Introduction to Machine Learning

Nicolas Keriven
CNRS, IRISA, Rennes

ENSTA 2024

The presenter

Nicolas Keriven

- 2010-2014 : Ecole polytechnique (X10), Master MVA
- 2014-2017 : Ph.D. at Inria Rennes
- 2017-2019 : Post-doc at ENS Ulm
- 2019 : Chargé de Recherche CNRS at Gipsa-lab, Grenoble
- 2023 : join IRISA, Rennes

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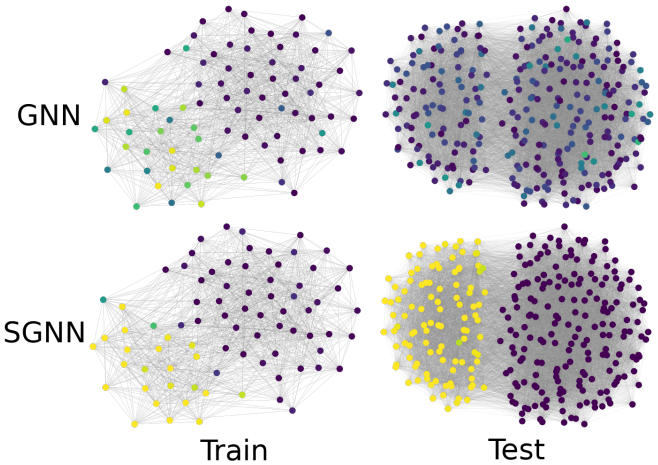
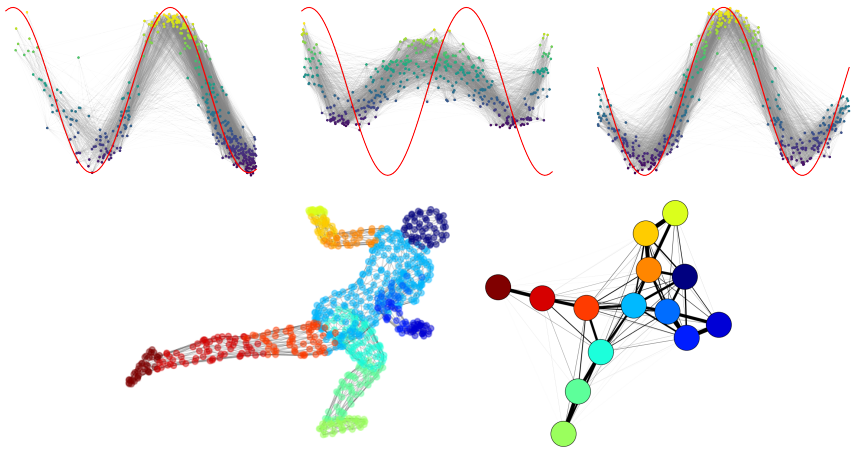
- 2023 : join IRISA, Rennes
- Research interest : ML theory, dimensionality reduction, Graph ML, Graph Neural Networks





Organization

- $8 \times 3h$ lecture and practices sessions

	17/02	18/02	19/02	20/02	21/02
09h30-12h45	Intro	Linear models + Regul.	Clustering	Time series, RL and RNN	Adv. Deep Learning + Exam. QCM
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Objectives

- Understand the theoretical basis of data science/machine learning/AI
- Implement/apply data science algorithms and models using classical frameworks
- Learn how to learn : (of course) not exhaustive, and somewhat subjective !

The material

- Slides (pdf) and notebooks available here :
  `https://github.com/nkeriven/ensta-mt12`

- Jupyter notebooks are available to illustrate concepts and methods in Python (.ipynb files)

- Notebooks can be run remotely on Google Colab

Part of this material is from previous years' presenters, Florent Chatelain (McF, GIPSA-lab) and Olivier Michel (CNRS, GIPSA-lab).

Reference books


Christopher M. Bishop (2007) Pattern Recognition and Machine Learning *Springer*


Kevin P. Murphy (2012) Machine Learning. A Probabilistic Perspective *MIT Press*


Shai Shalev-Schwartz, Shai Ben-David (2014) Understanding Machine Learning : From Theory to Algorithms *Cambridge University Press*


Francis Bach (2021) Learning Theory from First Principles Draft

Supplementary materials, datasets, online courses, ...


`https://www.coursera.org/course/ml` *very popular MOOC (Andrew Ng)*


`https://work.caltech.edu/telecourse.html` *more involved MOOC (Y. Abu-Mostafa)*


`https://scikit-learn.org/stable/auto_examples/index.html` **Doc from the sklearn library**


`https://huggingface.co/` **Treasure trove of open models, datasets, tutorials...**

Many (many) more material online, learn how to find it, interpret it, use it !
Always with a grain of salt

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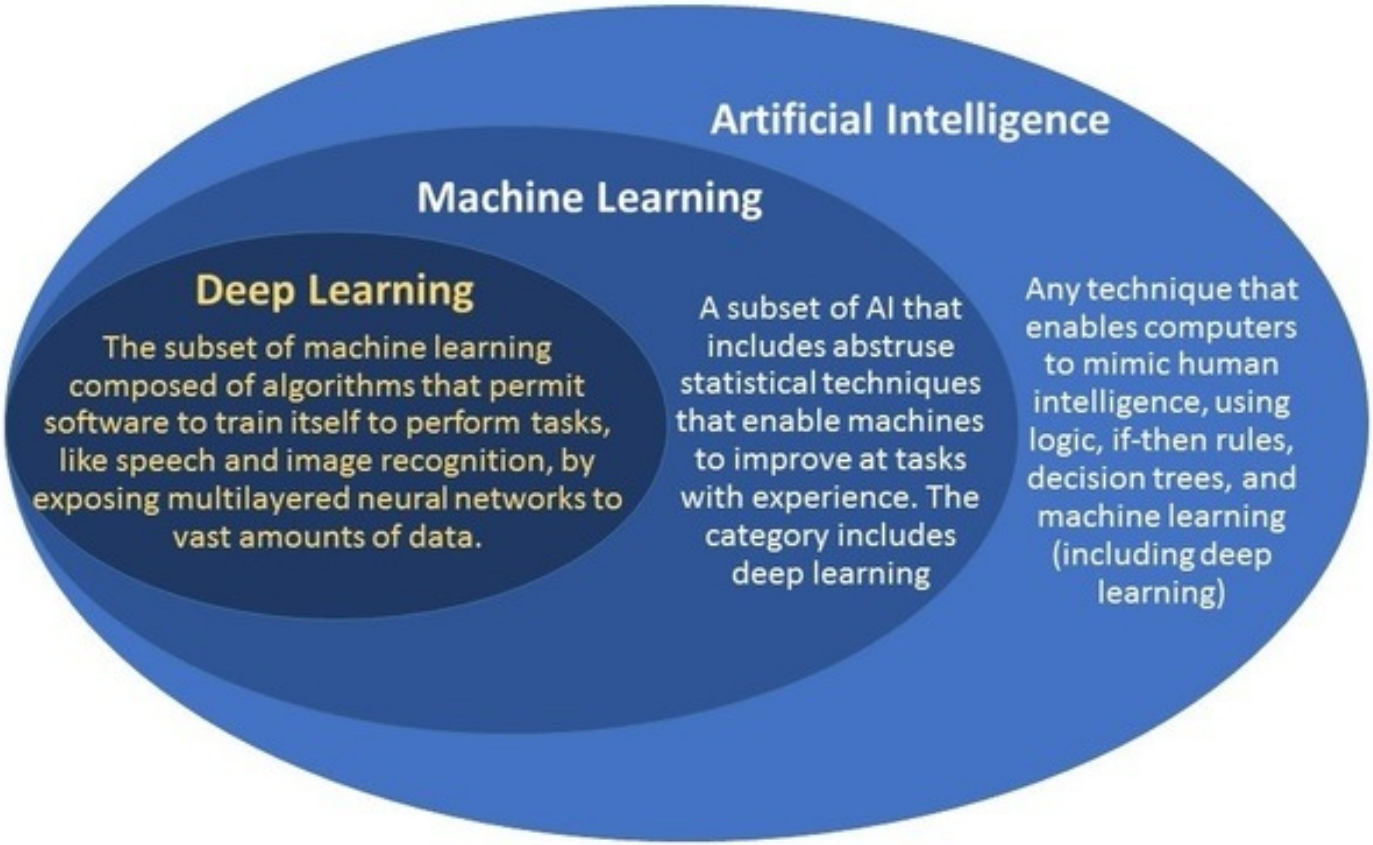
Machine Learning ⊂ Artificial Intelligence

A (simplified) picture...



Data Science Objective

A (simplified !) picture...

Objective of ML/Data Science

- How to extract knowledge or insights from data ?
- How to use it to solve real-life problems ?

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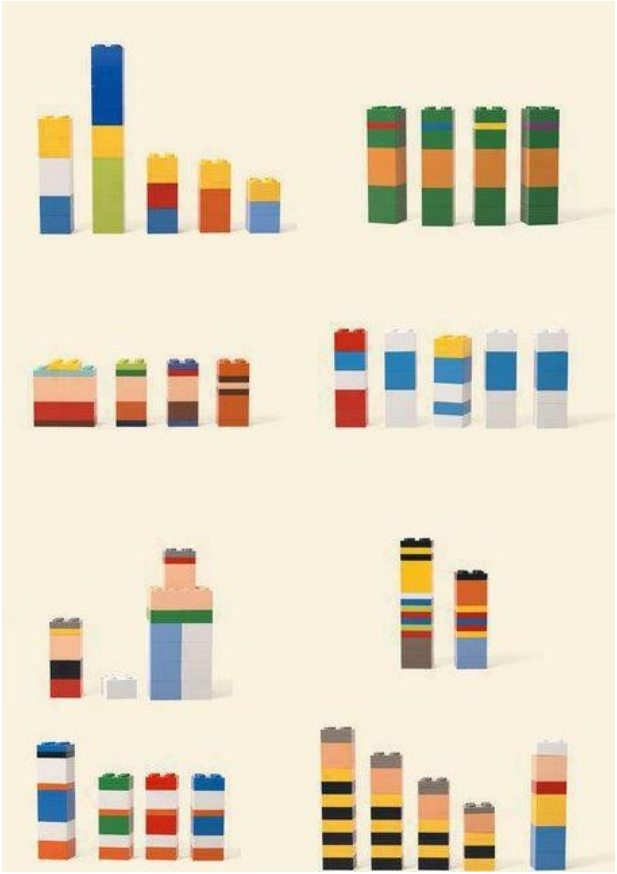
ie, you do a linear regression in Excel/Python (nothing wrong with that !), you sell it to investors as "Artificial Intelligence"

The vocabulary is not so important

Learning problem

Often a problem of discovering/learning relevant features, and making "sense" of them...



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Definitions of Learning

Machine Learning in Computer Science

Tom Mitchell (The Discipline of Machine Learning, 2006)

A computer program CP is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

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Key points

- Experience E : data and algorithms
- Performance measure P : mathematical loss function... or intuitive observation !
- tasks T : utility
  - classifying pictures (not easy)
  - automatic translation (hard)
  - playing Go (very hard)
  - ... doing what human does (what does that even mean ?)

Experience E : the data !

Type of data : qualitatives / ordinales / quantitatives variables

text	strings
speech	time series
images/videos	2/3d dependences
networks	graphs
games	interaction sequences
	...

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Too much data ?

Data are available "in the wild" but...

- importance of preprocessings (cleaning up, normalization, coding,...) Data preparation is a science in itself !
- importance of a good representation : from raw data to (usually) vectors

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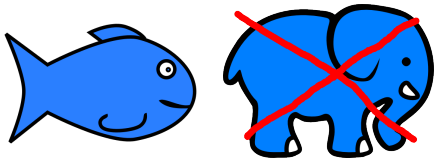

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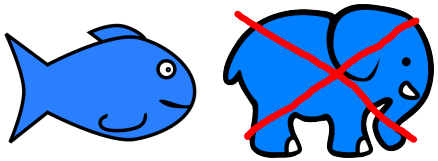

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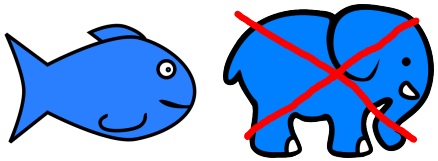

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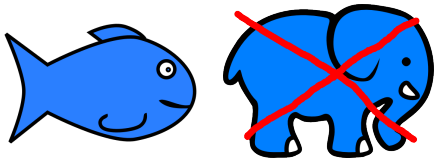

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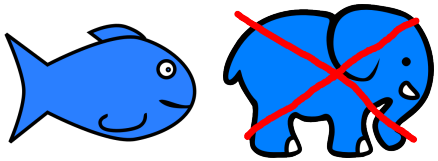

Generalization

- Perform well (minimize P) on new data (fresh data, i.e. unseen during training)

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Classification vs regression

Variable terminology

"Most often" :

- **observed data** called input variables, predictors or features, usually x
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Type of prediction problem : regression vs classification

Depending on the type of the output variables y

- quantitative data (continuous, e.g. age, height) : regression
- categorical data (discrete variables, e.g. cat/dog) : classification

Two very close problems. Many hybrid/not-as-easity-categorized tasks !

Training, testing, generalization

- Training set : labelled data $(x_1, y_1), \ldots, (x_n, y_n)$

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- "Learning" : deriving a function of prediction / rule of classification $\hat{f} : \mathcal{X} \to \mathcal{Y}$ using only the training data
- Generalization : obtaining a good performance on test data

Three main categories of ML

- Supervised learning : $\mathcal{T} = ((x_1, y_1), \ldots, (x_n, y_n))$ input/output couples are available to learn.
  - Goal : **Predict** y **on a new** x.
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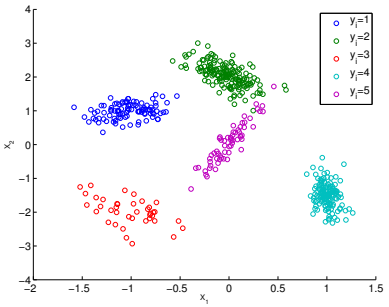

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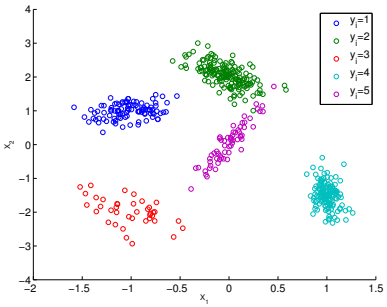

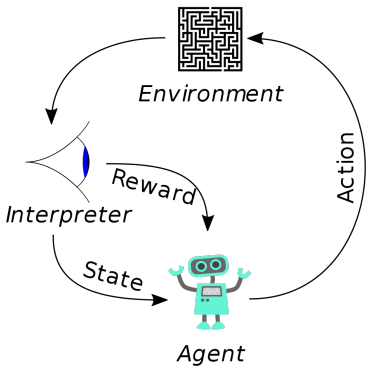

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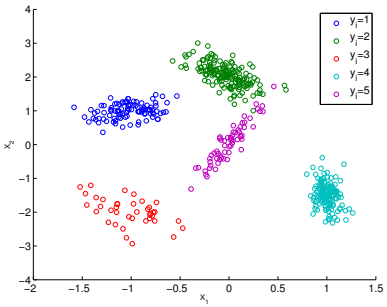
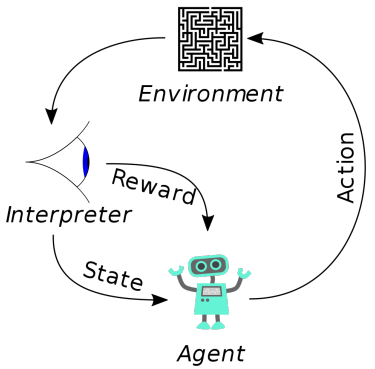
- Generative modelling : generally (...) unsupervised
  - Goal : **produce samples from a distribution**.
  - Ex : generate new interesting molecules...





Many variants/overlap

- Semi-supervised : some training data are labelled, some are unlabelled. Exploit both during training. → **Labelled data is expensive, unlabelled is cheap !**
- Transfer learning : use features from other tasks (pre-trained/foundational models).
- Self-supervised : unsupervised methods are used to produce "labels" used in downstream supervised training (often, go back and forth).
- etc, etc

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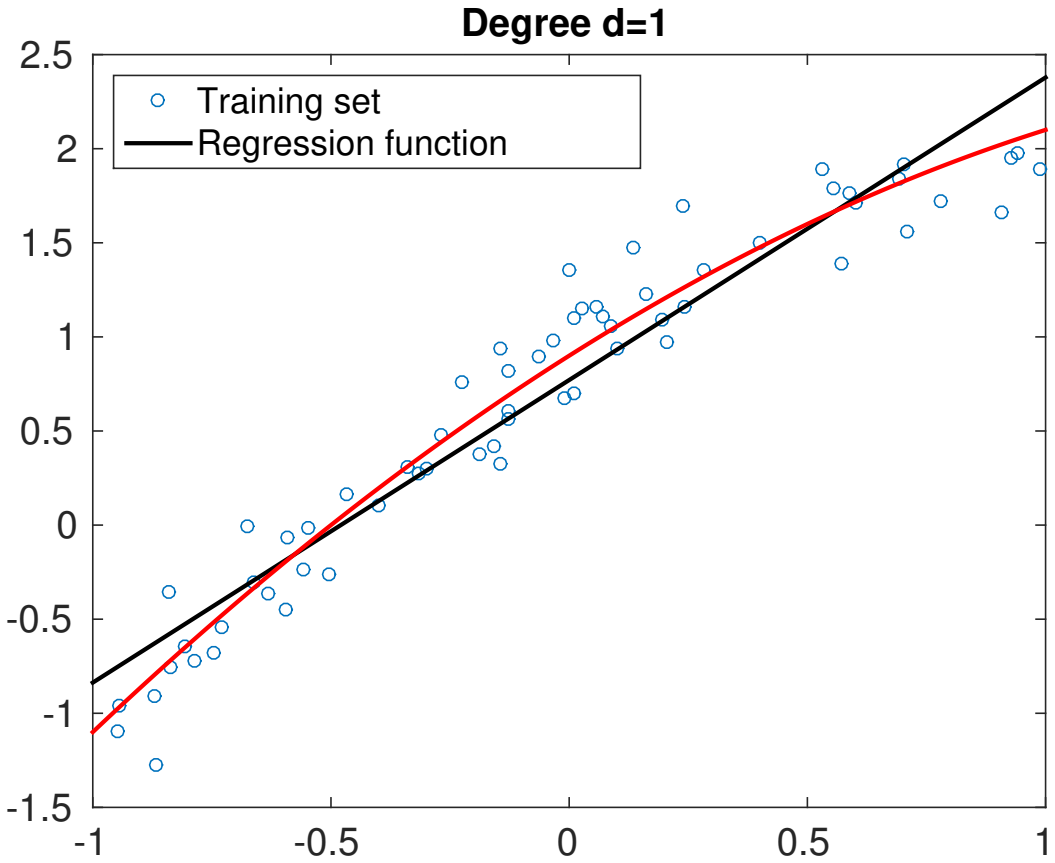
Linear regression

Fit an affine line to the data :



Linear regression

The prediction rule is :

$$\hat{f}(x) = f_{\beta,b}(x) = \beta^\top x + b$$

where $\beta \in \mathbb{R}^d$, $b \in \mathbb{R}$ are unknown parameters.

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Learning problem $\Leftrightarrow$ Estimation of β, b

Done by *minimizing* the "empirical risk" on the training data

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for some loss function L.

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- Least-Square :

$$L(\hat{y}, y) = (\hat{y} - y)^2$$

One of the most classical choice for regression.

- NB : in this case, β, b have an explicit expression. It is generally not the case, and they must be found with optimization algorithms like gradient descent.

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$$\hat{y} = \begin{cases} +1 & \text{if } \hat{f}(x) \geq 0 \\ -1 & \text{if } \hat{f}(x) < 0 \end{cases}$$

- Black solid line is the decision boundary $\hat{f}(x) = \beta^\top x + b = 0$.

Example of a binary classification problem in $\mathbb{R}^2$.

Parametric classification : simple linear model

We still use the empirical risk approach

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- Least-Square : $L(f(x), y) = (f(x) - y)^2$ makes more "sense" for regression, but still give reasonable results.
- Logistic-Regression : transform $f(x)$ into a probability that $y = 1$

$$p(x) = \frac{1}{1 + e^{-f(x)}} \in [0, 1]$$

such that $p(x) \to 1$ when $f(x) \to \infty$, and $p(x) \to 0$ when $f(x) \to -\infty$.Then, use the negative log-likelihood of a Bernoulli variable that takes value 1 with probability $p(x)$ (see later) :

$$L(f(x), y) = \begin{cases} -\log p(x) & \text{if } y = 1, \\ -\log(1 - p(x)) & \text{if } y = -1 \end{cases}$$

or, more succintly, $L(f(x), y) = \log(1 + e^{-yf(x)})$

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Parametric vs. non-parametric

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  - Linear models
  - Discriminant analysis
  - Neural networks, etc.

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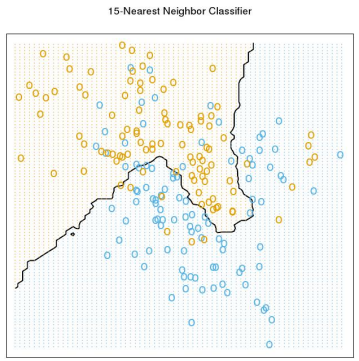
- Some algorithms are non-parametric : the number of "parameters" to learn depend on the number of samples in the training set
  - k-NN (just after)
  - Decision tree (not in this course)
  - Kernel methods



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☞ the number of neighbors k is an *hyperparameter* of the algorithm : its value must be fixed (positive integer) prior to applying the algorithm.

k-NN : remarks

- "Closest" depend on a notion of distance (metric) between points $d(x, x')$. Euclidean distance $\|x - x'\|$ is a classic choice, but many other exist depending on the type of data (tabular, text, images, etc.)

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Linear Reg. (naive)	$O(nd^2 + d^3)$	$O(n'd)$
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- k-NN can be (very) costly for big datasets, there are *numerous* ways of accelerating it : trees to compute approximate distance (not lazy anymore !), dimension reduction, sketching...

Nadaraya-Watson estimator

- Idea : Instead of taking the k-closest samples, take all samples, but with a weighted average, where the weights are lower for points that are far :

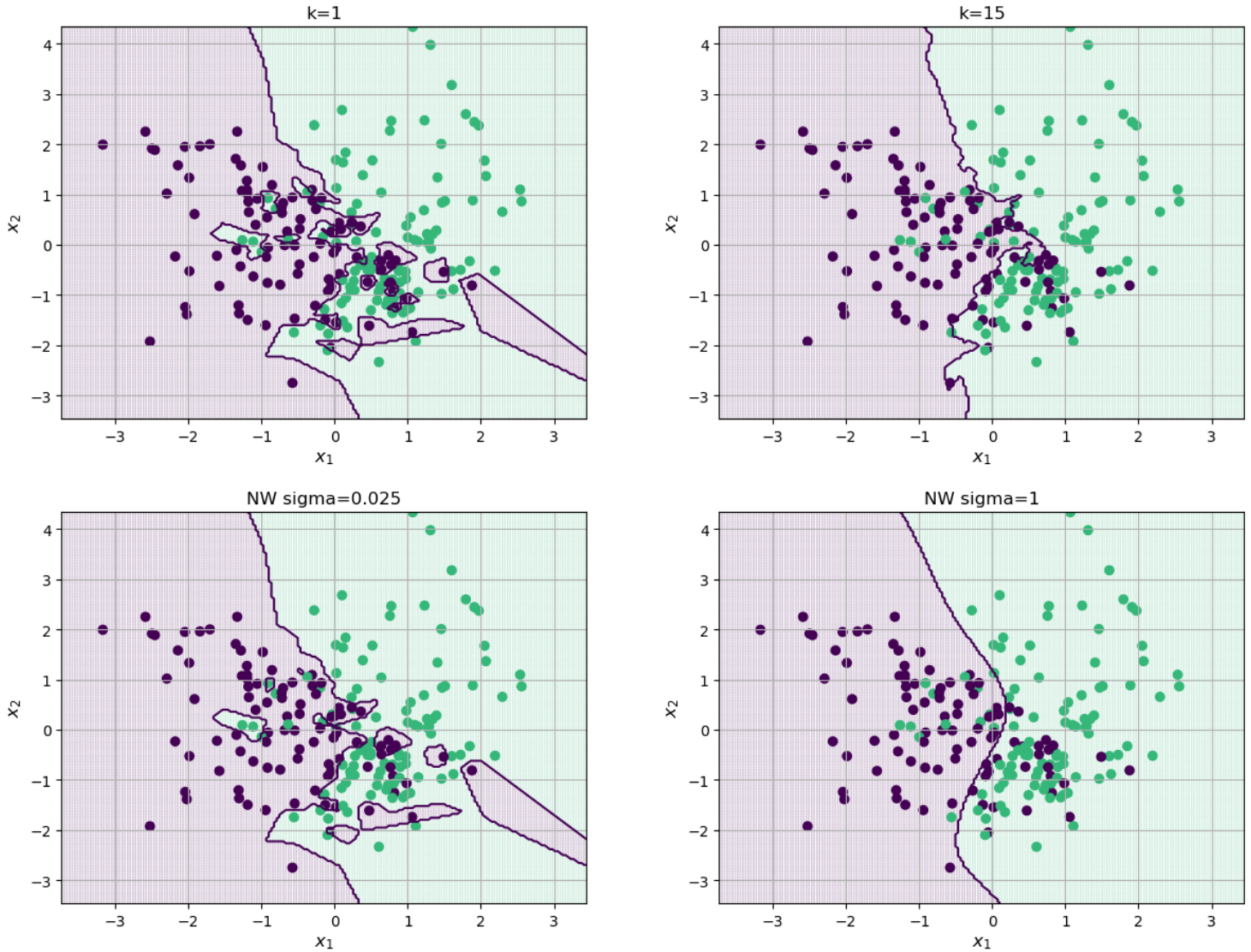
$$f_{NW}(x) = \sum_{i=1}^{n} w_i(x) x_i \text{ with } \sum_i w_i(x) = 1$$

for classification : $\hat{f}(x) = 1$ if $f_{NW}(x) \geq 0$.

- $w_i(x)$ are generally defined through a kernel function $k_\sigma(x, x_i)$ that decreases with the distance between points, which is then normalized. Eg Gaussian

$$k_\sigma(x, x_i) = e^{-\frac{\|x - x_i\|^2}{2\sigma^2}}, \quad w_i(x) = \frac{k_\sigma(x, x_i)}{\sum_{j=1}^{n} k_\sigma(x, x_j)}$$

K Nearest-Neighbors vs NW



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Empirical Risk Minimization (ERM) : a systematic approach

- Parametric model : seek a function $f_\theta(x)$ parametrized by $\theta \in \Theta$ such that $y \approx f_\theta(x)$ (for regression), or $yf_\theta(x) \gg 0$ (for classification)
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- Generally done through a loss function $L : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_+$. The ultimate goal is to minimize the expected risk (expected error, generalization error...) :

$$\mathcal{R}(\theta) = \mathbb{E}_{(x,y)} L(f_\theta(x), y)$$

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  where the expectation is taken over the joint distribution of (x, y). This ensure good generalization (theoretically, the best possible).
- Since the true expectation is not known in practice, we use the empirical risk over the training data (training error) :

$$\hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_i L(f_\theta(x_i), y_i)$$

  - if (x_i, y_i) are independently and identically distributed (i.i.d.), the expected risk and empirical risk are "close" (law of large numbers)

Loss functions

- $L(f(x), y)$ is often of the form $L(f(x) - y)$ for regression and $L(yf(x))$ for (binary) classification

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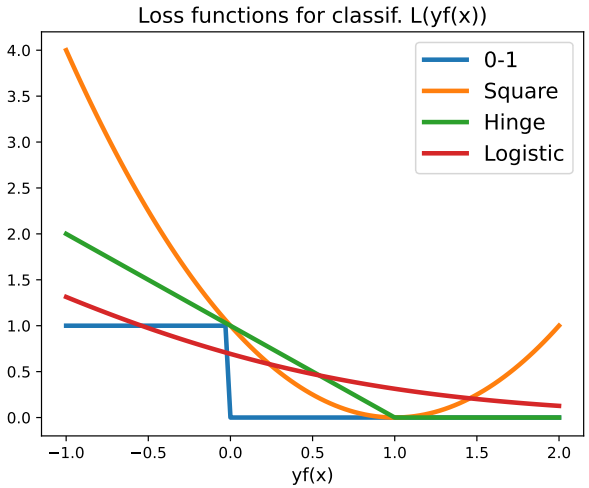
Binary classification

- 0-1 loss : $1_{yf(x)>0}$. "Ideal" in some sense, but combinatorial and NP-hard to optimize.
- Square loss : $(1 - yf(x))^2$. Easy to optimize, but not very natural for classification.
- Logistic loss : $\log(1 + e^{-yf(x)})$. Very popular (in particular for multiclass classif.), also called "Cross-entropy"
- etc. `https://en.wikipedia.org/wiki/Loss_functions_for_classification`



Exercise : True error rate

Consider a binary classification problem $y \in \{0, 1\}$ with scalar data $x \in \mathbb{R}$. The $0-1$ loss gives the misclassification probability :

$$\mathcal{R} = \mathbb{E}_{x,y}(1_{f(x)\neq y}) = \mathbb{P}(f(x) \neq y)$$

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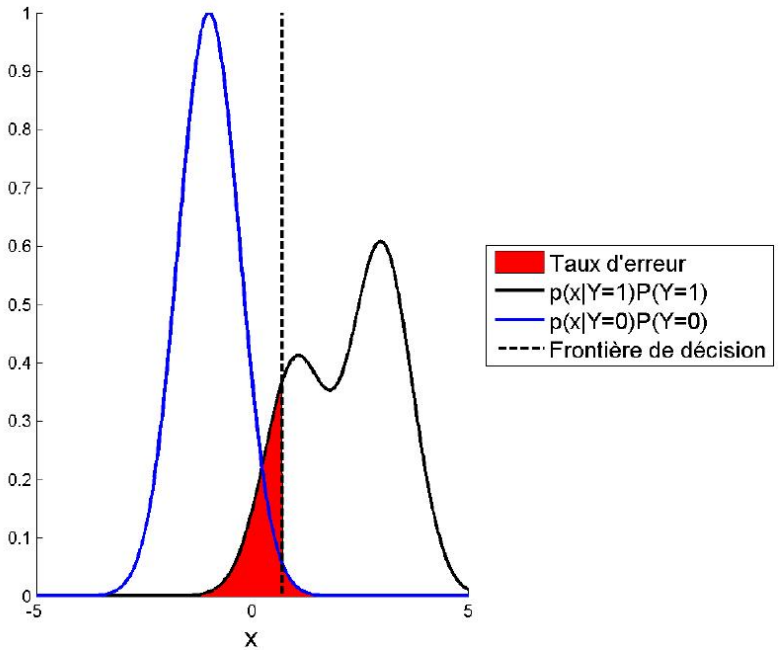
$$\mathcal{R} = \mathbb{E}_{x,y}(1_{f(x)\neq y}) = \mathbb{P}(f(x) \neq y)$$

For a prediction rule $f(x) = 0$ if $x \leq t$, 1 otherwise, where t is a given threshold, and based on the

- class weights $\Pr(y = 0)$, $\Pr(y = 1)$
- class pdf's $p(x|y = 0)$, $p(x|y = 1)$

how can we compute the misclassification probability ?



The optimal classifier for the $0-1$ loss is called the Bayes classifier (see next session).

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Optimization

How to find the minimum $\min_\theta \hat{\mathcal{R}}(\theta)$?

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- This is done through optimization algorithms.
  - Optimization is at the core of modern ML !
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Optimization

How to find the minimum $\min_\theta \hat{\mathcal{R}}(\theta)$?

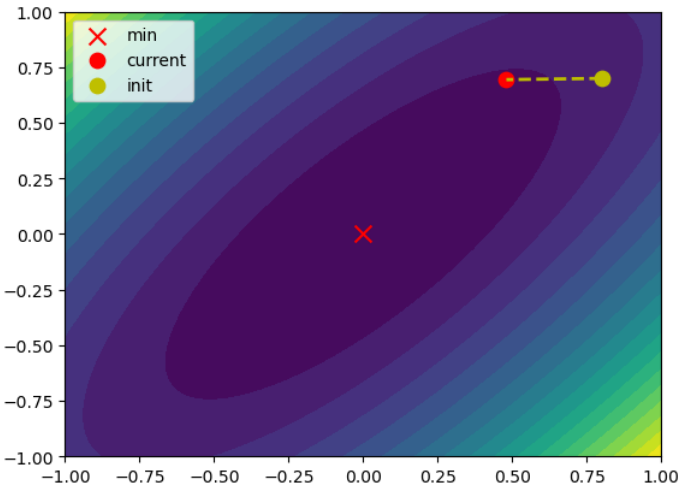
- This is done through optimization algorithms.
  - Optimization is at the core of modern ML !
  - The computational load ("GPU war") is vastly due to training through optimization.
- Overwhelmingly, the dominant approach is gradient descent (and its billions of variants). It is an iterative algorithm that start with some $\theta^{(0)}$ and take a step at each iteration in the direction of steepest descent :

$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla_\theta \hat{\mathcal{R}}(\theta^{(t)})$$

Gradient descent

$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla_\theta \hat{\mathcal{R}}(\theta^{(t)})$$

Quadratic example : $f : x \mapsto x^\top \Sigma x$



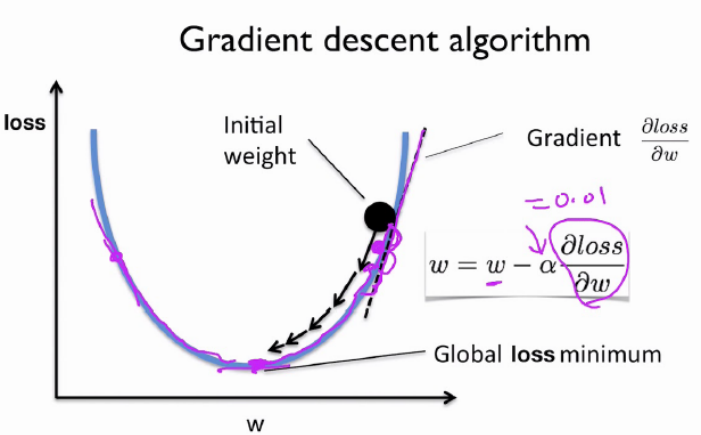
Remarks

- Modern AI is largely due to the fact that nowadays (Python) libraries can compute gradient automatically through "auto-differentiation". This can be done extremely efficiently with GPUs.

```
import torch
theta = torch.tensor(something, requires_grad=True)
loss = f(theta) # some function f using only basic operations
loss.backward() # compute the gradient by backprop
theta.grad # contains the gradient

```

- Most of the theory applies to convex optimization. Non-convex optimization is "not supposed to work", but it "does" for modern neural networks. It is still very mysterious !



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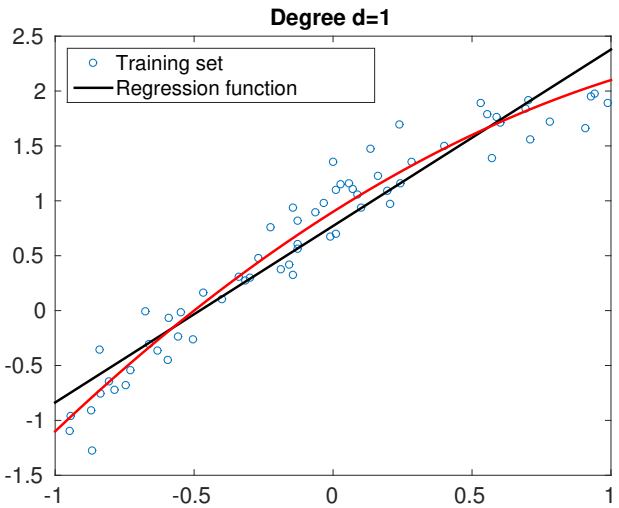
Simple linear model classification

A major problem in ML is choosing the function class/hyperparameters of the model.
For instance, consider the linear regression problem



- Is there a room for improvement of the classification performance ?

Feature engineering

One simple idea is to compute more features, and apply again a linear model in higher dimension.

Linear regression : model order p

E.g. qth degree polynomial regression : $p = q + 1$ parameters β_k s.t.

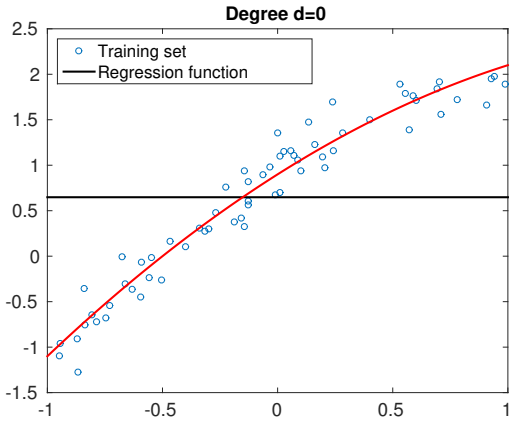
$$\hat{f}(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_q x^q = x_q^\top \beta$$

where

$$x_q = \left[1, x, x^2, \ldots, x^q\right],$$
$$\beta = [\beta_0, \beta_1, \beta_2, \ldots, \beta_q]$$

Linear regression : complexity vs stability

How to choose q ?



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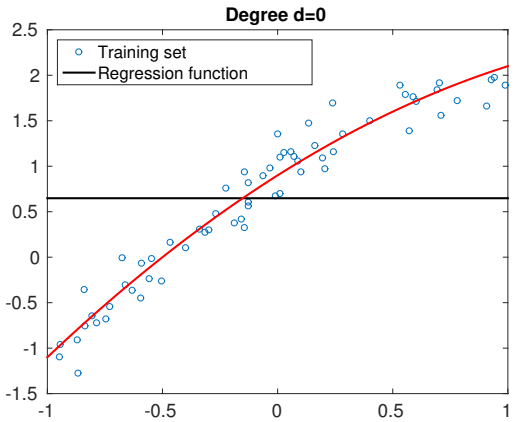

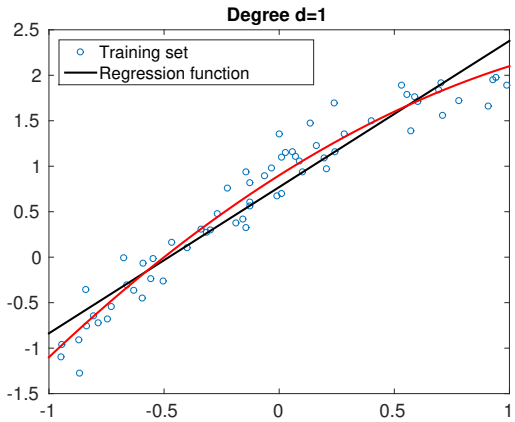

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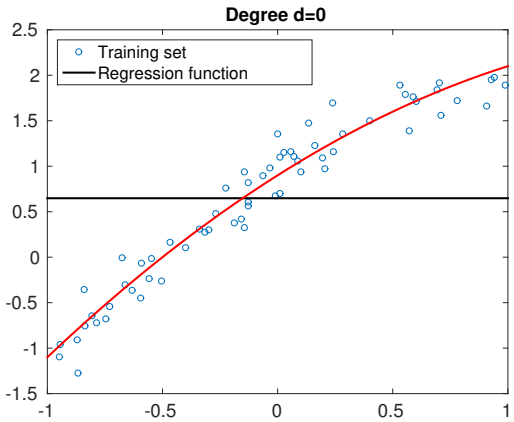

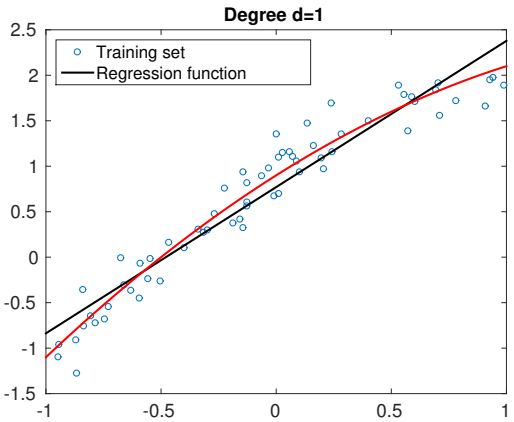

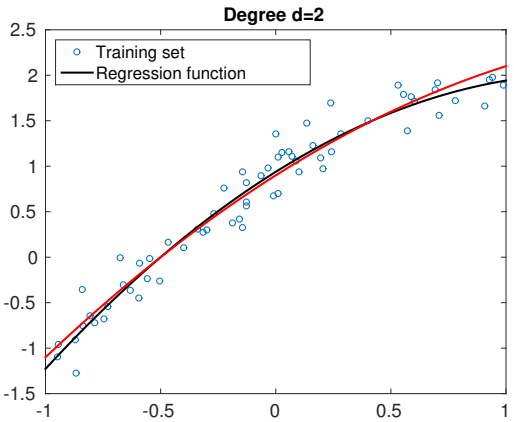

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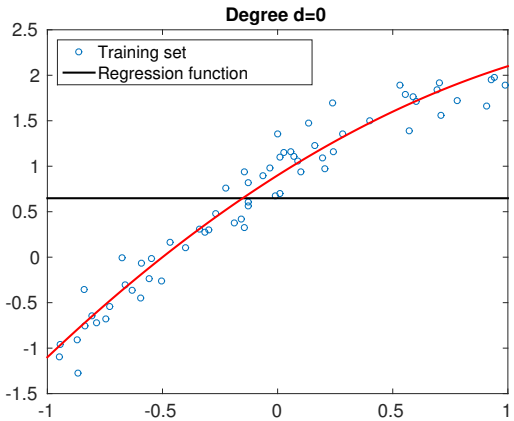

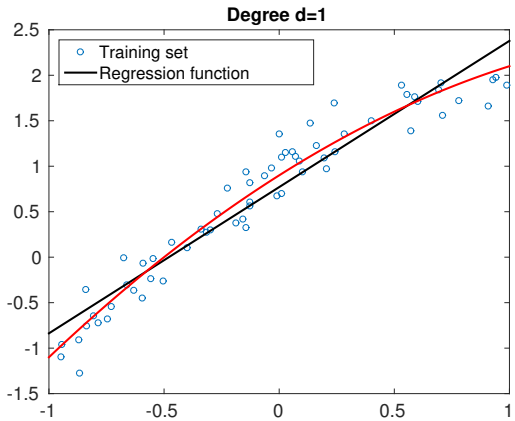

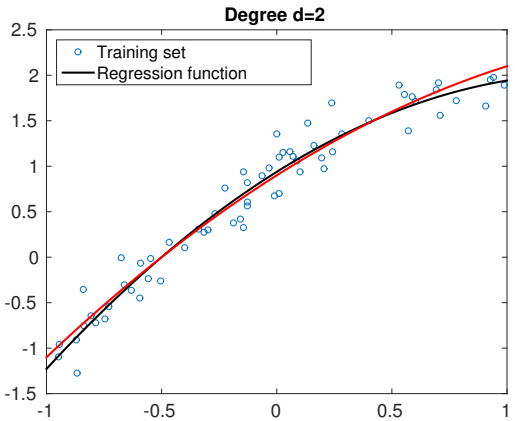

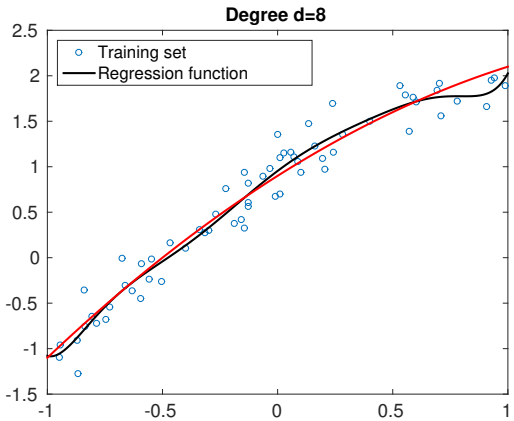

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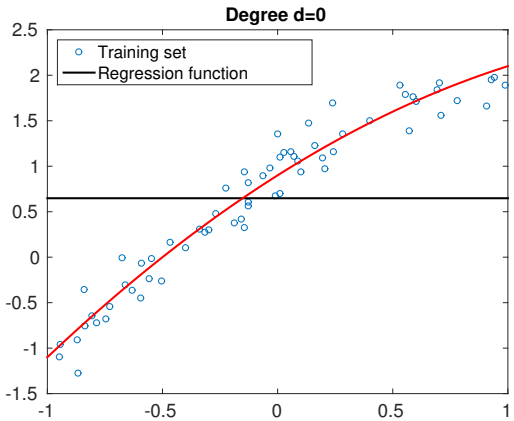

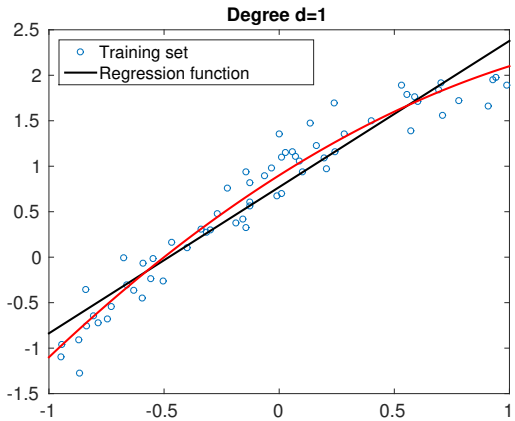

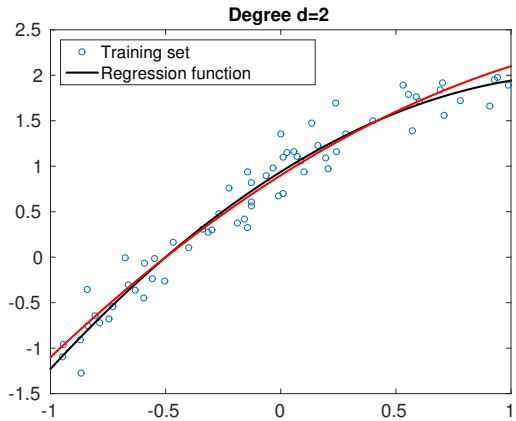

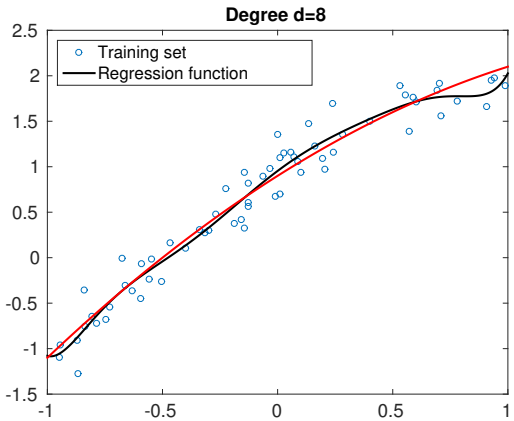

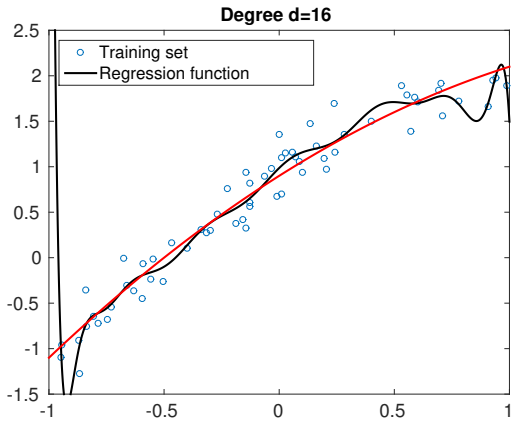

Linear regression : complexity vs stability

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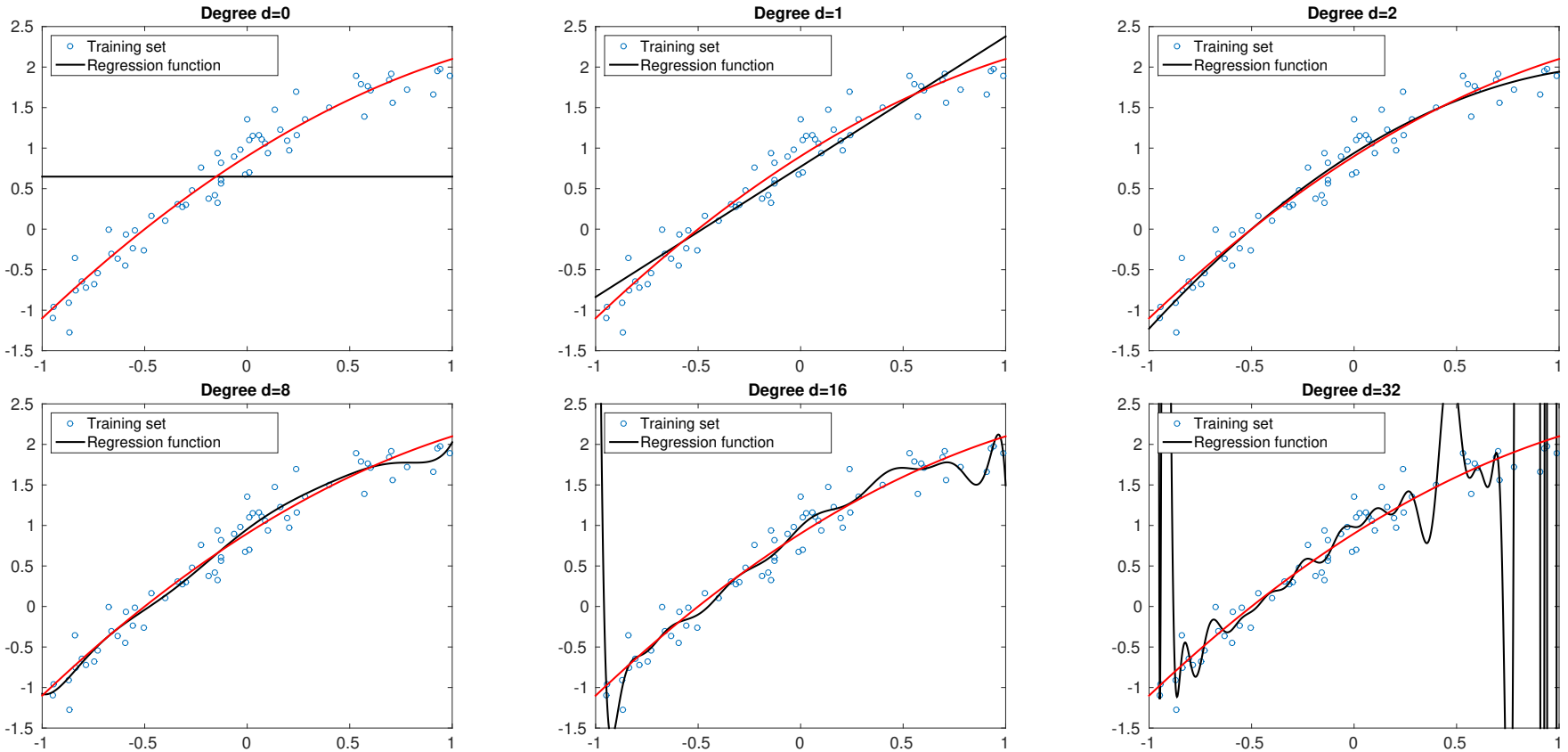
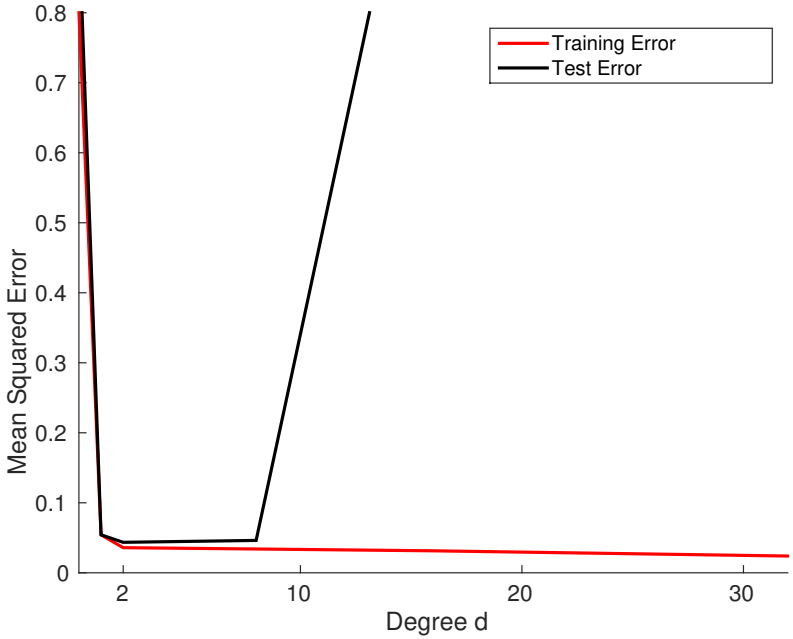


Linear Regression : Test error vs Train Error

When q increases, the training error descreases, but the test error increases. This is the over-fitting phenomenon : the model fits "too much" the training data, and generalizes poorly.

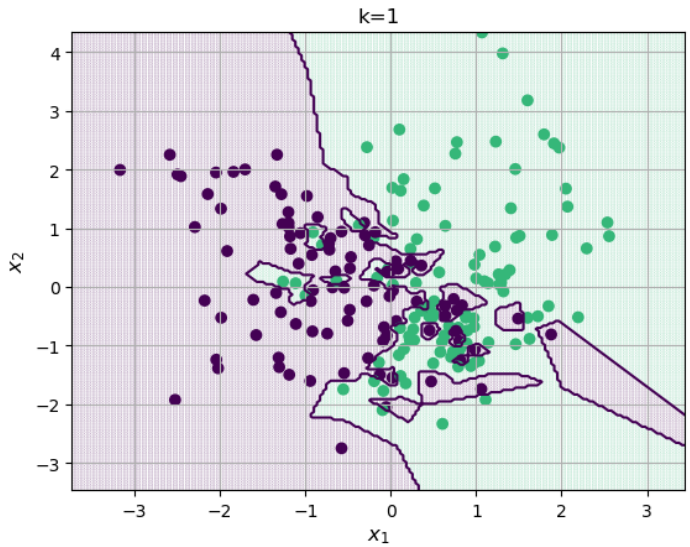


- True error rate (i.e. error rate for test data not used for learning) minimized when $q = 2$ ...
- ... true generative model : order $q = 2$ polynomial (+ white noise)

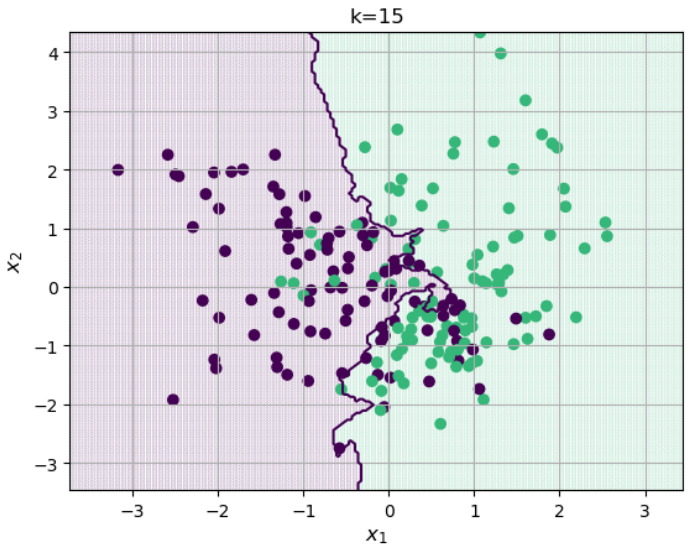
☞ One cannot use the training error to select the model !

Model Selection : under/over-fitting tradeoff

Is it also true for non-parametric models like k-NN ?
Recall the pictures



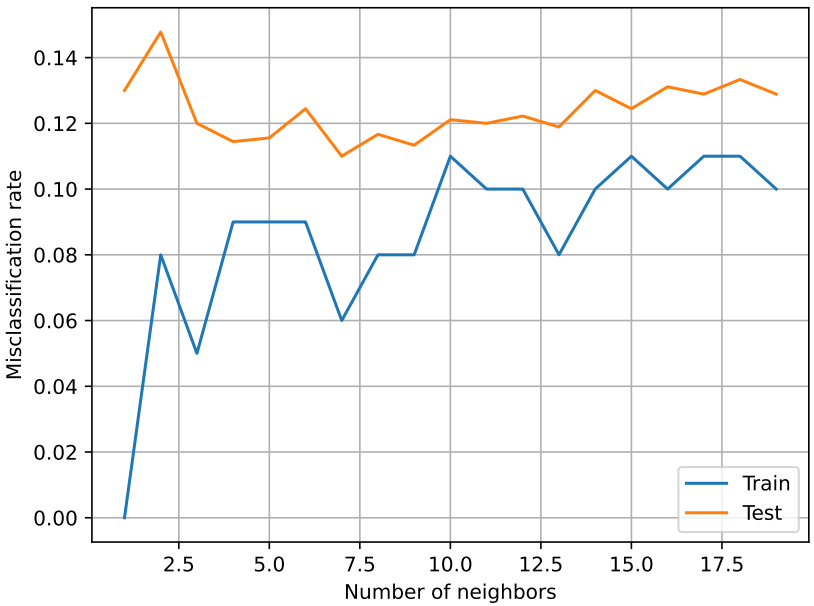
$k = 1$



$k = 15$

- $k = 1 \rightarrow$ training error is always 0 ! Explain why.
- Question : in your opinion, which one gives the best classification rule ?

k-NN : train vs test



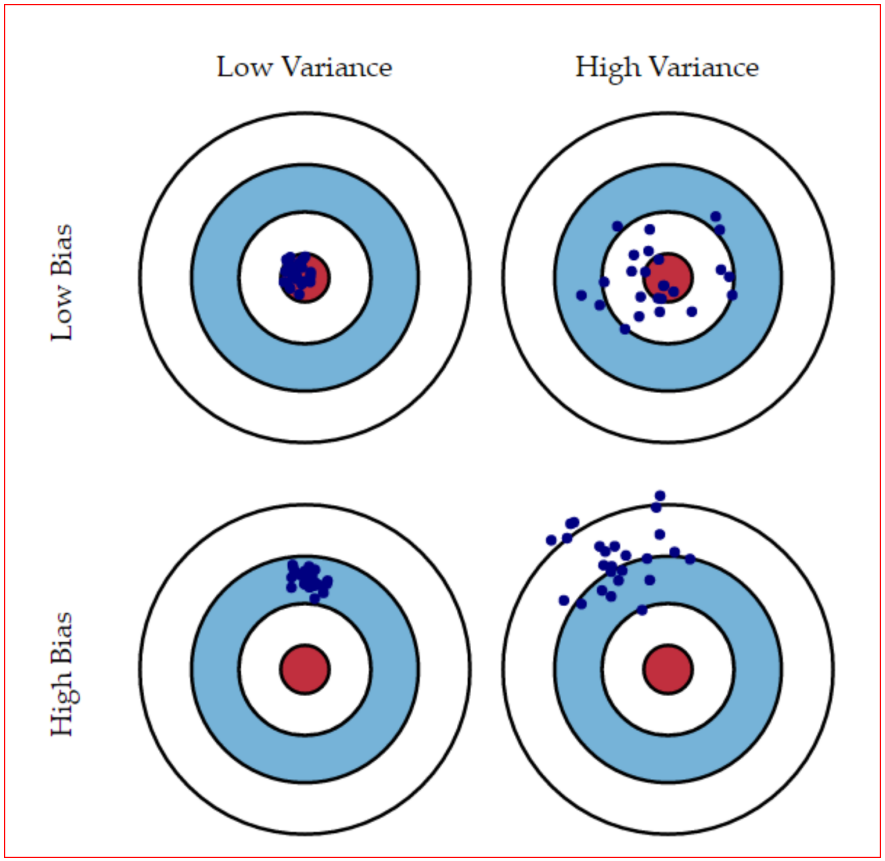
Train and test error (misclassification rate) vs the flexibility of the k-NN algorithm

- when $k = 1$, the model becomes too flexible ← over-fitting
- when k is large, the model becomes too simple ← under-fitting
- $k = 7$ is the optimal choice for this dataset

Fundamental trade-off : Bias vs Variance

Definition

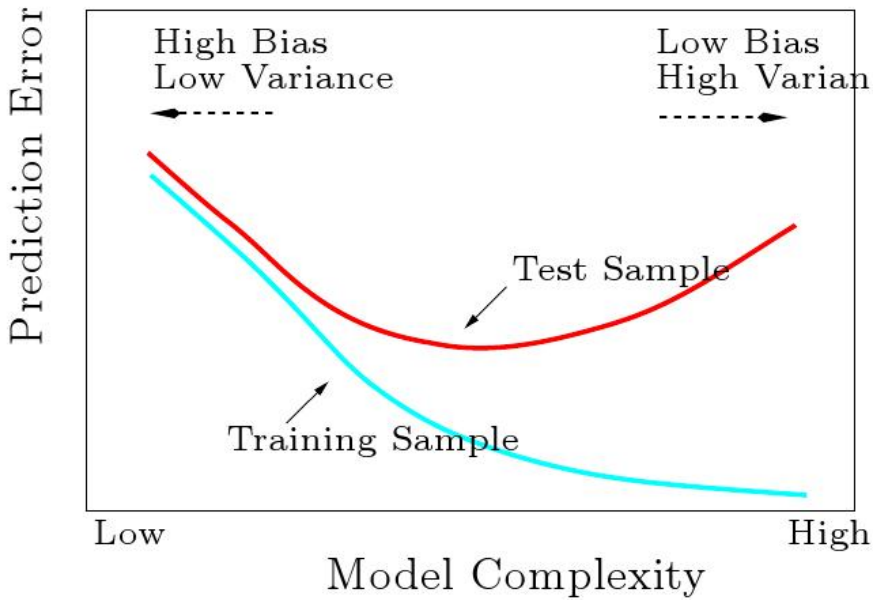
- Bias : how much the model is centered on the true answer
- Variance : how much the model has high stochastic variations



Fundamental trade-off : Bias vs Variance

Relation with over/under-fitting

- too simple model (high bias) → under-fitting
  - the model is too simple to fit the true function
- too complex model (high variance) → over-fitting
  - the model overfits the training data, and gives random garbage on test data



Bias/variance : mathematical definition

- Consider a model
$$y = f^\star(x) + \epsilon,$$
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- Where :
  - $\mathrm{Bias}_D\left[\hat{f}_D(x)\right] = \mathbb{E}_D(\hat{f}_D(x)) - f^\star(x)$ reflects how much the model is centered on $f^\star$
  - $\mathrm{Var}_D\left[\hat{f}_D(x)\right] = \mathbb{E}_D\left[\left(\hat{f}_D(x) - \mathbb{E}_D(\hat{f}_D(x))\right)^2\right]$ reflects how much the model varies with D
  - $\mathrm{Var}\left[\epsilon\right]$ is the irreducible part, the level of noise.

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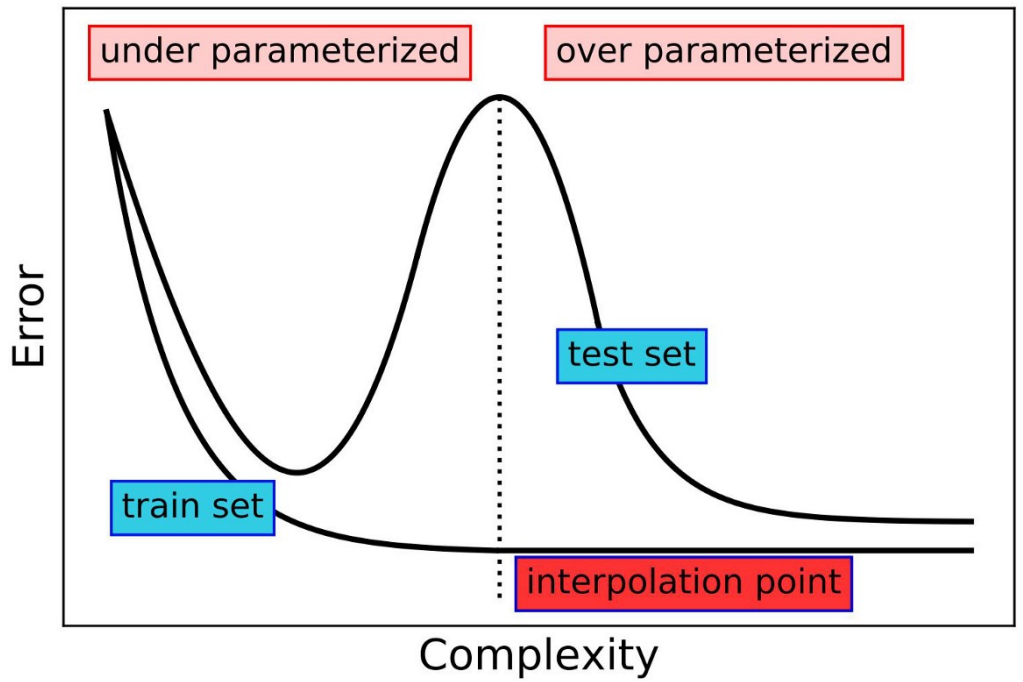
A grain of salt

- "Modern" deep learning largely counters the classical overfitting paradigm
  - Models are largely interpolating, but still generalize well !
- Implications both mathematical and more"philosophical" (what are test data ? How do we use them in modern paradigms ?...)
  - see `https://www.argmin.net/p/thou-shalt-not-overfit`



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Model Assessment/Validation

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- But
  - only part of the data is used to train the model : to preserve performance, the validation set must not be too large
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- standard solution : cross-validation, e.g. K-fold Cross-Validation

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- Idea : take several different validation sets, for each train a model, average the validation errors.
- In practice split the data in K-folds, here $K = 5$:

$\hat{\mathcal{R}}_1(\hat{f}_1, \lambda)$	Validation	Train	Train	Train	Train
$\hat{\mathcal{R}}_2(\hat{f}_2, \lambda)$	Train	Validation	Train	Train	Train
$\hat{\mathcal{R}}_3(\hat{f}_3, \lambda)$	Train	Train	Validation	Train	Train
$\hat{\mathcal{R}}_4(\hat{f}_4, \lambda)$	Train	Train	Train	Validation	Train
$\hat{\mathcal{R}}_5(\hat{f}_5, \lambda)$	Train	Train	Train	Train	Validation

  where λ is some hyperparameter of the model/method
- Estimate of Test error :

$$\mathrm{CV}(\hat{f}, \lambda) = \frac{1}{K} \sum_{k=1}^{K} \hat{\mathcal{R}}_k(\hat{f}_k, \lambda)$$

- Usually K=5 or 10 is a good trade-off (K=n is called leave-one-out)

Conclusions

Model assesment methods are an essential tool for data analysis, especially for big datasets involving many predictors

Cross-validation

- generic and simple procedure that can be used for any supervised problem
- provides a direct estimate of the test error.
- Can be used for model selection and/or hyperparameter tuning
- K-fold (with $K = 5$, or $K = 10$) is a standard choice, but there exists many variants depending on the problem, e.g.
  - *stratified* K-fold to ensure that all the folds have roughly the same average response value $\leftarrow$ useful for classification to be sure that each fold contains roughly the same proportions of class labels.
  - *hold-out* cross-validation for time-series where a subset (split temporally) of the data is reserved for validating the model performance

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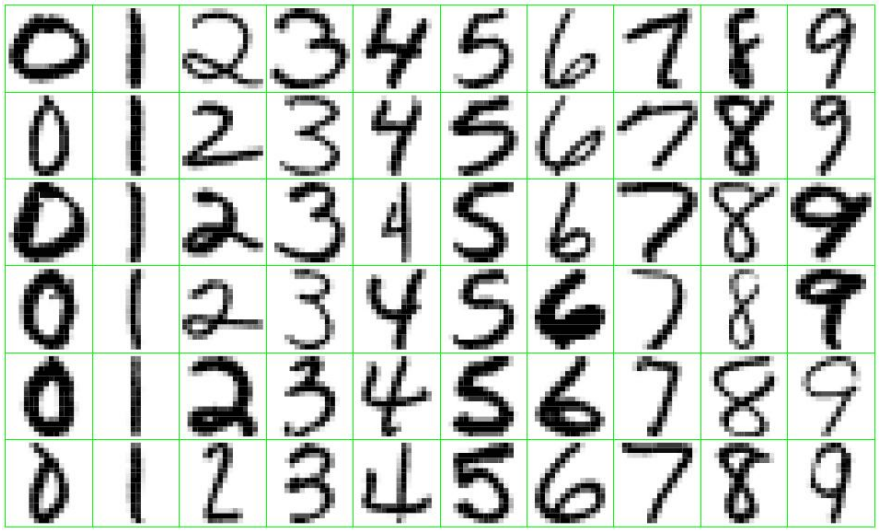
Examples of Tasks

Recognition of handwritten digits (US postal envelopes)



- ☞ Predict the class (0,...,9) of each sample from an image of 16 × 16 pixels, with a pixel intensity coded from 0 to 255
- Low error rate to avoid wrong allocations of mails !
- Historically one of the first, most popular image dataset : MNIST

Supervised classification

Examples of Tasks

Spams Recognition

Spam

```
WINNING NOTIFICATION
We are pleased to inform you of the result
of the Lottery Winners International
programs held on the 30th january 2005.
[...]  You have been approved for a lump sum
pay out of 175,000.00 euros.
CONGRATULATIONS!!!
```

No Spam

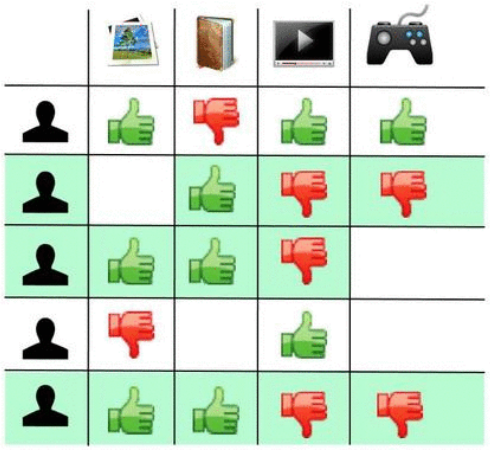
```
Dear George,
Could you please send me the report #1248 on
the project advancement?
Thanks in advance.

Regards,
Cathia
```

- ☞ Define a model to predict whether an email is spam or not
- Low error rate to avoid deleting useful messages, or filling the mailbox with useless emails
- One of the most deployed application today ! !

supervised classification

Examples of Tasks

Recommender systems

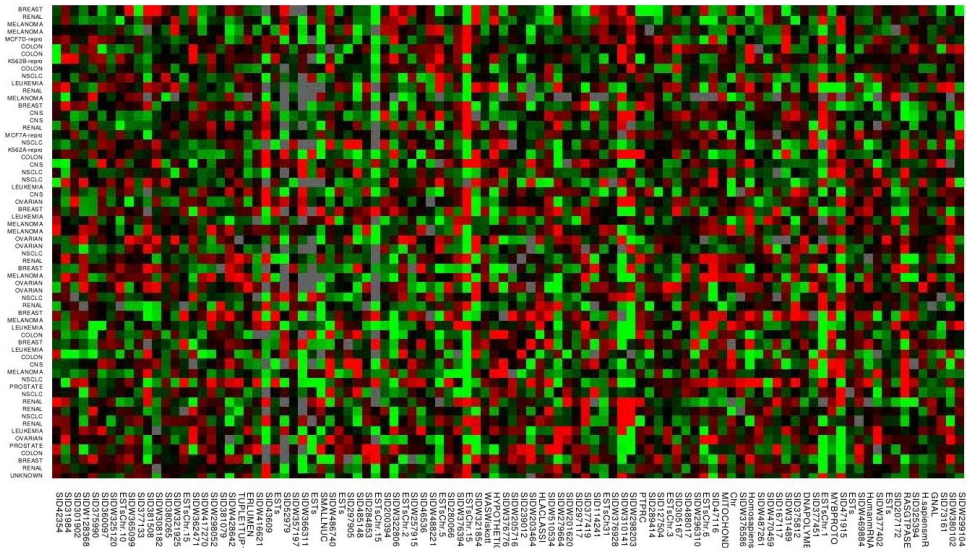


- ☞ Make personalized user recommendation of : movies, music, purchase, advertisements, social network friends...
- ▶ User-based (collaborative filtering), content-based, often hybrid
- ▶ (mis)Used all over the Internet, by every large website
- ▶ Historically, also important : the Netflix challenge

unsupervised classification/regression

Examples of Tasks

DNA-microarrays

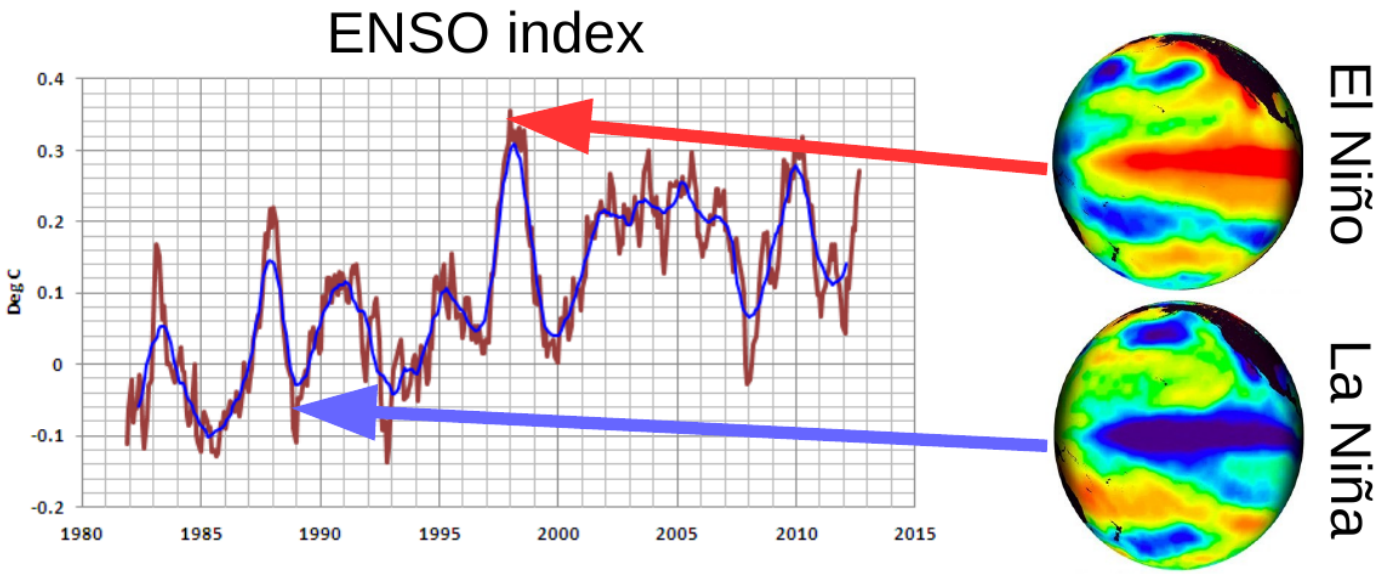


- Genes expression dataset for several thousand individual genes (columns) and tens of samples (rows) $d \gg n$ (huge challenge ! !)
- ☞ Clustering of genes (resp. samples) with similar expression profiles across samples (resp. genes)

unsupervised classification

Examples of Tasks in Geosciences

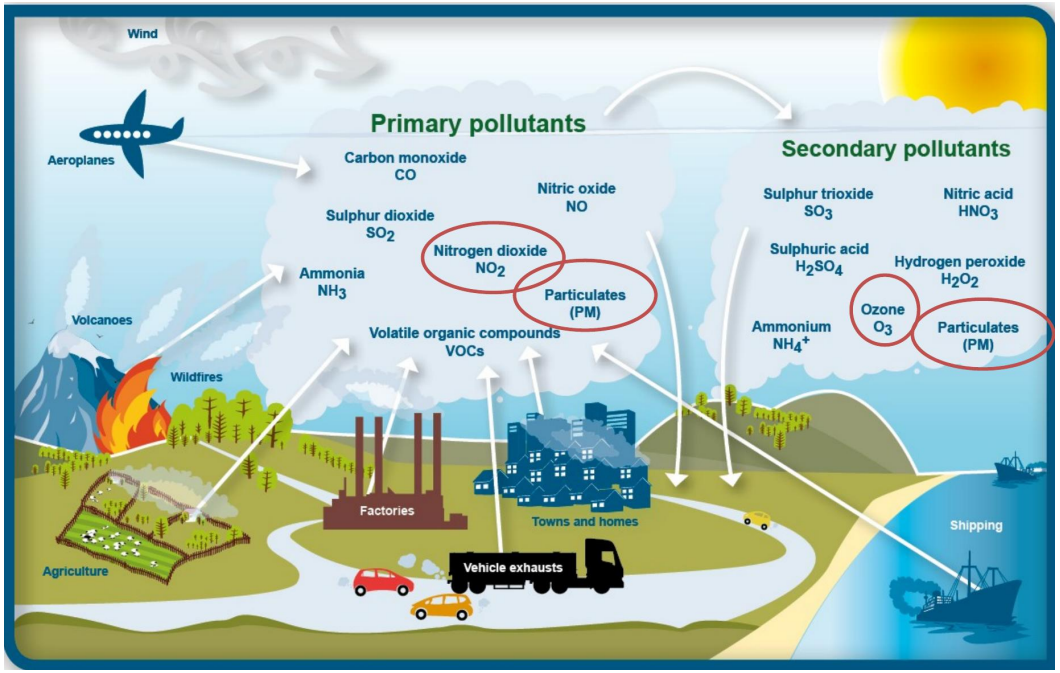
Prediction of El Niño southern oscillation



- Predict, 6 months in advance, the intensity of an El Niño Southern Oscillation (ENSO) event from ocean-atmosphere datasets (sea level pressure, surface wind components, sea surface temperature, surface air temperature, cloudiness...)

supervised regression (on time series)

Prediction of pollutant concentrations



- Predict pollutant concentrations (0_3,$N0_2$,PM10,PM2.5) at time D_0+1,+2,+3 from hourly measures timeseries + weather data + chemistry based forecasting models

supervised regression (pollutant concentration prediction) / classification (pollution alert or not)