Introduction to Machine Learning

Formation ENSTA ParisTech
Conférence IA

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Organization

Volume

- 2 × 7h lecture and practices sessions

	Monday 4 feb.	Tuesday 5 feb.
9:30-12:30	General intro, Classification	Model-free methods
13:30-17:30	Classification, Regression, Model Selection	Unsupervised learning

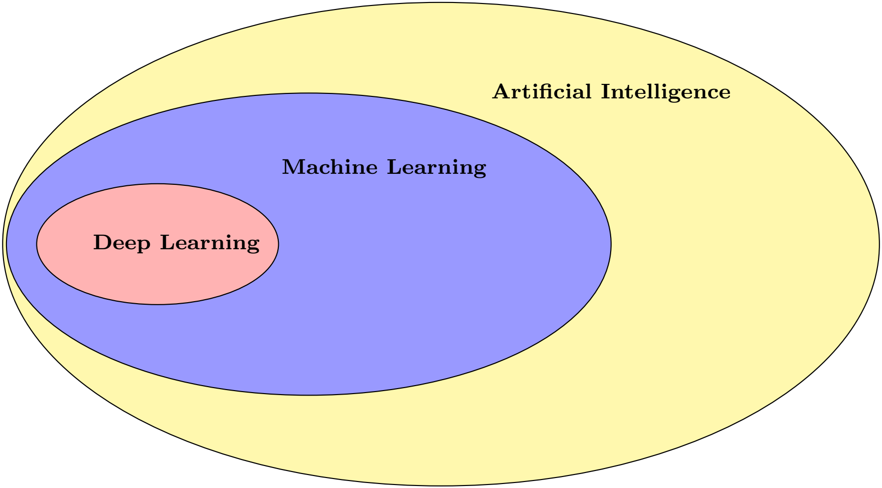
Objectives

- model/algorithm analysis for supervised learning
- assess the quality of predictions and inferences
- application of these algorithms on different datasets from geosciences : ecology, geography, ocean-atmosphere, astrophysics, etc. . .

The material

- Slides (pdf) and notebooks available here :
  `https://gricad-gitlab.univ-grenoble-alpes.fr/chatelaf/conference-ia/`
- Jupyter notebooks are available to illustrate concepts and methods in Python (.ipynb files)
- Binders are also available to run them remotely and interactively (no need to install Python and its dependencies, see `README.md`)

Machine Learning $\subset$ Artificial Intelligence



Data Science

How to extract knowledge or insights from data ?

Learning problems are at the cross-section of several applied fields and science disciplines

- *Machine learning* arose as a subfield of
  - Artificial Intelligence,
  - Computer Science.

  Emphasis on large scale implementations and applications : algorithm centered
- *Statistical learning* arose as a subfield of
  - Statistics,
  - Applied Maths,
  - Signal Processing, ...

  Emphasizes models and their interpretability : model centered

☞ There is much overlap : Data Science

References

Reference books

- Trevor Hastie, Robert Tibshirani et Jerome Friedman (2009), The Elements of Statistical Learning (2nd Edition), *Springer Series in Statistics*
- Christopher M. Bishop (2007), Pattern Recognition and Machine Learning, *Springer*
- Kevin P. Murphy (2012), Machine Learning : a Probabilistic Perspective, *MIT press*

Supplementary materials, datasets, online courses, ...

- `http://www-stat.stanford.edu/~tibs/ElemStatLearn/`
- `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` *Examples from the sklearn library*

Learning problem

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

Key points

- Experience E : data and statistics
- Performance measure P : optimization
- tasks T : utility
  - automatic translation
  - playing Go
  - ... doing what human does

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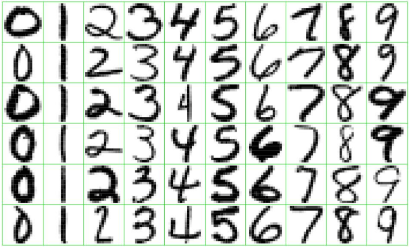
Examples of Tasks

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 !

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 (Ham)

Dear George,

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

Regards,
Cathia

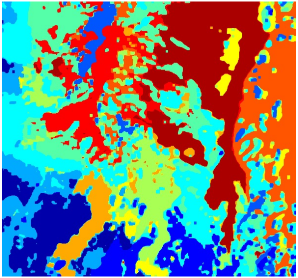
☞ Define a model to predict whether an email is spam or not

- Low error rate to avoid deleting useful messages, or filling the mailbox with useless emails

supervised classification

Examples of Tasks in Geosciences

Recognition of Hekla Volcano landscape, Iceland

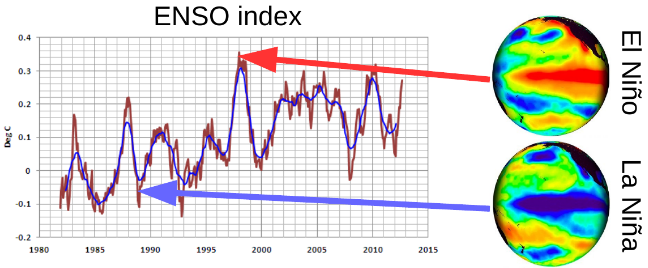


☞ Predict the class of landscape $\in$ { Lava 1970, Lava 1980 I, Lava 1980 II, Lava 1991 I, Lava 1991 II, Lava moss cover, hyaloclastite formation, Tephra lava, Rhyolite, Scoria, Firn-glacier ice, Snow } from digital remote sensing images

supervised or unsupervised classification

Examples of Tasks in Geosciences

Prediction of El Niño southern oscillation

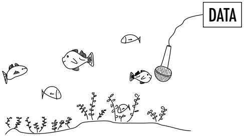


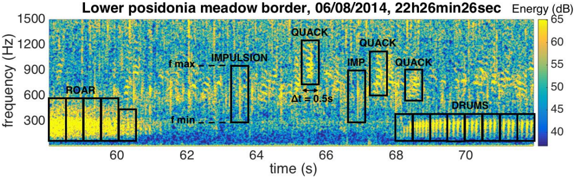
☞ Predict, 6 months in advance, the intensity of an El Niño Southern Oscillation (ENSO) event from ocean-atmosphere datasets (sea level pressure, surface wind components, sea surface temperature, surface air temperature, cloudiness...)

supervised regression

Examples of Tasks in Geosciences

Recognition of fish sounds



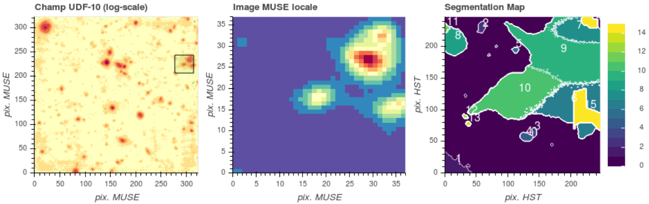


☞ Predict the class of underwater sounds (roar,quack,drums,impulsion) from times series recorded by hydrophones ($f_s = 156kHz$)

supervised or unsupervised classification

Examples of Tasks in Geosciences

Prediction of galaxy spectrum

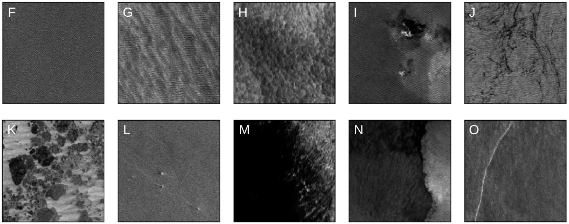


☞ Predict galaxy spectra from both hyperspectral MUSE datacubes and Hubble Space Telescope images for better understanding of the early unviverse

supervised regression

Examples of Tasks in Geosciences

Recognition of climate-ocean events



- ☞ Predict the classes of SAR images of the ocean (convective cells in I, sea ice in K, weather front in N,...) to detect climate-ocean events from water surface roughness

supervised or unsupervised classification

Definitions

Variable terminology

- observed data referred to as *input* variables, *predictors* or *features* $\leftarrow$ usually denoted as X
- data to predict referred to as *output* variables, or *responses* $\leftarrow$ usually denoted as Y

Type of prediction problem : regression vs classification

Depending on the type of the *output* variables

- when Y are quantitative data (continuous variables, e.g. ENSO intensity index values) $\leftarrow$ regression
- when Y are categorical data (discrete qualitative variables, e.g. handwritten digits $Y \in \{0, \dots, 9\}$) $\leftarrow$ classification

Two very close problems

Prediction problem

Assumptions

- inputs X_i are vectors in $\mathbb{R}^p$:

$$X_i = (X_{i,1}, \ldots, X_{i,p})^T \in \mathcal{X} \subset \mathbb{R}^p$$

- output variables Y_i take values :
  - in $\mathcal{Y} \subset \mathbb{R}$ (regression)
  - in a finite set $\mathcal{Y}$ (classification)
- $Y = f(X) + \epsilon$

Prediction rule

function of prediction / rule of classification $\equiv$ function $f : \mathcal{X} \to \mathcal{Y}$ to get predictions

$$\widehat{Y} = f(X)$$

of new elements Y given X

Supervised or unsupervised learning

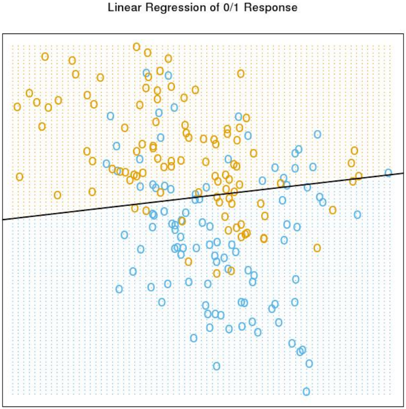
Training set $\equiv$ available sample $\mathcal{T}$ to learn the prediction rule f

For a sized n training set, different cases :

- Supervised learning : $\mathcal{T} \equiv ((X_1, Y_1), \ldots, (X_n, Y_n))$ input/output couples are available to learn the prediction rule f
- Unsupervised learning : $\mathcal{T} \equiv (X_1, \ldots, X_n)$ only the inputs are available
- Semi-supervised : mixed scenario (often encountered in practice, but less information than in the supervised case)

Toy example of binary classification

- Binary output variables : $Y_i \in \{0, 1\}$,
- Input variables $X_i \in \mathbb{R}^2$, for $i = 1, \ldots, N$



Example of a binary classification problem in $\mathbb{R}^2$. The 2 classes are coded as a binary variable : ORANGE=1, BLUE=0.

Simple linear model for classification

We seek a prediction model based on the linear regression of the outputs $Y \in \{0, 1\}$:

$$Y = \beta_1 X_1 + \beta_2 X_2 + \epsilon,$$

where $\boldsymbol{\beta} = (\beta_1, \beta_2)^T$ is a 2D unknown parameter vector

Learning problem $\Leftrightarrow$ Estimation of $\boldsymbol{\beta}$

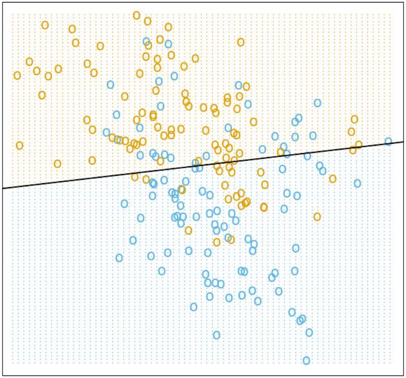
Least Squares Estimator $\hat{\boldsymbol{\beta}} = (\hat{\beta}_1, \hat{\beta}_2)^T$: minimize the training error rate (quadratic cost sense)

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^{N} (Y_i - \beta_1 X_{i,1} - \beta_2 X_{i,2})^2$$

Classification rule based on least squares regression

$$f(X) = \begin{cases} 1 \text{ if } \widehat{Y} = \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 \geq 0.5, \\ 0 \text{ otherwise} \end{cases}$$

Simple linear model for classification (Cont'd)



Example of classification in $\mathbb{R}^2$*. The 2 classes are coded as a binary variable : ORANGE=1, BLUE=0. The line is the decision boundary* $z = \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 = 0.5$ *: BLUE decision region below, ORANGE one above*

[Notebook]

'Black Box' method : k Nearest-Neighbors (k-NN)

The prediction model is directly defined, for $X = x$, as :

$$\widehat{Y}(x) = \frac{1}{k} \sum_{X_i \in N_k(x)} Y_i,$$

where $N_k(x)$ is the neighborhood of x defined by the k closest inputs X_i in the training set $\{(X_i, Y_i)\}_{i=1\dots n}$

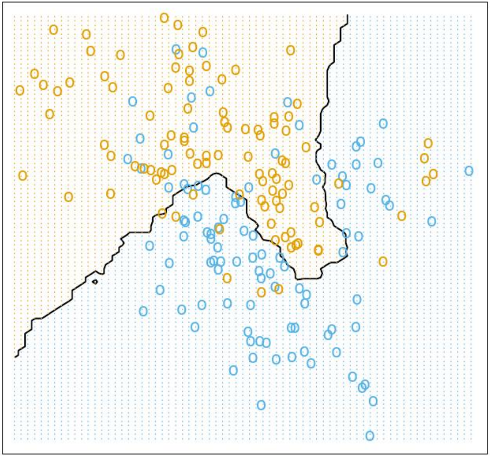
Classification rule associated with k-NN

$$f(x) = \begin{cases} 1 \text{ if } \widehat{Y}(x) > \frac{1}{2}, \\ 0 \text{ otherwise} \end{cases}$$

$\Leftrightarrow$ majority vote among the k closest neighbors of the testing point x

K Nearest-Neighbors (Cont'd)

15-Nearest Neighbor Classifier



Model complexity

Most of methods have a complexity related to their *effective* number of parameters

Linear regression : model order p

E.g. dth degree polynomial regression : $p = d + 1$ parameters a_k s.t.

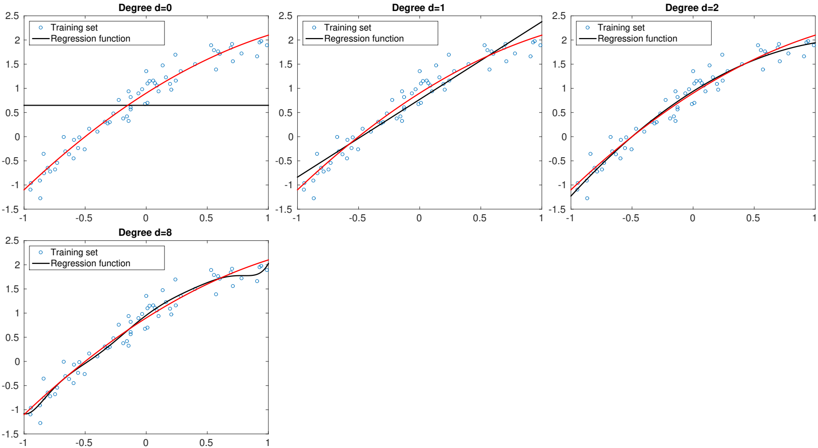
$$\begin{aligned} Y &= a_0 + a_1 x + a_2 x^2 + \ldots + a_d x^d + \epsilon, \\ &= \boldsymbol{X}_d \boldsymbol{a}_d + \epsilon, \end{aligned}$$

where

$$\begin{aligned} \boldsymbol{X}_d &= \left[1,\ x,\ x^2, \ldots, x^d\right], \\ \boldsymbol{a}_d &= \left[a_0, a_1, a_2, \ldots, a_d\right]^T. \end{aligned}$$

Linear regression : complexity vs stability

Polynomial degree d influence



Linear regression : complexity vs stability

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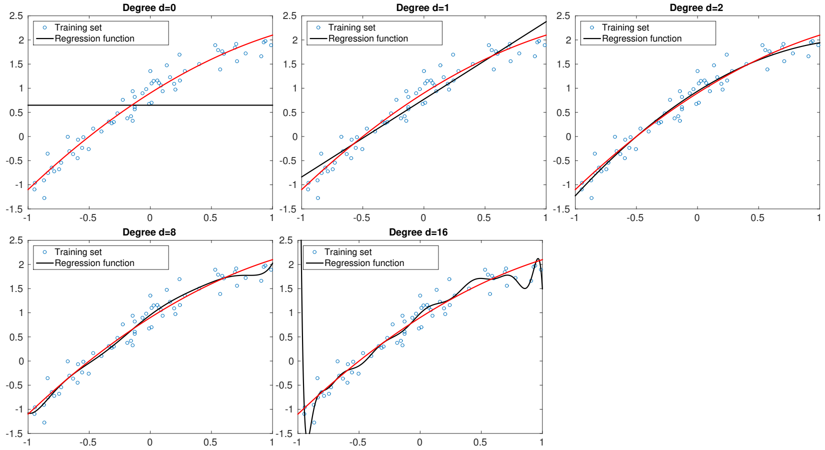
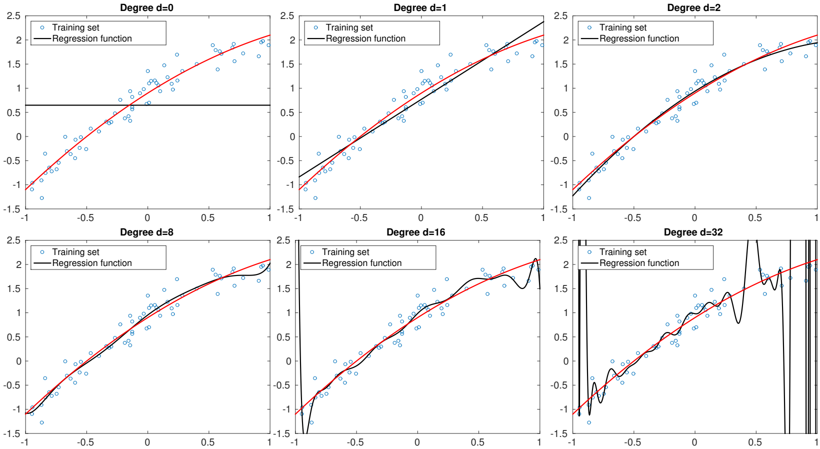


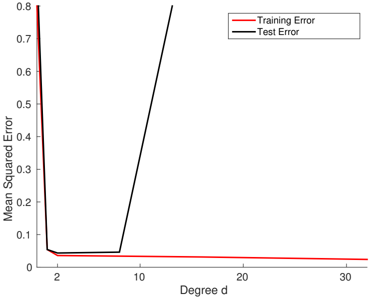
Linear regression : complexity vs stability

Polynomial degree d influence ← over-fitting



Linear Regression : Test error vs Train Error

Error rate vs polynomial order d



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

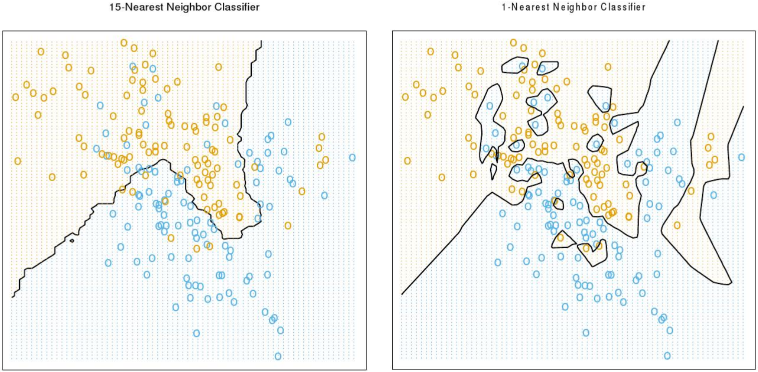
☞ Training error always decrease with the model complexity. Can't use alone to select the model !

[Notebook]

K Nearest-Neighbors

k-NN : complexity parameter k

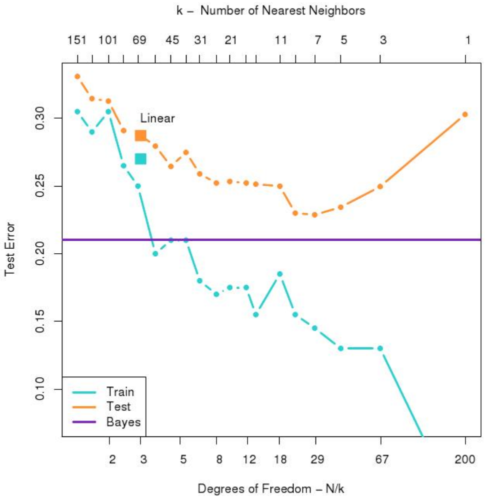
The effective number of parameters expresses as $N_{\text{eff}} = \frac{N}{k}$, where N is the size of the training sample



$k = 15,\ N_{\text{eff}} \approx 13$ $\qquad$ $k = 1,\ N_{\text{eff}} \approx 200$

- $k = 1 \rightarrow$ training error is always 0 !

Model Selection

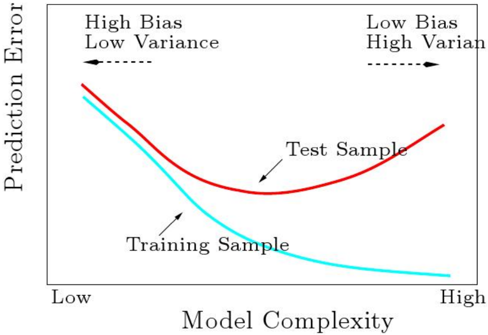


[Notebook]

Model Selection (Cont'd)

Fundamental trade-off

- too simple model (high bias) → under-fitting
- too complex model (high variance) → over-fitting



Fundamental Bias-Variance trade-off

if the true model is

$$Y = f(X) + \epsilon,$$

then for any prediction rule $\widehat{f}(X)$, Mean Squared Error (MSE) expresses as

$$E\left[\left(Y - \widehat{f}(x)\right)^2\right] = \text{Var}\left[\widehat{f}(x)\right] + \text{Bias}\left[\widehat{f}(x)\right]^2 + \text{Var}\left[\epsilon\right]$$

- Var $[\epsilon]$ is the *irreducible* part
- as the flexibility of $\widehat{f} \nearrow$, its variance $\nearrow$ and the bias $\searrow$

☞ overfitting/underfitting trade-off