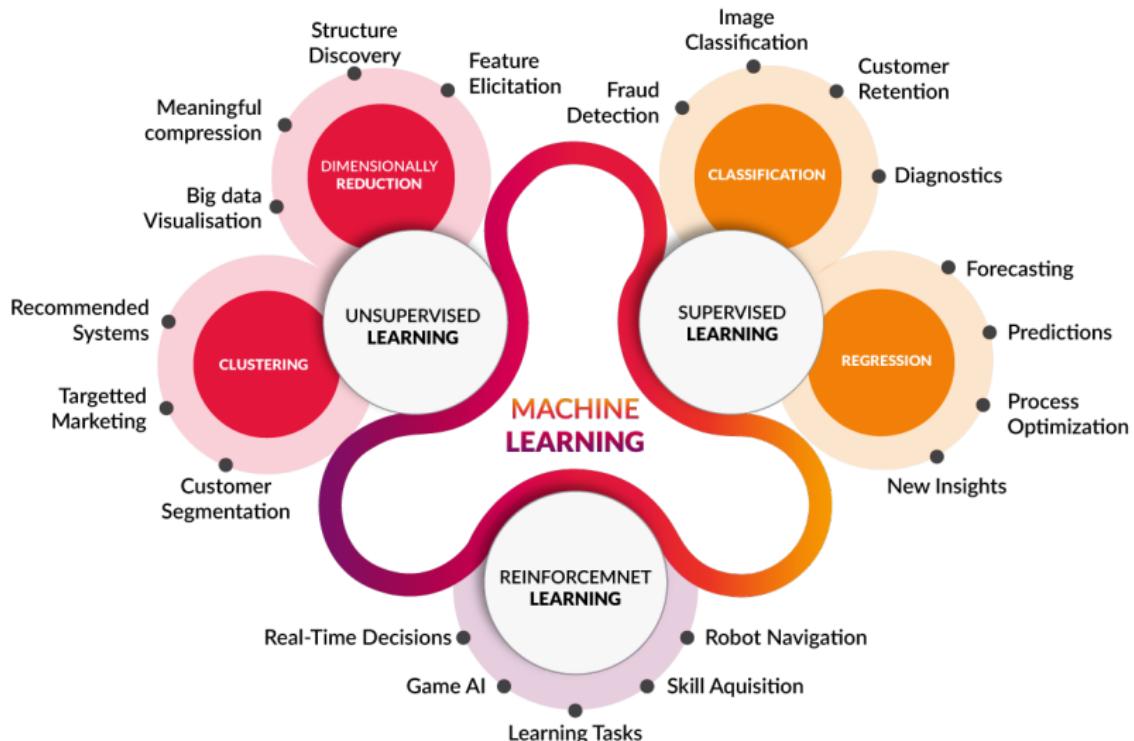
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- **Methodological advancement** to analyze complex datasets: high dimensional statistics, deep learning, reinforcement learning, . . .

# Overview of Machine Learning



# Overview of Machine Learning



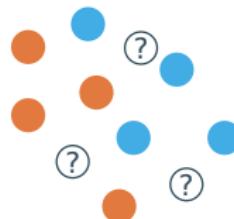
# Overview of most popular machine learning methods

Two main categories of machine learning algorithms:

- **Supervised learning:** predict output  $Y$  from some input data  $X$ . The training data has a known label  $Y$ .

Examples:

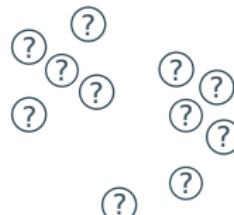
- $X$  is a picture, and  $Y$  is a cat or a dog
- $X$  is a picture, and  $Y \in \{0, \dots, 9\}$  is a digit
- $X$  is are videos captured by a robot playing table tennis, and  $Y$  are the parameters of the robots to return the ball correctly
- $X$  is a music track and  $Y$  are the audio signals of each instrument



- **Unsupervised learning:** training data is not labeled and does not have a known result

Examples:

- detect change points in a non-stationary time-series
- detect outliers
- cluster data in homogeneous groups
- compress data without loosing much information
- density estimation



- **Others:** reinforcement learning, semi-supervised learning, online learning,...

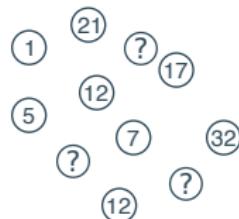
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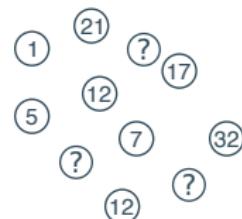
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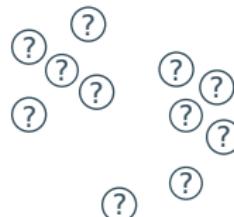
- **Supervised learning:** predict output  $Y$  from some input data  $X$ . The training data has a known label  $Y$ .

Classification	Regression
SVM	Lasso, Ridge
Logistic regression	Nearest Neighbors
Random Forest	Neural Networks



- **Unsupervised learning:** training data is not labeled and does not have a known result

Clustering	Dimensionality reduction
K-means, the Apriori algorithm, Birch, Ward, Spectral Cluster	PCA, ICA word embedding



- **Others:** reinforcement learning, semi-supervised learning, online learning,...

## Supervised learning

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**Goal:** from **training data**, we want to **predict an output  $Y$**  (or the best action) from the observation of some **input  $X$** .

**Difficulties:**  $Y$  is not a deterministic function of  $X$ . There can be some noise:

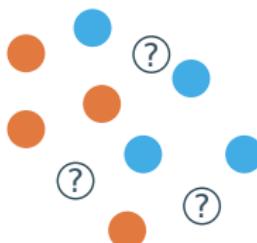
$$Y = f(X) + \varepsilon$$

The function  $f$  is unknown and can be sophisticated.

→ hard to perform well systematically

**Possible theoretical approaches:** perform well

- in the **worst-case**: minimax theory, game theory
- in average, or with high probability



**Algorithmic approaches:**

- **local averages**:  $K$ -nearest neighbors, decision trees
- **empirical risk minimization**: linear regression, lasso, spline regression, SVM, logistic regression
- **online learning**
- **deep learning**
- **probabilistic models**: graphical models, Bayesian methods

# Supervised learning: theory

Some **data**  $(X, Y) \in \mathcal{X} \times \mathcal{Y}$  is distributed according to a probability distribution  $P$ .

We observe training data  $D_n := \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ .

We must form prediction into a **decision set**  $\mathcal{A}$  by choosing a prediction function

$$f : \underbrace{\mathcal{X}}_{\text{observation}} \rightarrow \underbrace{\mathcal{A}}_{\text{decision}}$$

Our performance is measured by a **loss function**  $\ell : \mathcal{A} \times \mathcal{Y} \rightarrow \mathbb{R}$ . We define the risk

$$R(f) := \mathbb{E}[\ell(f(X), Y)] = \text{expected loss of } f$$

**Goal:** minimize  $R(f)$  by approaching the performance of the **oracle**  $f^* = \arg \min_{f \in \mathcal{F}} R(f)$

	Least square regression	Classification
$\mathcal{A} = \mathcal{Y}$	$\mathbb{R}$	$\{0, 1, \dots, K - 1\}$
$\ell(a, y)$	$(a - y)^2$	$1_{a \neq y}$
$R(f)$	$\mathbb{E}[(f(X) - Y)^2]$	$\mathbb{P}(f(X) \neq Y)$
$f^*$	$\mathbb{E}[Y X]$	$\arg \max_k \mathbb{P}(Y = k X)$

## Supervised learning: theory

# Outline

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Introduction

Supervised learning

Empirical risk minimization: OLS, Logistic regression, Ridge, Lasso, Quantile regression

Calibration of the parameters: cross-validation

Local averages

Deep learning

Unsupervised learning

Clustering

Dimensionality Reduction Algorithms

Planning of the class

# Empirical risk minimization

Idea: estimate  $R(f)$  thanks to the training data with the empirical risk

$$\hat{R}_n(f) := \underbrace{\frac{1}{n} \sum_{i=1}^n \ell(f(X_i), Y_i)}_{\text{average error on training data}} \approx \underbrace{R(f) = \mathbb{E}[\ell(f(X), Y)]}_{\text{expected error}}$$

We estimate  $\hat{f}_n$  by minimizing the empirical risk

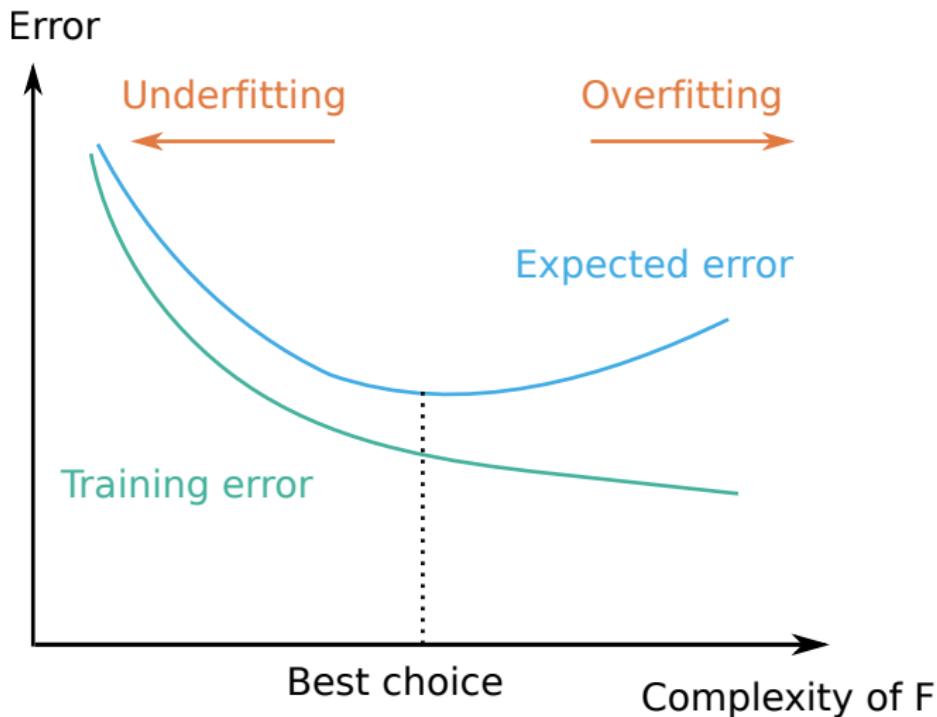
$$\hat{f}_n \in \arg \min_{f \in \mathcal{F}} \hat{R}_n(f).$$

Many methods are based on empirical risk minimization: ordinary least square, logistic regression, Ridge, Lasso,...

**Choosing the right model:**  $\mathcal{F}$  is a set of models which needs to be properly chosen:

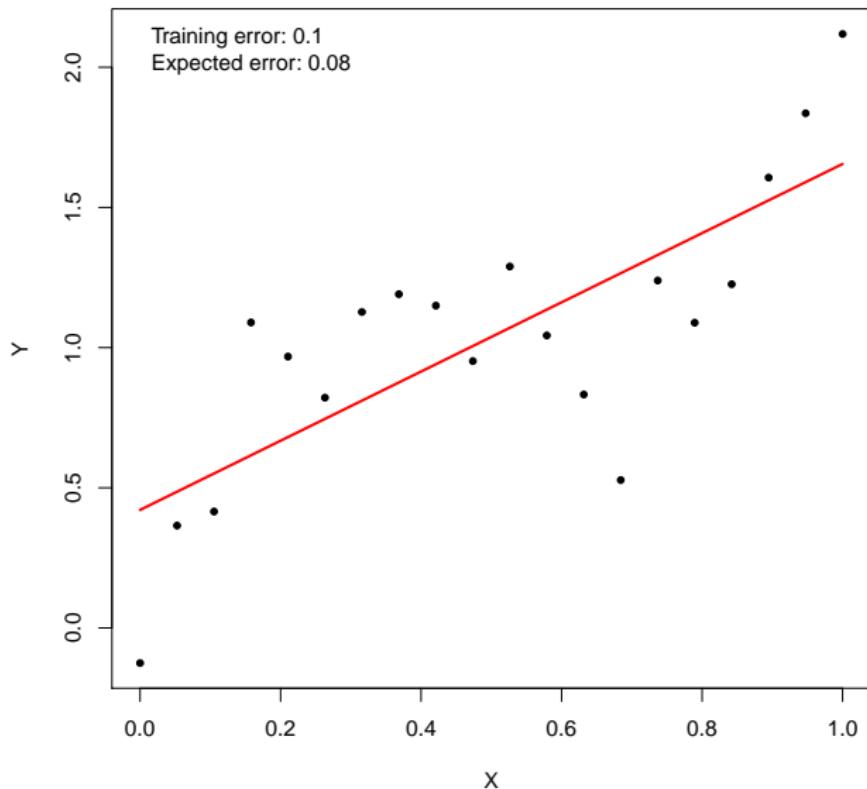
$$R(\hat{f}_n) = \underbrace{\min_{f \in \mathcal{F}} R(f)}_{\text{Approximation error}} + \underbrace{R(\hat{f}_n) - \min_{f \in \mathcal{F}} R(f)}_{\text{Estimation error}}$$

## Overfitting



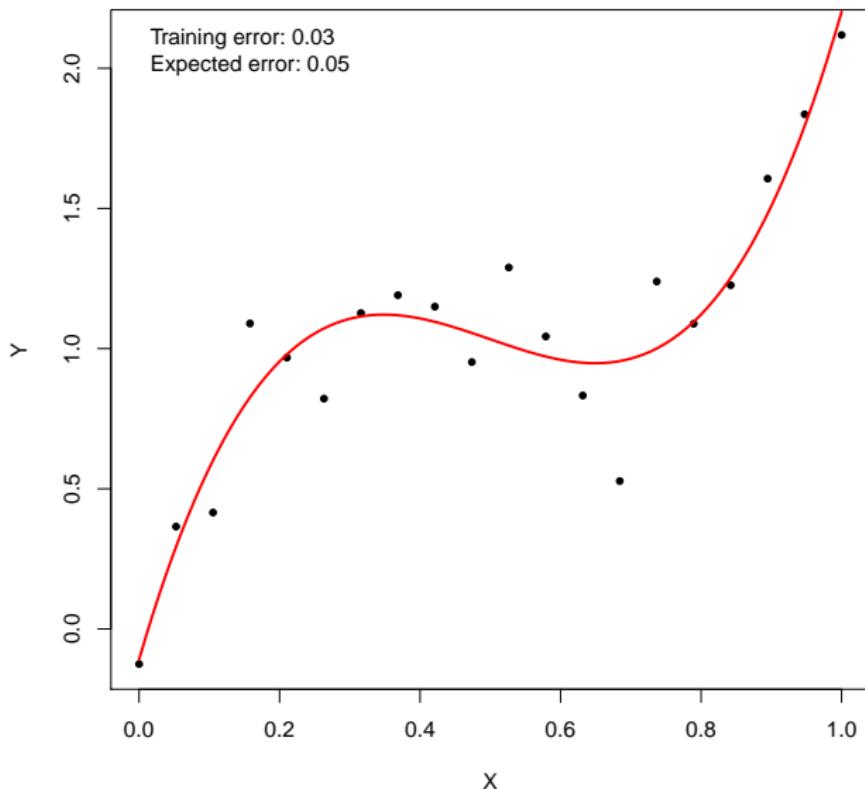
## Overfitting: example in regression

Linear model:  $Y = aX + b$



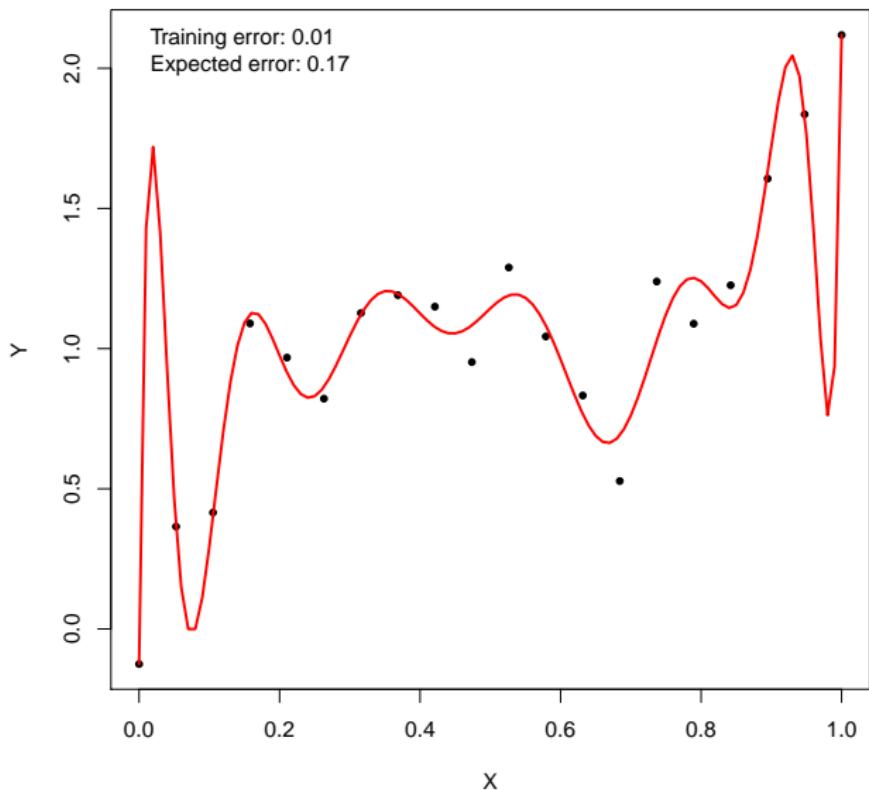
## Overfitting: example in regression

$$\text{Cubic model: } Y = aX + bX^2 + cX^3 + d$$



## Overfitting: example in regression

Polynomial model: Degree = 14



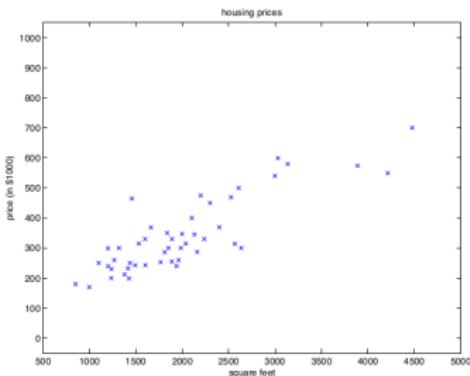
# Least square linear regression

## DATA

Living area (feet <sup>2</sup> )	Price (1000\$)
2104	400
1600	330
2400	369
1416	232
3000	540
:	:

$$(x_1, y_1), \dots, (x_n, y_n)$$

example taken from Coursera



Living area (feet <sup>2</sup> )	#bedrooms	Price (1000\$)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
:	:	:

## Least square Linear regression

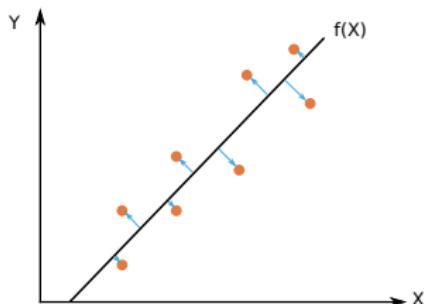
Given training data  $(X_i, Y_i)$  for  $i = 1, \dots, n$ , with  $X_i \in \mathbb{R}^d$  and  $Y_i \in \{0, 1\}$  learn a predictor  $f$  such that our expected square loss

$$\mathbb{E}[(f(X) - Y)^2]$$

is small.

We assume here that  $f$  is a linear combination of the input  $x = (x_1, \dots, x_d)$

$$f_w(x) = \sum_{i=1}^d w_i x_i = w^\top x$$



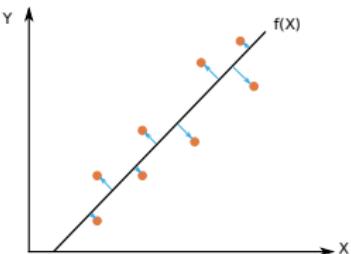
# Ordinary Least Square

Input  $X \in \mathbb{R}^d$ , output  $Y \in \mathbb{R}$ , and  $\ell$  is the square loss:  $\ell(a, y) = (a - y)^2$ .

The Ordinary Least Square regression (OLS) minimizes the empirical risk

$$\hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^n (Y_i - w^\top X_i)^2$$

This is minimized in  $w \in \mathbb{R}^d$  when  $\mathbf{X}^\top \mathbf{X} w - \mathbf{X}^\top \mathbf{Y} = 0$ , where  $\mathbf{X} = [X_1, \dots, X_n]^\top \in \mathbb{R}^{n \times d}$  and  $\mathbf{Y} = [Y_1, \dots, Y_n]^\top \in \mathbb{R}^n$ .

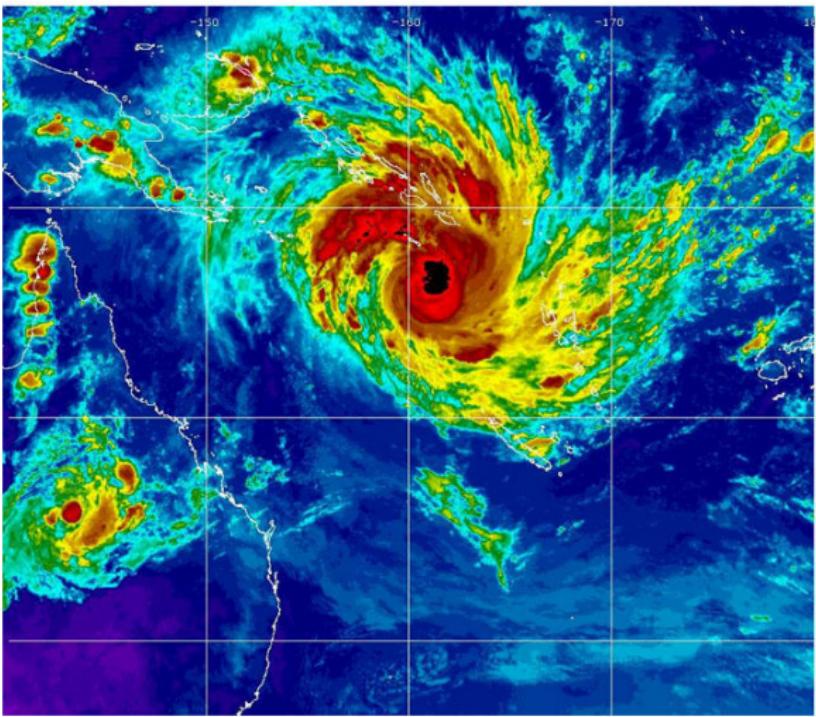


Assuming  $X$  is injective (i.e.,  $X^\top X$  is invertible) and there is an exact solution

$$\hat{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y}.$$



What happens if  $d \gg n$ ?



## Ordinary Least Square: how to compute $\hat{w}_n$ ?

If the design matrix  $X^\top X$  is invertible, the OLS has the closed form:

$$\hat{w}_n \in \arg \min_w \hat{R}_n(w) = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y}.$$

**Question:** how to compute it?

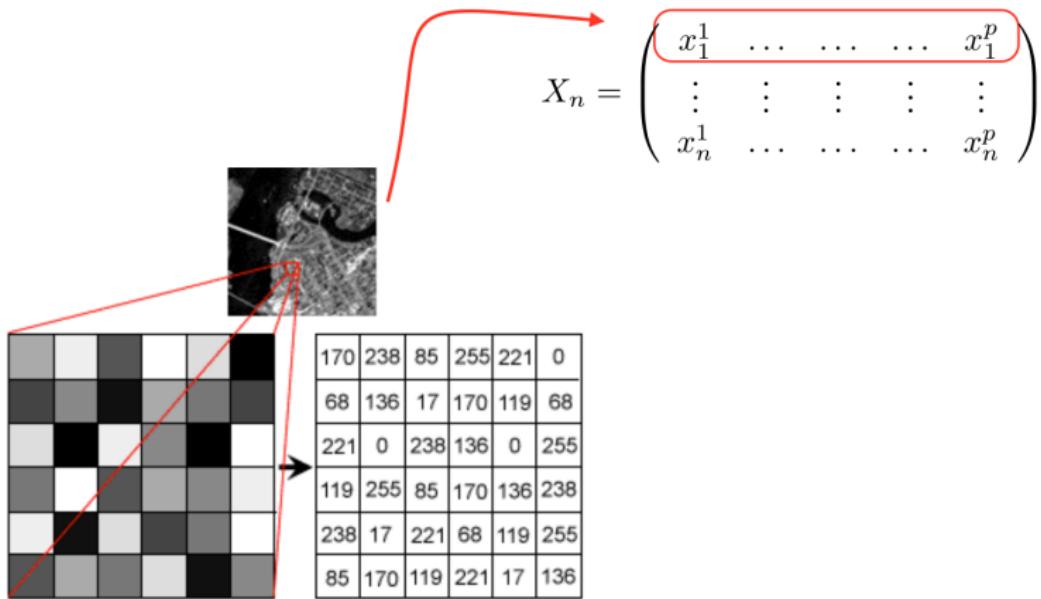
- inversion of  $(\mathbf{X}^\top \mathbf{X})$  can be prohibitive (the cost is  $\mathcal{O}(d^3)$ !)
- **QR-decomposition:** we write  $\mathbf{X} = \mathbf{Q}\mathbf{R}$ , with  $\mathbf{Q}$  an orthogonal matrix and  $\mathbf{R}$  an upper-triangular matrix. One needs to solve the linear system:

$$R\hat{w} = Q^\top \mathbf{Y}, \quad \text{with} \quad R = \begin{pmatrix} x & x & \cdots & x \\ \vdots & \ddots & & \vdots \\ 0 & & \ddots & x \end{pmatrix}$$

- iterative approximation with convex optimization algorithms [Bottou, Curtis, and Nocedal 2016]: (stochastic)-gradient descent, Newton,...

$$w_{i+1} = w_i - \eta \nabla \hat{R}_n(w_i)$$

## Beyond vectors?



## Beyond vectors?



**$n$  patients  $p$  gene expression measurements**

...



$i$



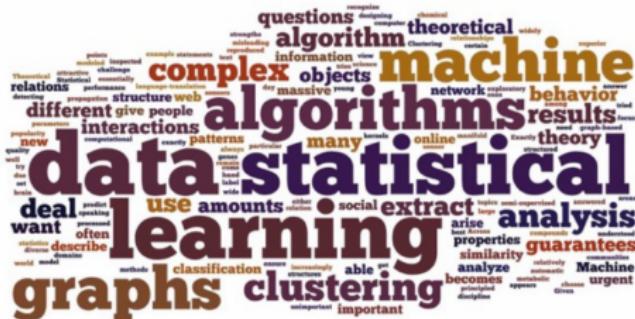
...



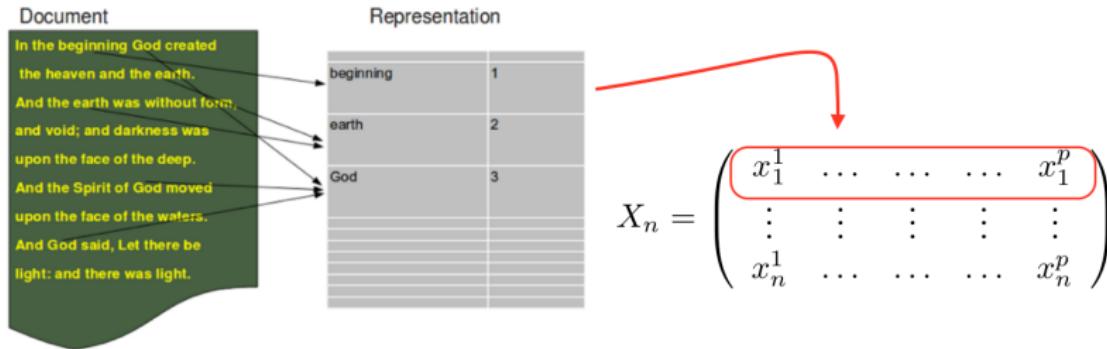
$$X_n = \begin{pmatrix} x_1^1 & \dots & \dots & \dots & x_1^p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^1 & \dots & \dots & \dots & x_n^p \end{pmatrix}; Y_n = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$



## Beyond vectors?



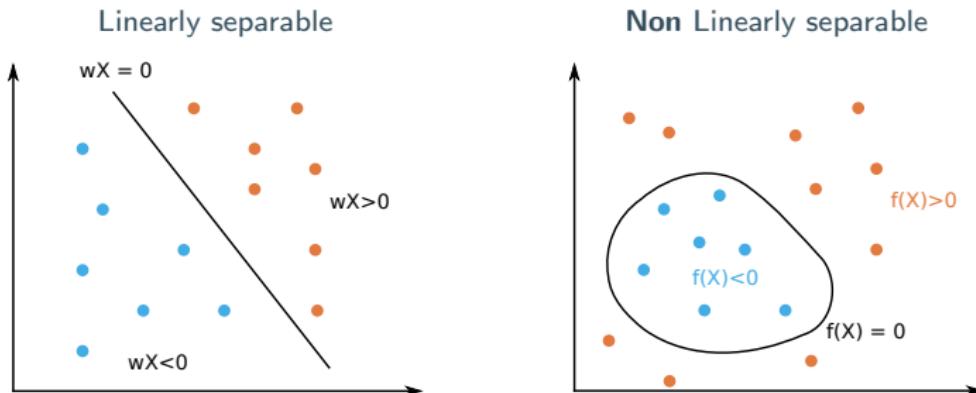
$$Y_n = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$



# Classification

Given training data  $(X_i, Y_i)$  for  $i = 1, \dots, n$ , with  $X_i \in \mathbb{R}^d$  and  $Y_i \in \{0, 1\}$  learn a classifier  $f(x)$  such that

$$f(X_i) \begin{cases} \geq 0 & \Rightarrow Y_i = +1 \\ < 0 & \Rightarrow Y_i = 0 \end{cases}$$



# Linear classification

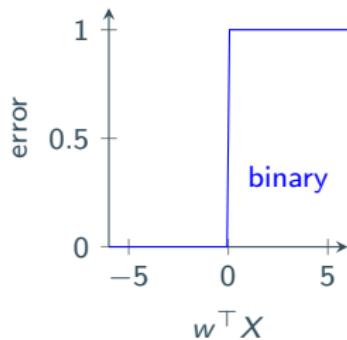
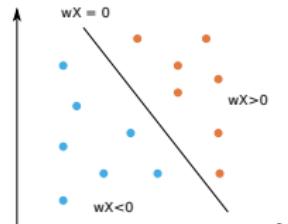
We would like to find the best linear classifier such that

$$f_w(X) = w^\top X \begin{cases} \geq 0 & \Rightarrow Y = +1 \\ < 0 & \Rightarrow Y = 0 \end{cases}$$

**Empirical risk minimization** with the binary loss?

$$\hat{w}_n = \arg \min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{Y_i \neq \mathbb{1}_{w^\top X_i \geq 0}}.$$

👎 This is **not convex** in  $w$ . Very hard to compute!



# Spam filters



2007-05-22 18:33 - News in English  
**Soccer: Milan weighs attack options**  
Gilardino tipped to lead the line, Inzaghi late card

2007-05-22 17:29 - News in English  
**Wine wards off senile dementia**  
A glass a day stops mild impairment worsening, Italians say

2007-05-22 16:12 - News in English  
**Treasury may sell all of Alitalia**  
Formal bids for carrier due by July 2

2007-05-22 15:58 - News in English  
**Afghanistan: Rome cold on Bush call**  
'We respond to parliament, no one else,' FM says

2007-05-22 14:11 - News in English  
**Electronic nose sniffs asthma**  
Device developed by Italian researcher in Netherlands

**Sport** (football)

**Health**

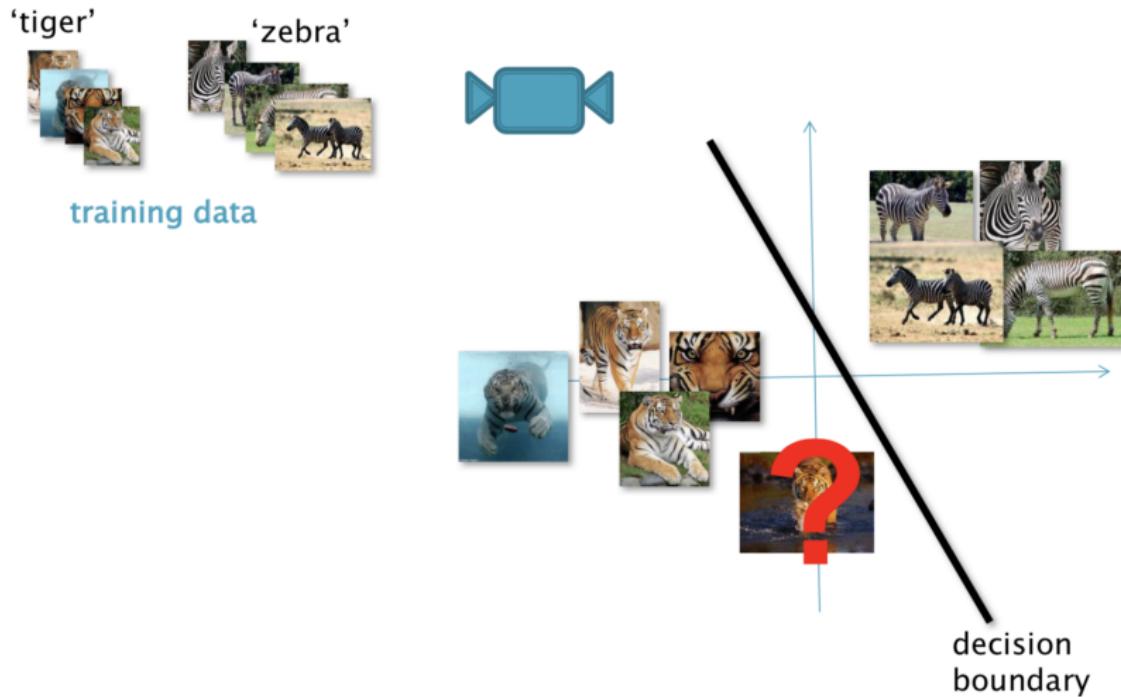
**Politics** (economy)

**Politics** (foreign)

**Technology**

Subject	Date	Time	Body	Spam?
I has the viagra for you	03/12/1992	12:23 pm	Hil I noticed that you are a software engineer so here's the pleasure you were looking for...	Yes
Important business	05/29/1995	01:24 pm	Give me your account number and you'll be rich. I'm totally serial	Yes
Business Plan	05/23/1996	07:19 pm	As per our conversation, here's the business plan for our new venture Warm regards...	No
Job Opportunity [A few thousand rows omitted]	02/29/1998	08:19 am	Hil am trying to fill a position for a PHP ...	Yes
Call mom	05/23/2000	02:14 pm	Call mom. She's been trying to reach you for a few days now	No

# Image recognition



# Pedestrian recognition

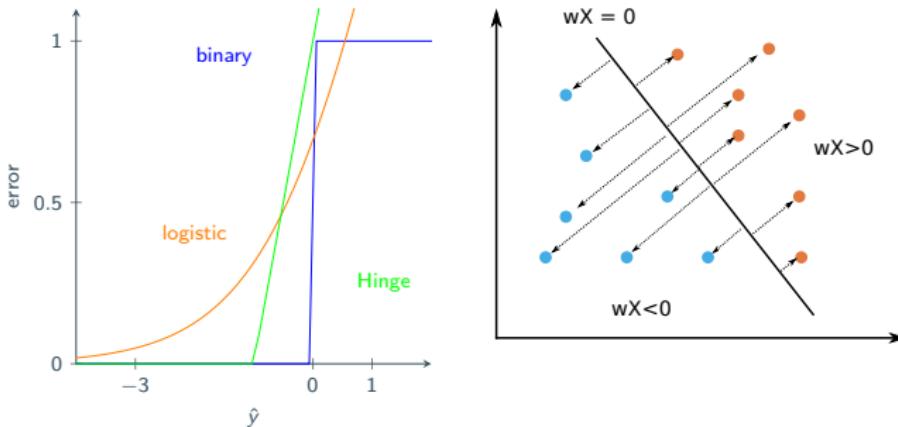


<https://youtu.be/lU4w0o-caFM>

# Logistic regression

Idea: replace the loss with a convex loss

$$\ell(w^\top X, y) = y \log(1 + e^{-w^\top X}) + (1 - y) \log(1 + e^{w^\top X})$$



**Probabilistic interpretation:** based on likelihood maximization of the model:

$$\mathbb{P}(Y=1|X) = \frac{1}{1 + e^{-w^\top X}} \in [0, 1]$$

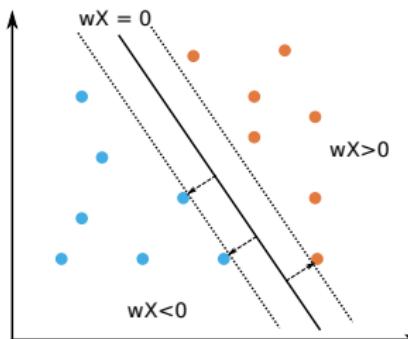
Satisfied for many distributions of  $X|Y$ : Bernoulli, Gaussian, Exponential, ...

**Computation of the minimizer of the empirical risk** (No closed form of the solution)

- Use a convex optimization algorithm (Newton, gradient descent, ...)

# Support Vector Machine (SVM)

In SVM, the linear separator (hyperplane) is chosen by **maximizing the margin**. Not by minimizing the empirical risk.



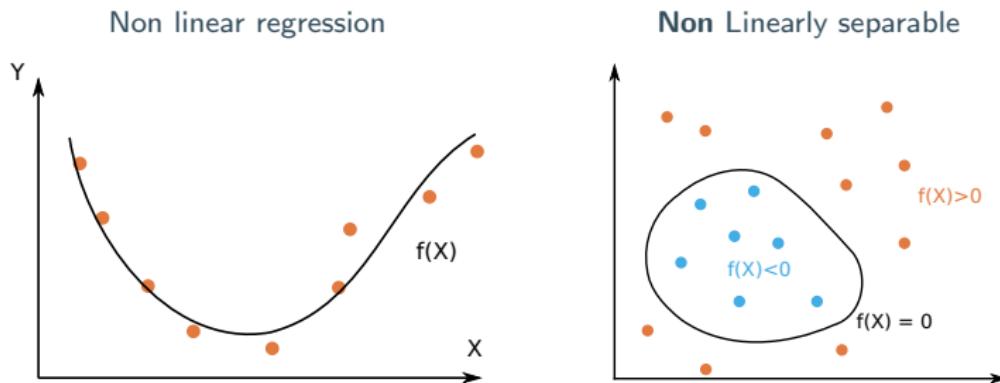
👍 **Sparsity:** it only depends on a few training points, called **the support vectors**  
In practice, we use **soft margins** because no perfect linear separation is possible.

## Non-linear regression/classification

Until now, we have only considered linear predictions of  $x = (x_1, \dots, x_d)$

$$f_w(x) = \sum_{i=1}^d w_i x_i .$$

But this can perform pretty bad... How to perform non-linear regression?



# Non-linear regression/classification

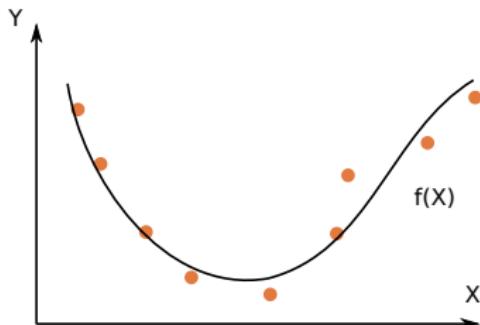
Idea: map the input  $X$  into a higher dimensional space where the problem is linear.

Example: given an input  $x = (x_1, x_2, x_3)$  perform a linear method on a transformation of the input like

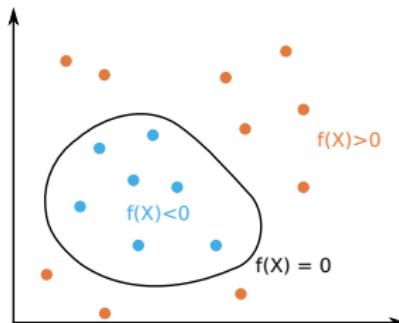
$$\Phi(x) = (x_1x_1, x_1x_2, \dots, x_3x_2, x_3x_3) \in \mathbb{R}^9$$

Linear transformations of  $\Phi(x)$  are polynomials of  $x$ ! The previous methods works by replacing  $x$  with  $\Phi(x)$ .

Non linear regression

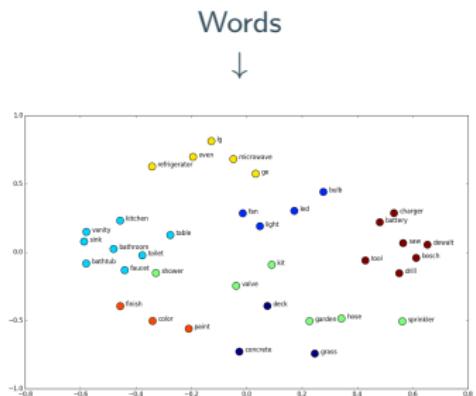


Non Linearly separable



# Example: Word Embedding (Word2Vec)

<http://wordrepresentation.appspot.com>



```
>>> print_analogy('Paris', 'France', 'Rome', words)
Paris-France is like Rome-Italy

>>> print_analogy('man', 'king', 'woman', words)
man-king is like woman-queen

>>> print_analogy('walk', 'walked', 'go', words)
walk-walked is like go-went

>>> print_analogy('quick', 'quickest', 'far', words)
quick-quickest is like far-furthest
```

A **spline of degree  $p$**  is a function formed by connecting polynomial segments of degree  $p$  so that:

- the function is continuous
- the function has  $D - 1$  continuous derivatives
- the  $p$ th-derivative is constant between knots

This can be done by choosing the good transformation  $\Phi_p(x)$  and the right regularization  $\|\Phi_p(x)\|$ .

**Difficulties:** choose the **number of knots** and the **degree**

# Regularization



How to avoid over-fitting if there is not enough data?



Control the complexity of the solution

- explicitly by choosing  $\mathcal{F}$  small enough: choose the degree of the polynomials,...
- implicitly by adding a **regularization term**

$$\min_{f \in \mathcal{F}} \hat{R}_n(f) + \lambda \|f\|^2$$

The higher the norm  $\|f\|$  is, the more complex the function is.

- 👍 We do not need to know the best complexity  $\mathcal{F}$  in advance
- 👎 Complexity controlled by  $\lambda$ , which need to be calibrated.

## Ridge regression

The most classic regularization in statistics for linear regression:

$$\hat{w}_n = \arg \min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (Y_i - w^\top X_i)^2 + \lambda \sum_{i=1}^d w_i^2$$

The exact solution is unique because the problem is now **strongly convex**:

$$\hat{w}_n = (\mathbf{X}^\top \mathbf{X} + n\lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{Y}$$

The regularization parameter  $\lambda$  controls the matrix conditioning:

- if  $\lambda = 0$ : ordinary linear regression
- if  $\lambda \rightarrow \infty$ :  $\hat{w}_n \rightarrow 0$

# The Lasso: how to choose among a large set of variables with few observations

The Lasso corresponds to  $L_1$  regularization:

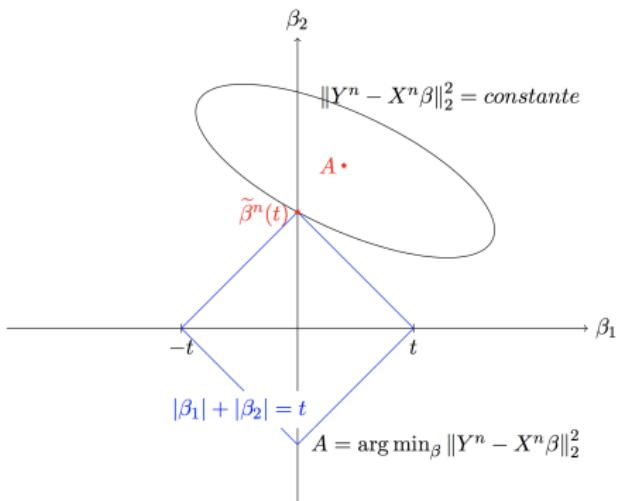
$$\hat{w}_n = \arg \min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (Y_i - w^\top X_i)^2 + \lambda \sum_{i=1}^d |w_i|$$

- 👍 Powerful if  $d \gg n$ : many potential variables, few observations
- 👍  $\hat{w}_n$  is sparse: most of its values will be 0 → can be used to choose variables

Other formulation of the Lasso:

$\exists \beta > 0$  such that

$$\hat{w}_n \in \arg \min_{\|w\|_1 \leq \beta} \frac{1}{n} \sum_{i=1}^n (Y_i - w^\top X_i)^2$$

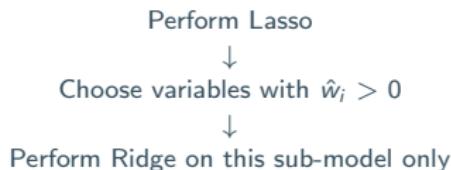


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- 👍 Powerful if  $d \gg n$ : many potential variables, few observations
- 👍  $\hat{w}_n$  is sparse: most of its values will be 0 → can be used to choose variables
- 👎 The Lasso is biased:  $\hat{w}_n^\top X \neq \mathbb{E}[Y|X]$ . Hence, it is better to:



Another solution is Elastic Net:

$$\hat{w}_n = \arg \min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (Y_i - w^\top X_i)^2 + \lambda_1 \sum_{i=1}^d |w_i| + \lambda_2 \sum_{i=1}^d w_i^2$$

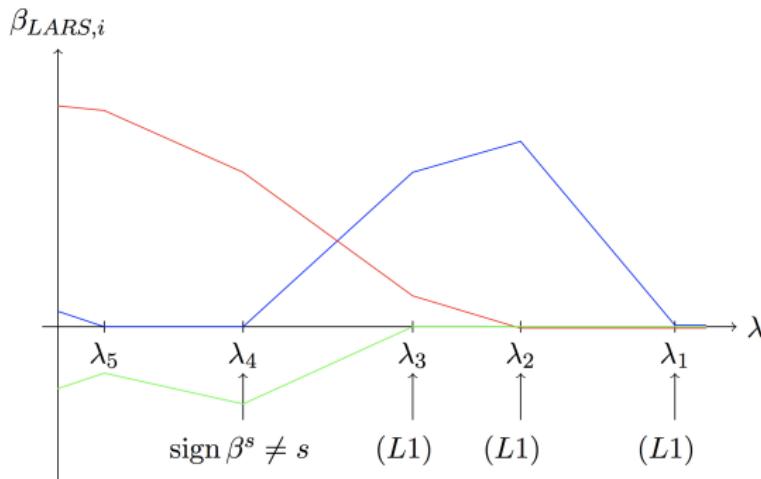
Many extensions of the Lasso exist: Group Lasso,...

## Lasso: the regularization path

The Lasso corresponds to  $L_1$  regularization:

$$\hat{w}_n = \arg \min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (Y_i - w^\top X_i)^2 + \lambda \sum_{i=1}^d |w_i|$$

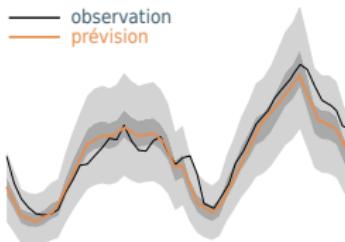
Plot of the evolution of the coefficients of  $\hat{w}_n$  as a function of  $\lambda$ :



In some situations, we are not interested in predicting the **average case**  $\mathbb{E}[Y|X]$  only, but by the **distribution of  $Y|X$** . → give a **measure of uncertainty** of our prediction

**Solution:** modify the loss function:

- square loss  $\ell(a, y) = (a - y)^2$ : prediction of the **expected value**
- absolute loss  $\ell(a, y) = |a - y|$ : prediction of the **median**  
(50% to be above  $Y$ , and 50% chance to be below)
- pinball loss  $\ell(a, y) = (a - y)(\tau - \mathbb{1}_{a < y})$ : prediction of the  **$\tau$ -quantile**  
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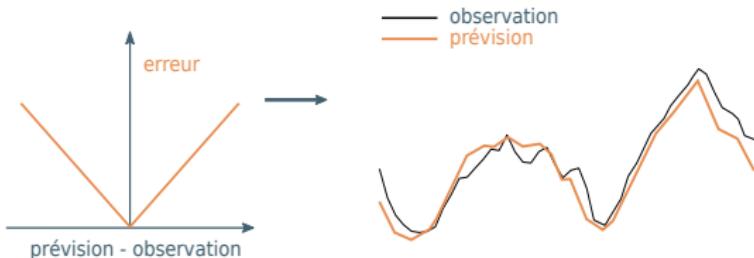


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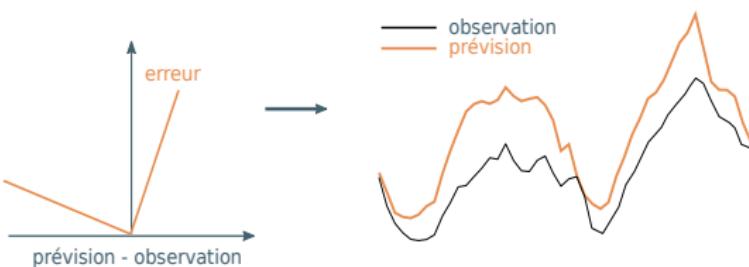


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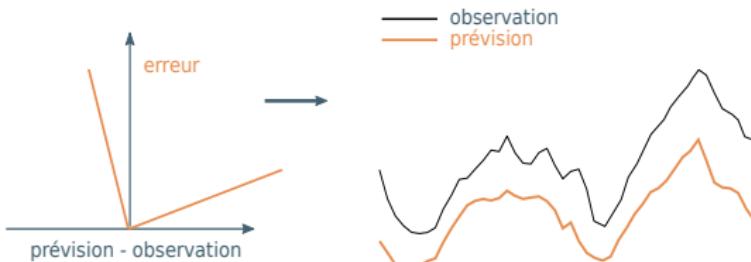


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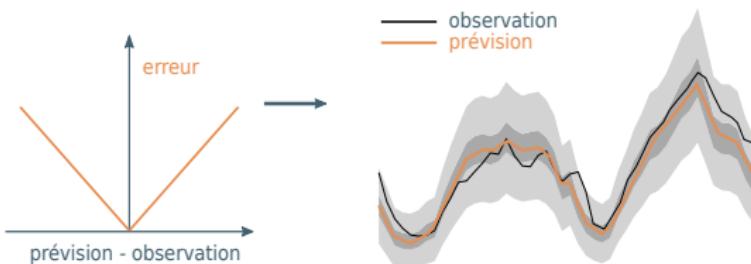


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# Outline

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Introduction

## Supervised learning

Empirical risk minimization: OLS, Logistic regression, Ridge, Lasso, Quantile regression

### Calibration of the parameters: cross-validation

Local averages

Deep learning

## Unsupervised learning

Clustering

Dimensionality Reduction Algorithms

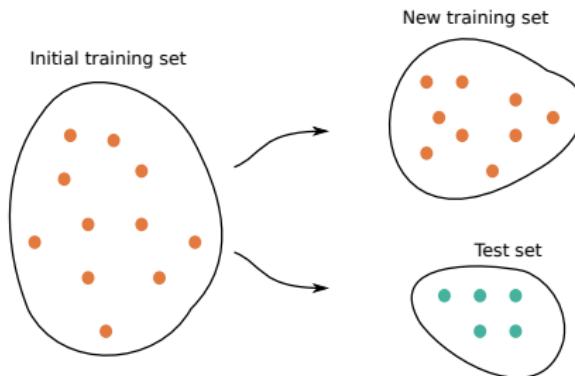
Planning of the class

## How to choose the parameters? Test set

All the methods in machine learning depend on **learning parameters**.

How to choose them? First solution: use a test set.

- randomly choose 70% of the data to be in the **training set**
- the remainder is a **test set**



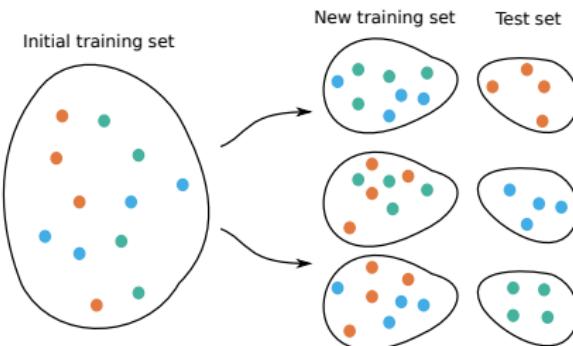
We choose the parameter with the smallest error on the test set.

- 👍 very simple
- 👎 waste data: the best method is fitted only with 70% of the data
- 👎 with bad luck the test set might be lucky or unlucky

# How to choose the parameters? Cross-validation

Cross-validation:

- randomly break data into  $K$  groups
- for each group, use it as a test set and train the data on the  $(K - 1)$  other groups



We choose the parameter with the smallest average error on the test sets.

- 👍 only  $1/K$  of the data lost for training
- 👎  $K$  times more expensive

In practice: choose  $K \approx 10$ .

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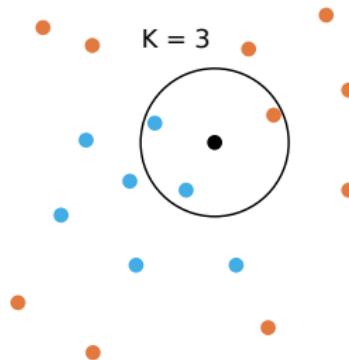
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# K-Nearest Neighbors

Classify data based on similarity with neighbors.

When observing a new input  $x$ , find the *k*-closest training data points to  $x$  and for

- classification: predict the most frequently occurring class
- regression: predict the average value

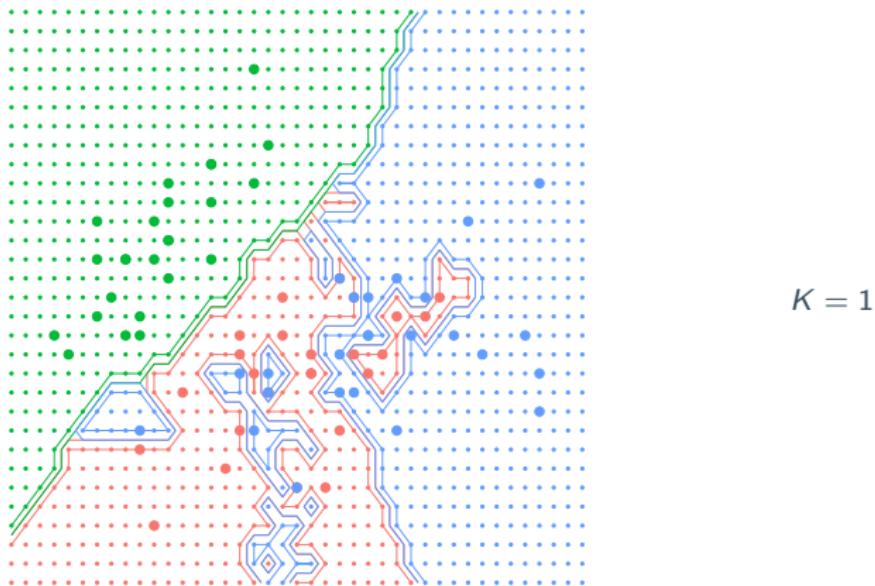


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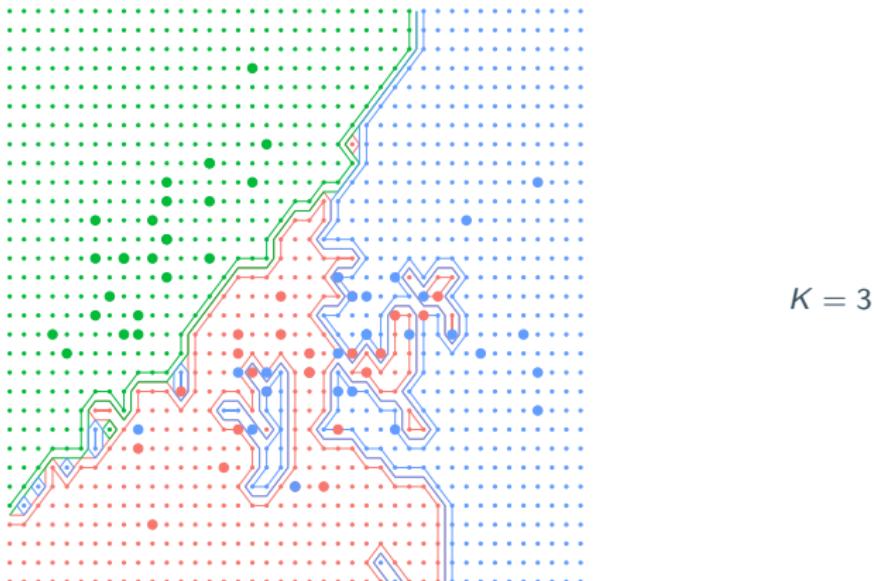


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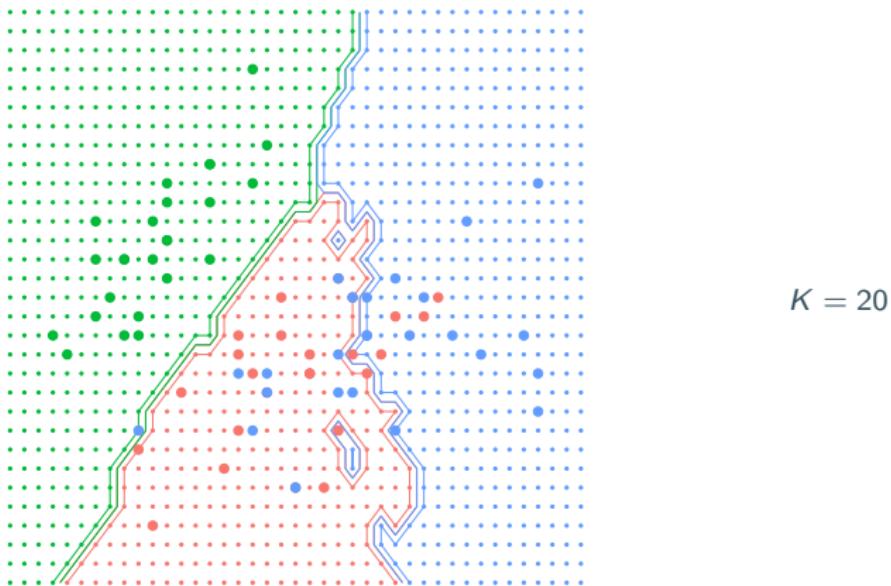


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## Advantages:

- No optimization or training
- Easy to implement
- Can get very good performance



## Drawbacks:

- Slow at query time: must pass through all training data at each
- Easily fooled by irrelevant inputs
- Bad for high-dimensional data ( $d > 20$ )



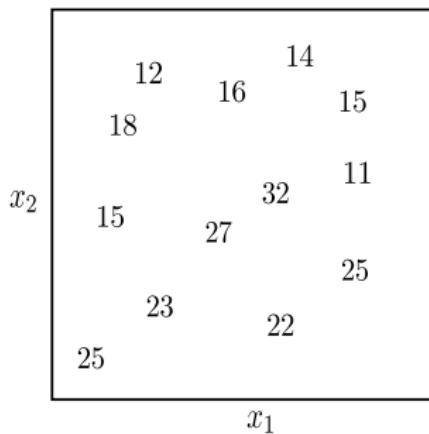
## Difficulties:

- choice of  $K$
- what distance for complex data?

# Decision Tree

Introduced by Breiman et al. 1984

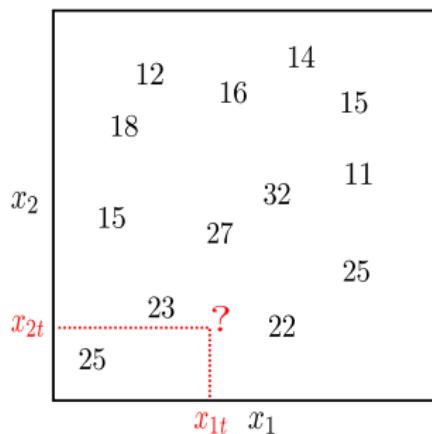
**Idea:** partitioned the input space in an inductive and diadic fashion.



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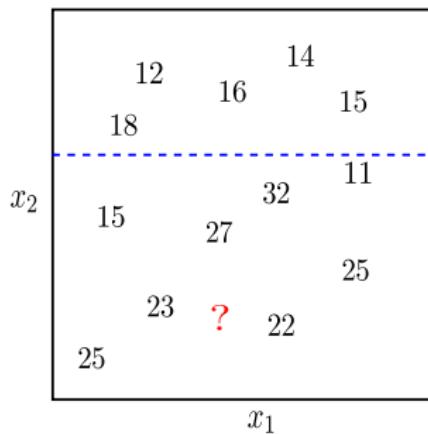
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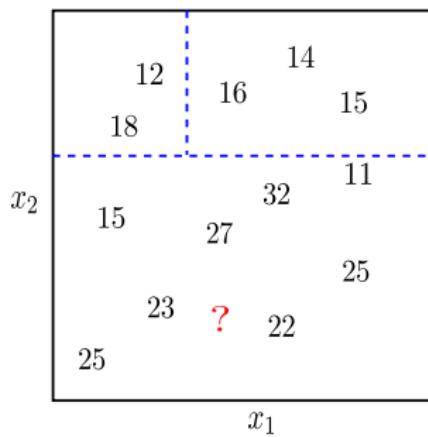
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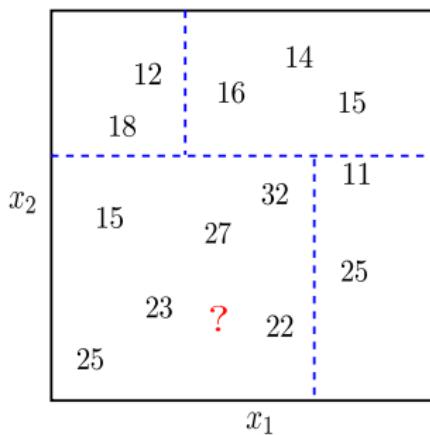
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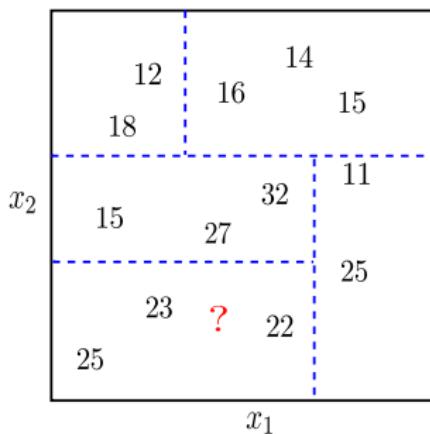
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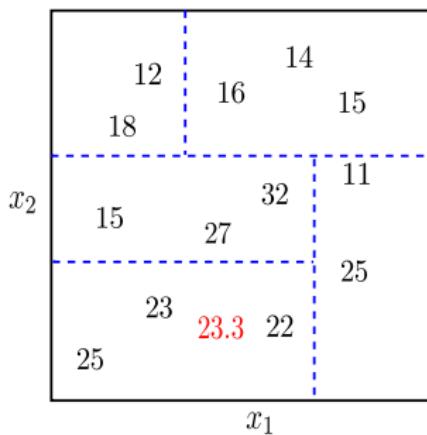
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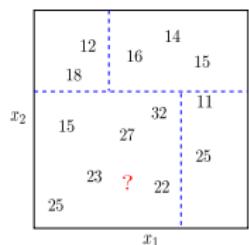
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# Decision Tree

Introduced by Breiman et al. 1984

**Idea:** partitioned the input space in an inductive and diadic fashion.



To construct the tree, we need to answer two questions:

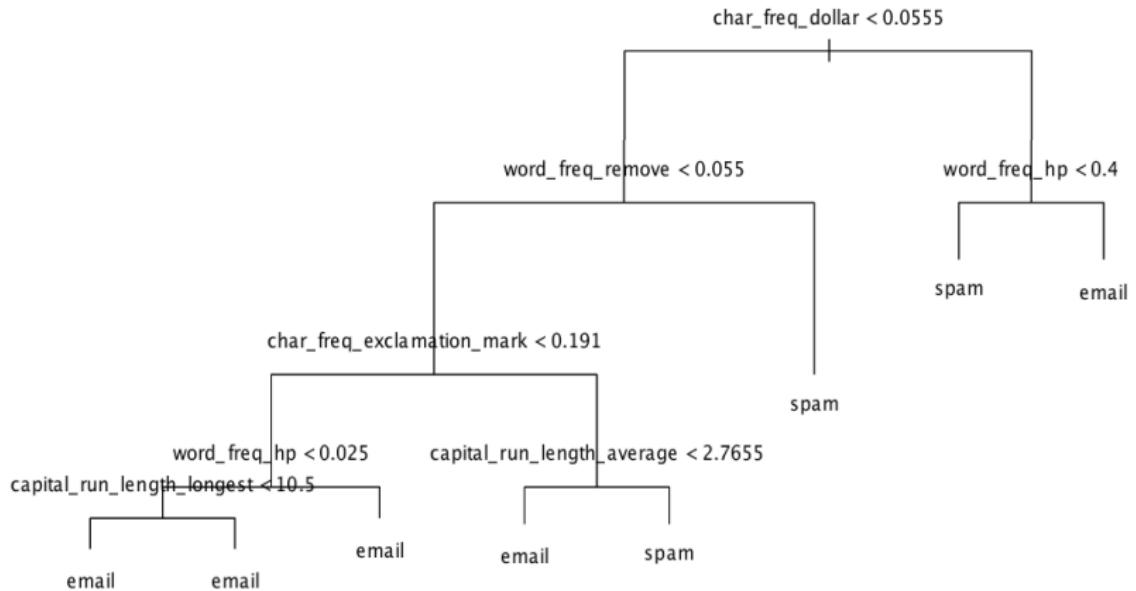
- **Location of the cuts:** which variable, what threshold?  
→ minimize the inter-groups variance
- **Depth of the tree:** when do we stop? Over-fitting risk!
  - continue while variance decreases enough
  - **pruning:** build a large tree and prune it by minimizing a penalized error:

$$\text{Test error}(T) + \lambda \text{size}(T)$$

Advantage: interpretable computational cost

Drawbacks: instable (butterfly effect),

## Decision trees: example for spam detection



Ensemble algorithms are based on the following idea: **averaging adds stability**.

**Example:** Assume that  $Y \in \{0, 1\}$  and that you have  $K$  independent classification methods  $f_k, k = 1, \dots, K$  such that  $\mathbb{P}(f_k(X) \neq Y) \leq \varepsilon$ . Then from Hoeffding's inequality:

$$\mathbb{P}(\text{majority voting of } f_k(X) \neq Y) \lesssim e^{-K\varepsilon^2}$$

→ exponential decrease to 0!

**Idea:** build base methods as independent as possible and average them.

1. split the training set into  $K$  subsets of size  $n/K$
2. train a different “base learner” on each subset

**Issue:**  $n$  may be too small → not enough data per “base learner” → **Bagging**

Introduced by Breiman 1996

## To fit a new “base learner”

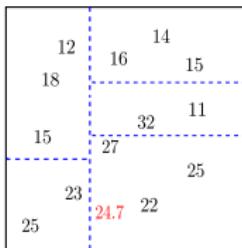
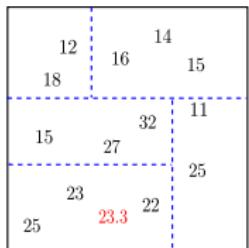
1. sample  $n$  data with replacement from the training set
2. train the “base learner” on this subset of observations

Each base learner gets  $\approx 36.8\%$  of the data. Remaining points are called “out-of-bag”.

We can estimate the performance of each base learner with the out-of-bag error

Introduced by Breiman 2001

Idea: build many ( $\approx 400$ ) random decisions trees and average their predictions.



predict  $\frac{24.7+23.3}{2} = 24$

## How to build uncorrelated trees?

- bagging: each tree is built over sample of training points
- random choice of the covariate to cut



### Advantages:

- No over-fitting (the more trees we build, the better)
- Easy computation of an error estimate: “out-of-bag”: no-need of cross validation
- efficient for small data sets  $n$



### Drawbacks: computational cost, black box

Random forests is a powerful tool to order explanatory variables by predictive importance.

First, we build the forest and compute  $E$  its “out-of-bag” error.

**For each variable  $X_i$ , we compute its importance as follows**

- randomly permute the values of  $X_i$  among training data
- update the “out-of-bag” error  $E_i$
- get the importance of  $X_i$  given by  $E_i - E$

# Outline

---

Introduction

## Supervised learning

Empirical risk minimization: OLS, Logistic regression, Ridge, Lasso, Quantile regression

Calibration of the parameters: cross-validation

Local averages

## Deep learning

Unsupervised learning

Clustering

Dimensionality Reduction Algorithms

Planning of the class

**Successful application domains:** **Image** (object recognition), **Audio** (speech recognition), **Text** (parsing)

## What is it used for?

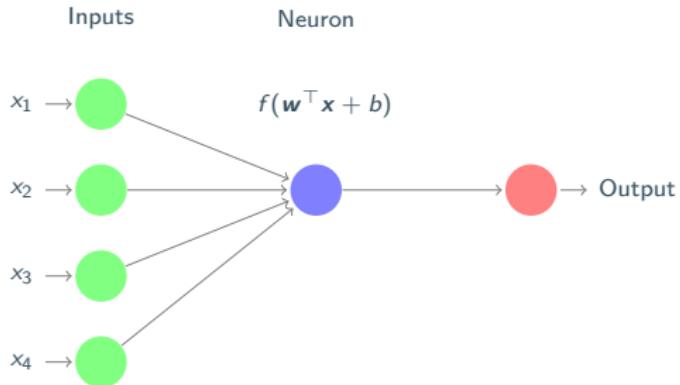
- **Prediction**: regression, classification,
- **Generation**: denoising, reconstruction of partial/missing data, generation of new data

## What is it?

- Models with graphs structure (networks) with multiple layers (deep)
- Typically non-linear models

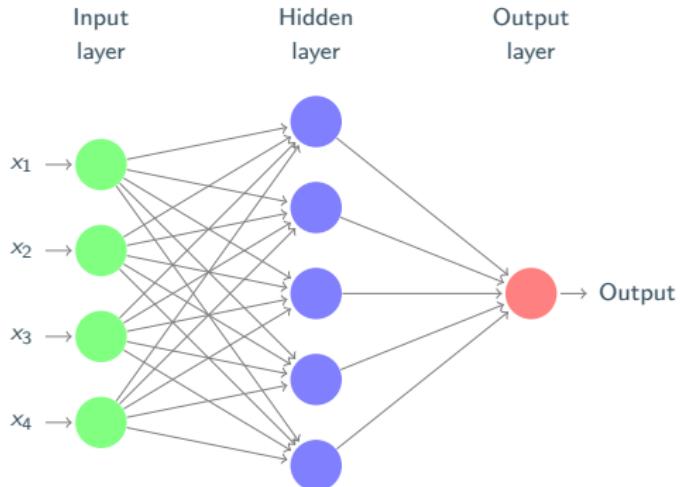
# Deep neural network

- A **neuron** is a **non-linear transformation** of a **linear combination** of inputs.
- A column of neurons taking the same input  $x$  forms a new **layer**



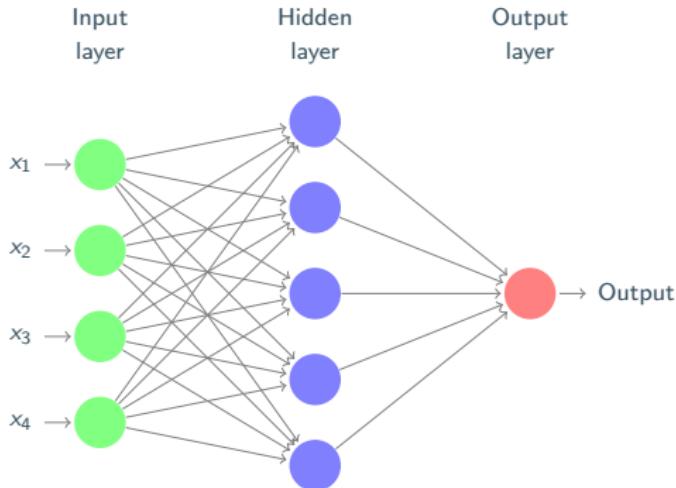
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# Deep neural network

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Training a neural networks: **backpropagation** (gradient descent using  $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$ ).

Avoid over-fitting: **dropout** [Hinton et al. 2012]

Build data-specific models: **convolutional** neural networks [LeCun et al. 1998]

# What can you do with DNN?

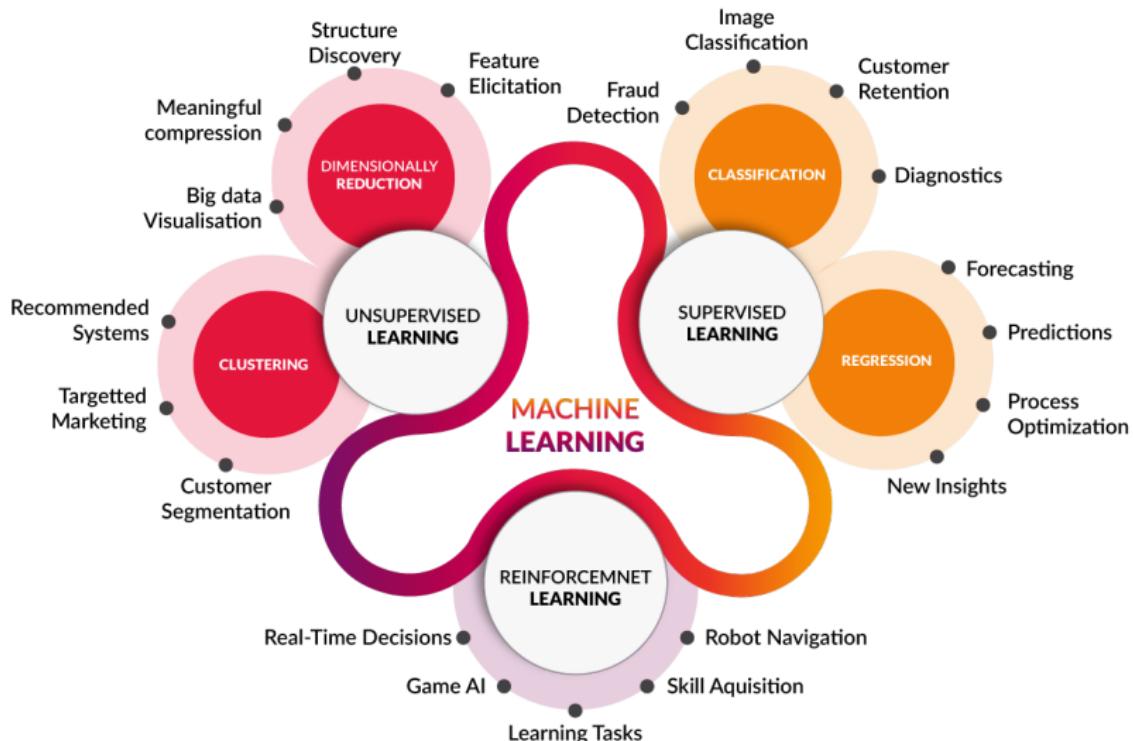


<https://youtu.be/Khuj4ASldmU>

## Unsupervised learning

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# Overview of Machine Learning



# Outline

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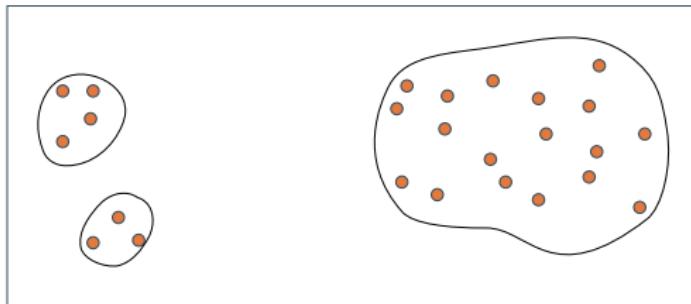
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# Clustering

- Idea: group together similar instances
- Requires data but no labels
- Useful when you don't know what you are looking for



The similarity is measured by a **metric** (ex:  $\|x - y\|_2^2$ ).

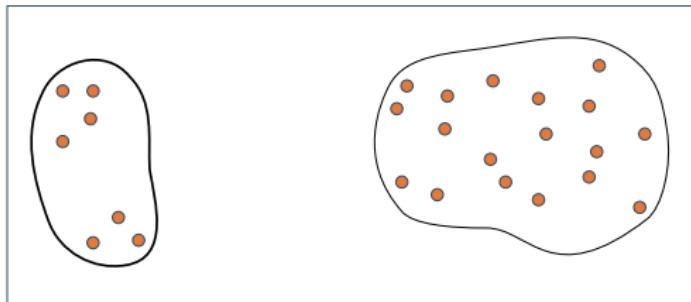
The results crucially depends on the metric choice: depends on data.

## Types of clustering algorithms:

- model based clustering (mixture of Gaussian)
- **hierarchical clustering**: a hierarchy of nested clusters is build using divisive or agglomerative approach
- Flat clustering: no hierarchy (**k-means**, spectral clustering)

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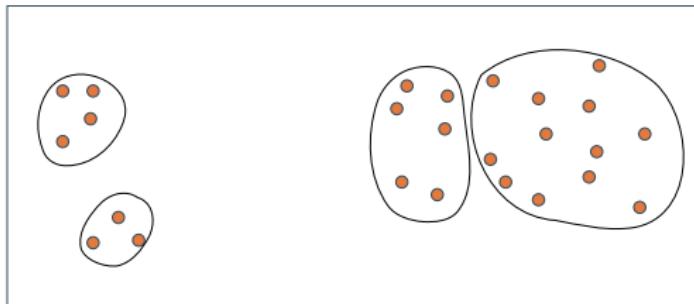
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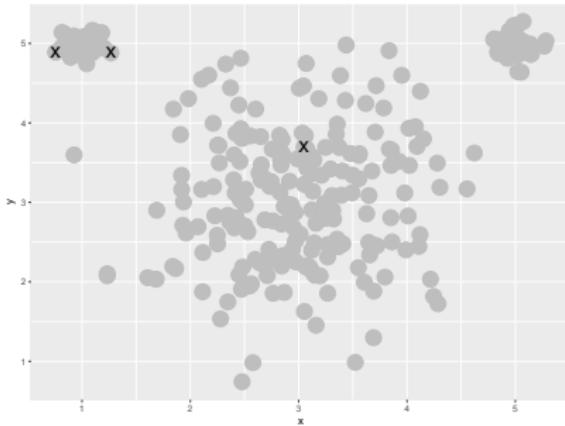
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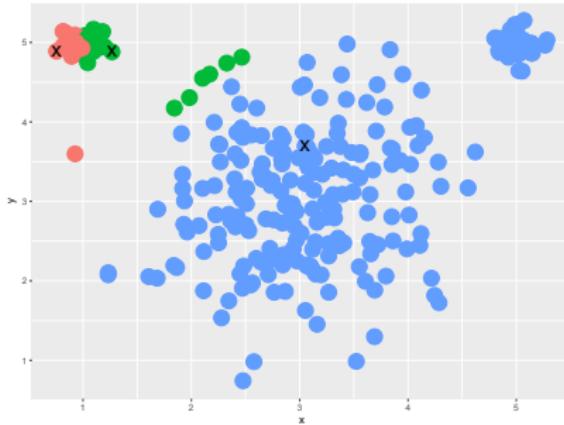
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# K-means



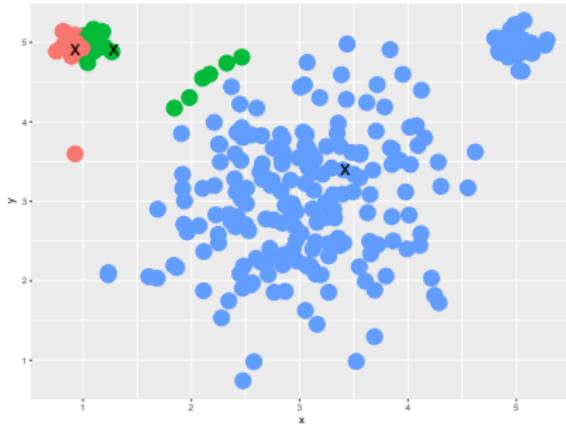
- **Initialization:** sample  $K$  points as cluster centers
- Alternate:
  1. Assign points to closest center
  2. Update cluster to the averaged of its assigned points
- Stop when no point's assignment change.

# K-means



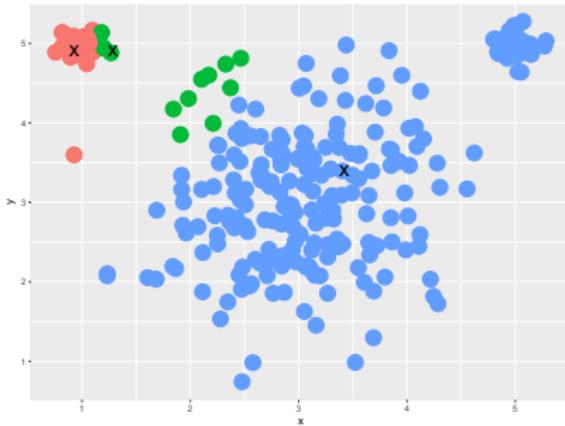
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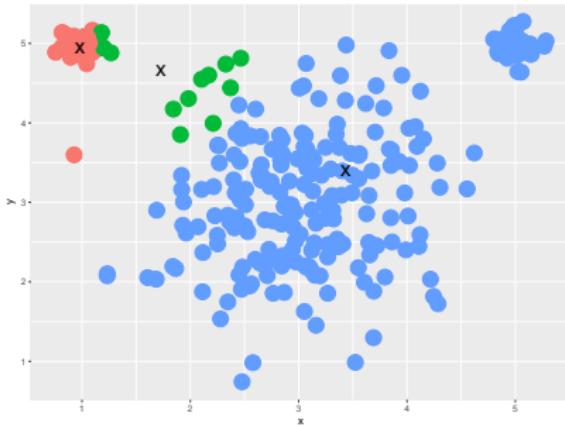
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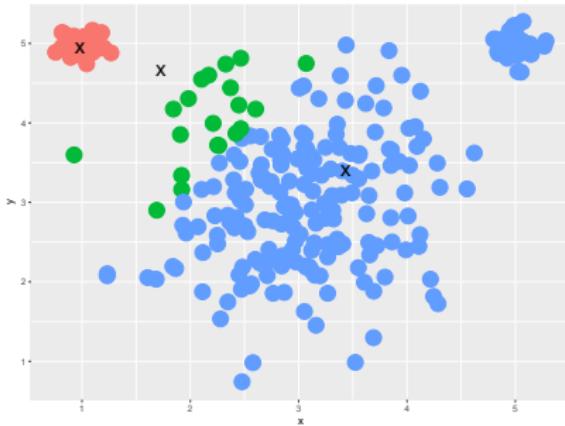
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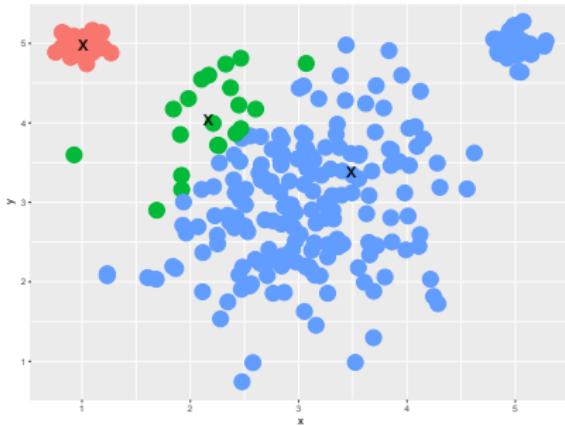
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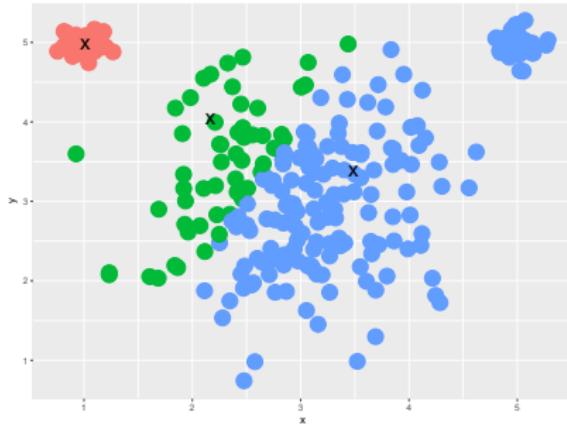
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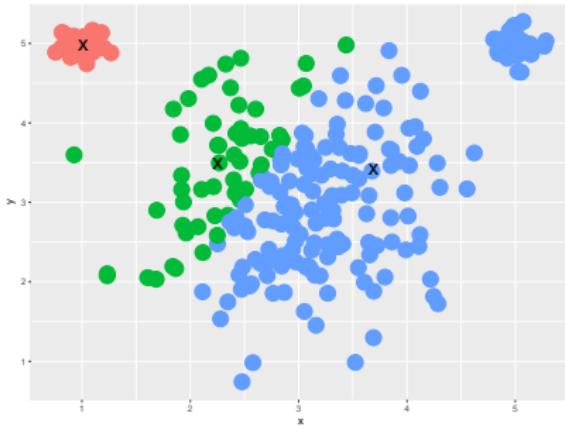
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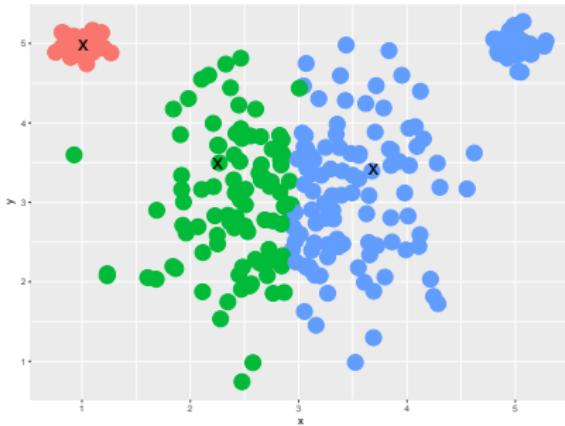
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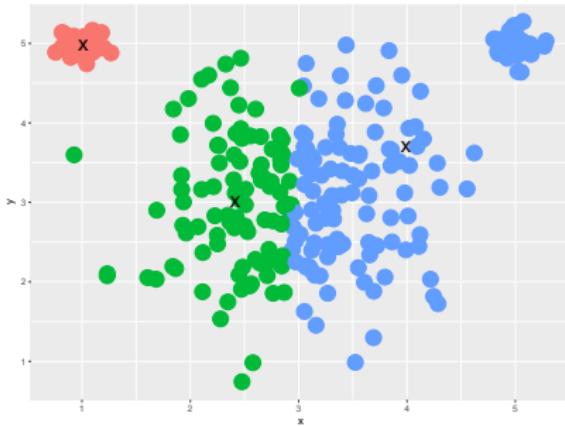
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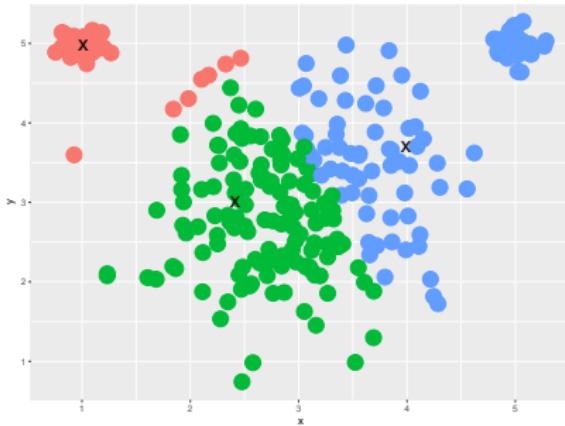
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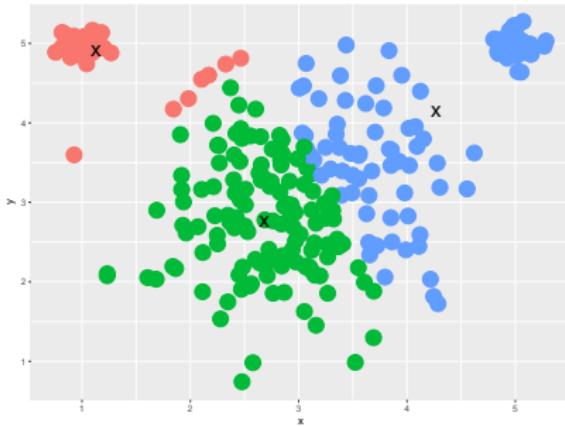
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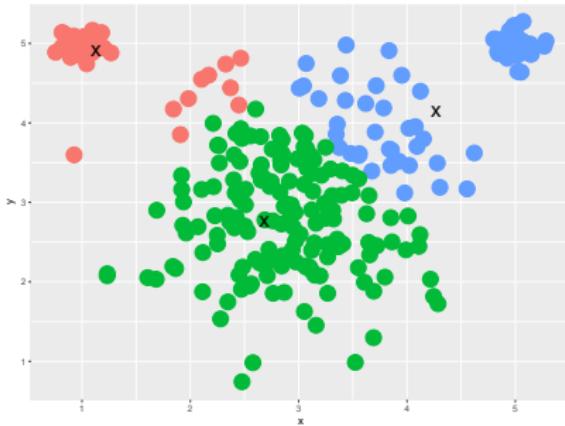
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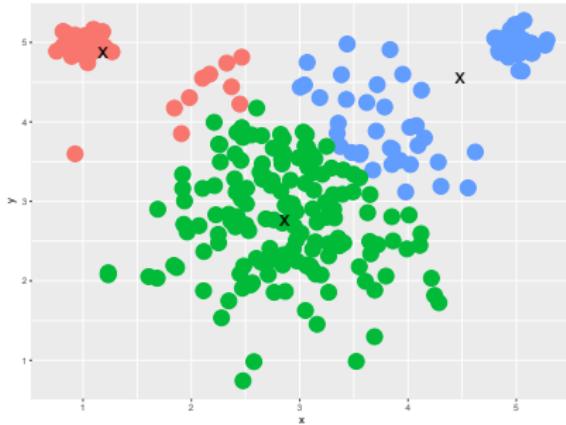
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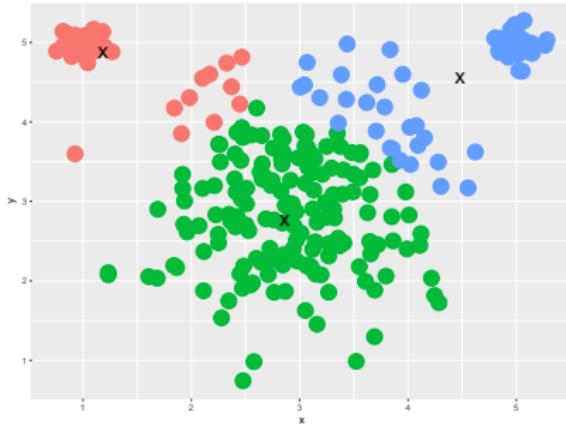
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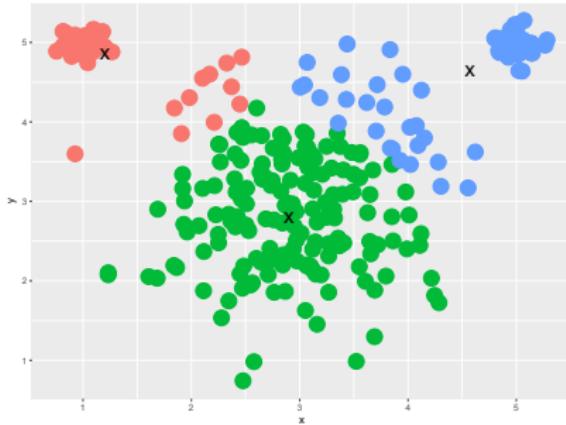
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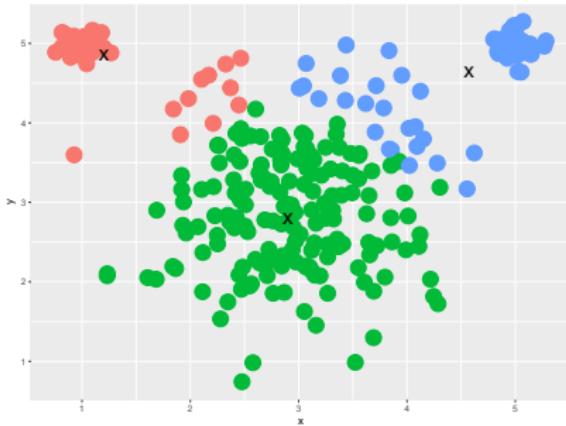
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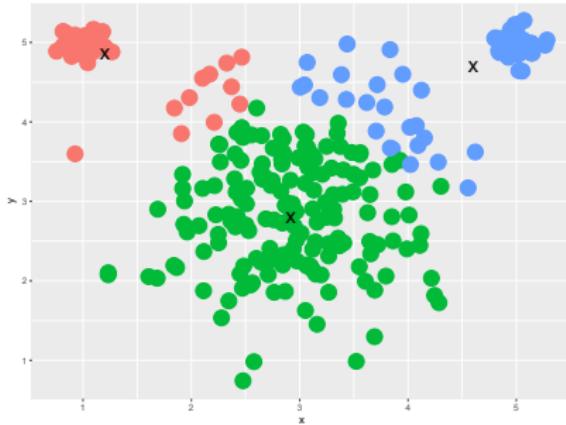
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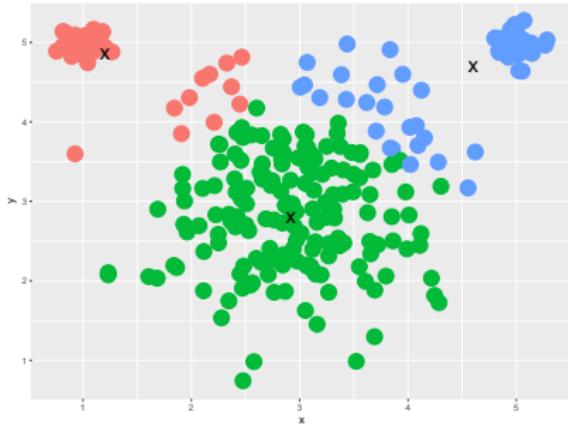
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Guaranteed to converge in a finite number of iterations.

Initialization is crucial.

## Example: Segmentation



<https://youtu.be/qWl9idsCuLQ>

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# Principal component analysis

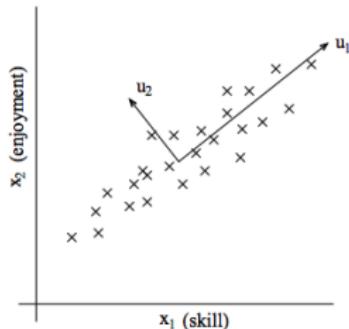
Assume that you have a data matrix (with column-wise zero empirical mean)

$$X := \begin{bmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,p} \\ \vdots & \vdots & \dots & \vdots \\ x_{n,1} & x_{n,2} & \dots & x_{n,p} \end{bmatrix}$$

If  $p$  is large, some columns (i.e., explanatory variables) may be linearly correlated.

- **bad statistical property:** risk minimization not identifiable, the covariance matrix ( $X^\top X$ ) is not invertible  $\rightarrow$  unstable estimators
- **bad computational property:** we need to store  $p \gg 1$  columns with redundant information

**PCA** reduces the  $p$  dimensions of the data set  $X$  down to  $k$  principal components.



# Principal component analysis

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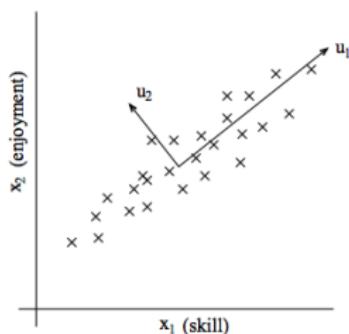
## How does it work?

1. Find the vector  $u_1$  such that the projection of the data on  $u$  has the greatest variance.

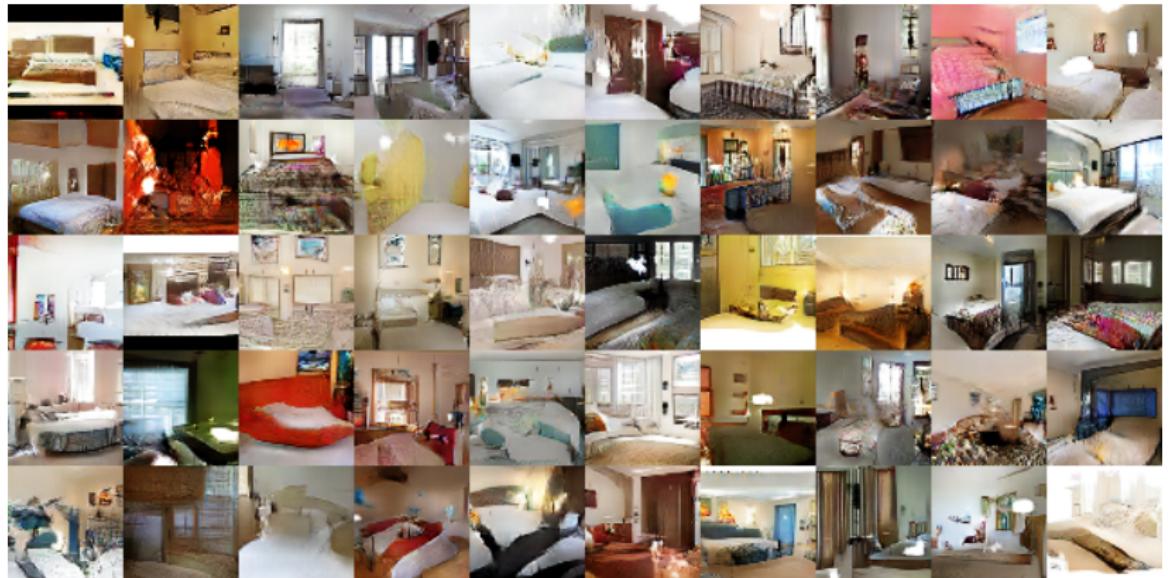
$$u_1 := \arg \max_{\|u\|=1} \|X^\top u\|^2 = u^\top X^\top X u$$

⇒ this is the principal eigenvector of  $X^\top X$ .

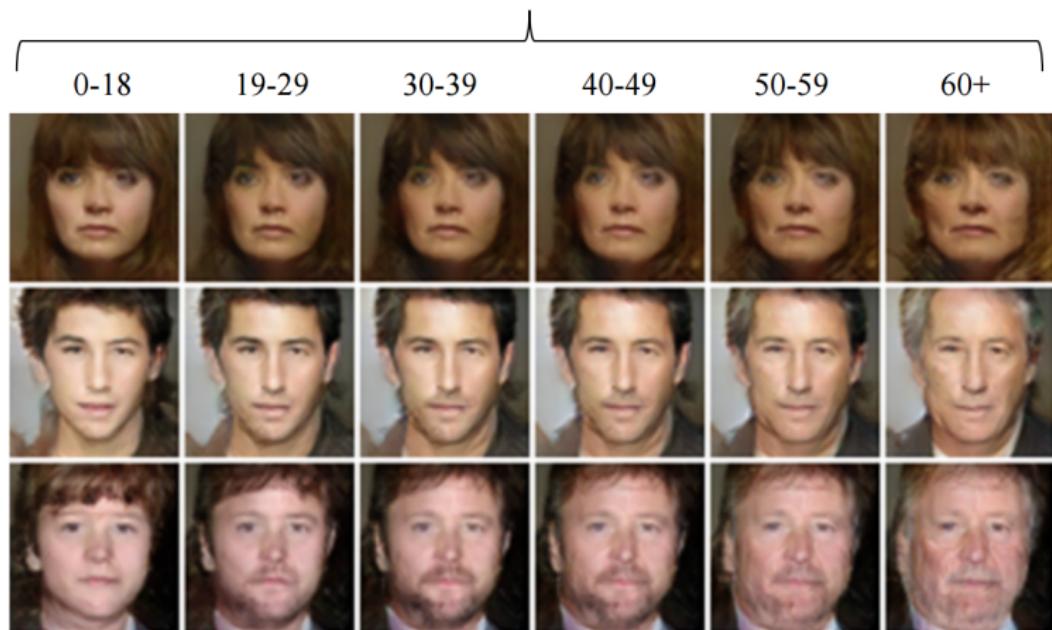
2. More generally, if we wish a  $k$ -dimensional subspace we choose  $u_1, \dots, u_k$  the top  $k$  eigenvectors of  $X^\top X$ .
3. The  $u_i$  form a new orthogonal basis of the data



# Generative Models



## Face Aging



# Generative Models

DeepBach: harmonization in the style of Bach generated using deep learning

Soprano  
Alto  
Tenor  
Bass

0:04 / 0:59

<https://youtu.be/QiBM7-5hA6o>

# Generative Models



<https://youtu.be/lcGYEXJqun8>

## **Planning of the class**

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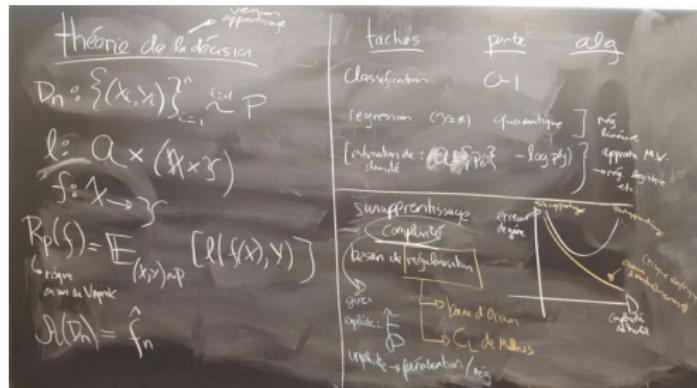
# Objective of the class

The goal of the class is to introduce the basics of machine learning. We will mix:

- **theory:** some theorems will be proved!
- **practice:** some algorithms will be implemented on real data

**Disclaimer:** at the end of the class, you will most likely not be able to reproduce all examples seen in this introduction!

Typical session will be a lecture from 8h30 to 10h20, followed by a 20min break and the practical work (PW) from 10h40 to 12h30. **2021: Online inverted classroom**



Voir <https://www.di.ens.fr/appstat/spring-2021/>

## For next week...

Prepare your personal laptops in practical sessions with python (jupyter, anaconda) working on it.

Check the crash-test Jupyter notebook:

<https://www.di.ens.fr/appstat/spring-2020/TP/TD0-prerequisites/crash-test.ipynb>

## References

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