Data Science for Geosciences

Introduction

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The presenters

Florent Chatelain

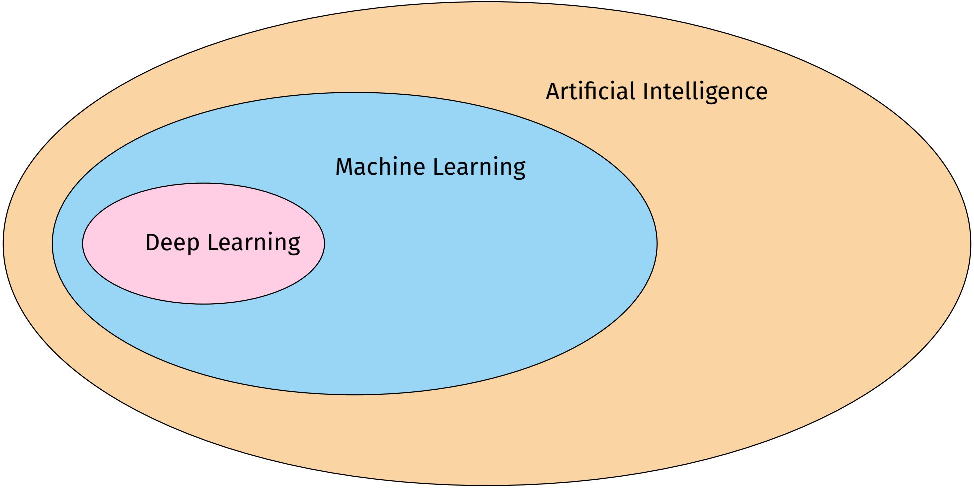
- Ph.D. degree in signal processing from the National Polytechnic Institute, Toulouse, France, in 2007
- Post-doc position at INRIA - ARIANA Team, 2007-2008
- Since 2008, Associate Professor at GIPSA-Lab, University of Grenoble, France.
- Research interests are centered around estimation, detection and large scale inference

Mathieu Fauvel

- Ph.D. degree in signal and image processing from the National Polytechnic Institute, Grenoble, France, and the University of Iceland, in 2007
- Post-doc position at INRIA - MISTIS Team, 2008-2010
- Assistant Professor (Grenoble, 2007-2008 & Toulouse, 2010-2011)
- Associate Professor at DYNAFOR, National Polytechnic Institute, Toulouse, between 2011-2018.
- Since 2018, Research (CR1) at CESBIO, INRA.
- Research interests are: machine learning for environmental/ecological monitoring

What is machine learning?

Machine Learning ⊂ Artificial Intelligence



Taken from `https://www.geospatialworld.net/blogs/difference-between-ai%EF%BB%BF-machine-learning-and-deep-learning/`

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

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

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Key points

- Experience E: data and statistics

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- Experience E: data and statistics
- Performance measure P: optimization

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Key points

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

Type of data: qualitatives / ordinales / quantitatives variables

- Text: strings
- Speech: time series
- Images/videos: 2/3d dependences
- Networks: graphs
- Games: interaction sequences
- ...

Big data (volume, velocity, variety, veracity)

Data are available without having decided to collect them!

- importance of preprocessings (cleaning up, normalization, coding,...)
- importance of a good representation : from raw data to vectors

Generalize

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

☞ Derive good (P/error rate) prediction functions

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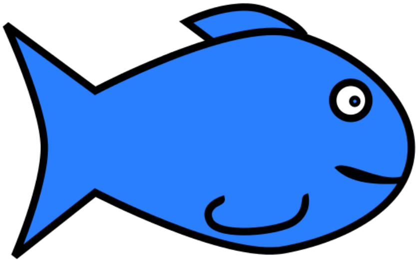
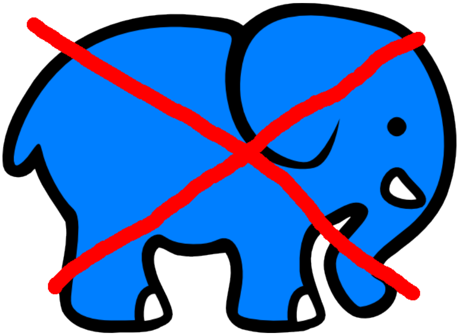


A fish



A fish

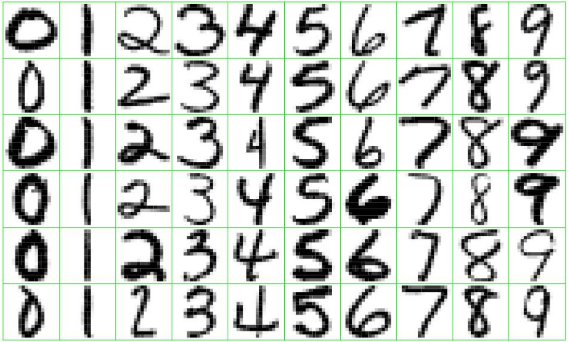
Reference books

- 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.cs.ubc.ca/~murphyk/MLbook/`
- `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*

Examples



☞ 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

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!!!

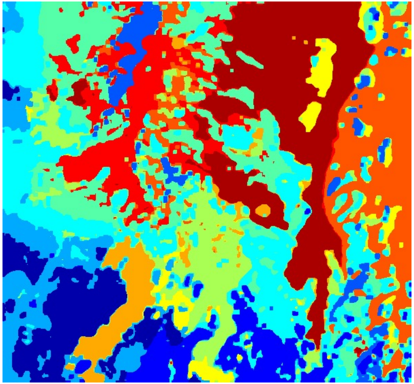
No Spam

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

Regards,
Cathia

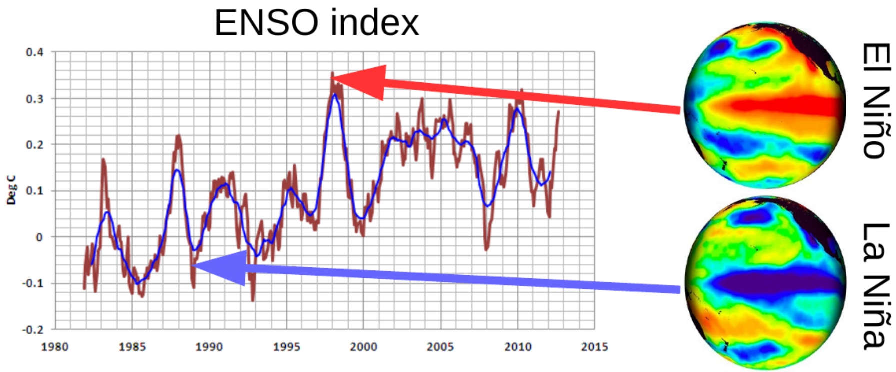
- ☞ Define a model to predict whether an email is spam or not
- Low error rate to avoid deleting useful messages, or filling the mailbox with useless emails

supervised classification



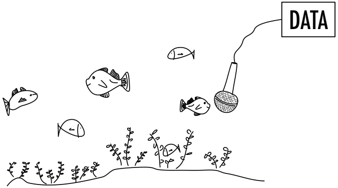
- Predict the class of landscape ∈ { Lava 1970, Lava 1980 I, Lava 1980 II, Lava 1991 I, Lava 1991 II, Lava moss cover, hyaloclastite formation, Tephra lava, Rhyolite, Scoria, Firn-glacier ice, Snow } from digital remote sensing images

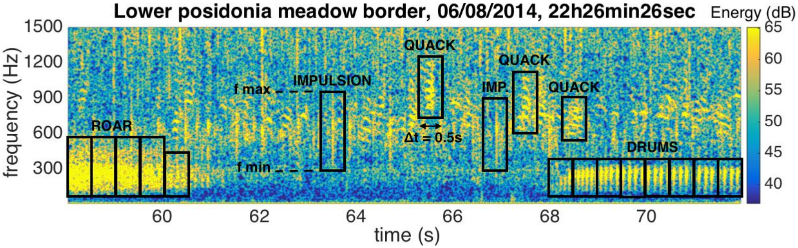
supervised or unsupervised classification



☞ 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...)

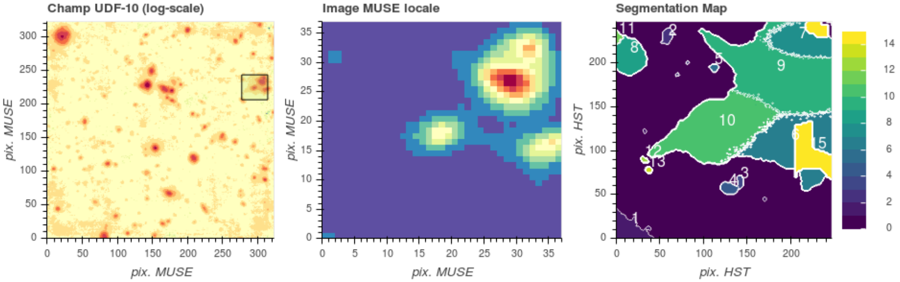
supervised regression





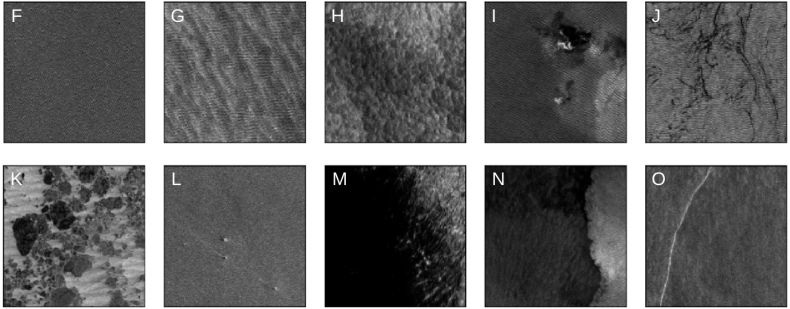
☞ Predict the class of underwater sounds (roar, quack, drums, impulsion) from times series recorded by hydrophones ($f_s = 156kHz$)

supervised or unsupervised classification



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

supervised regression



☞ 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

Basics

Variable terminology

- Observed data referred to as *input* variables, *predictors* or *features*: X
- Data to predict referred to as *output* variables, or *responses*: Y

Type of prediction problem: regression vs classification

Depending on the type of the *output* variables

- When Y are quantitative data (e.g. ENSO intensity index values): regression
- When Y are categorical data (e.g. handwritten digits $Y \in \{0, \dots, 9\}$): classification

Two very close problems

Assumptions

- Input variables 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 $\hat{f}: \ \mathcal{X} \to \mathcal{Y}$ to get predictions of new elements Y given X

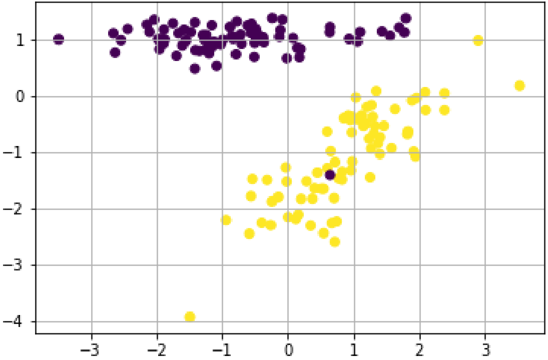
$$\widehat{Y} = \hat{f}(X)$$

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

For a sized n training set, different cases:

- Supervised learning: $\mathcal{T} \equiv \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ are available
- Unsupervised learning: $\mathcal{T} \equiv (X_1, \dots, X_n)$ are available only
- Semi-supervised: mixed scenario (often encountered in practice, but less information than in the supervised case)

Toy Example


1
0
−1
−2
−3
−4
−3
−2
−1
0
1
2
3

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

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

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

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

Notebook

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

Linear classification: model order p

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

$$\begin{aligned} Y &= \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_d x^d + \epsilon, \\ &= \mathbf{X}_d \boldsymbol{\beta}_d + \epsilon, \end{aligned}$$

where

$$\begin{aligned} \mathbf{X}_d &= \left[1,\ x,\ x^2, \ldots, x^d\right], \\ \boldsymbol{\beta}_d &= [\beta_0, \beta_1, \beta_2, \ldots, \beta_d]^T. \end{aligned}$$

Notebook

Error rate vs polynomial order d

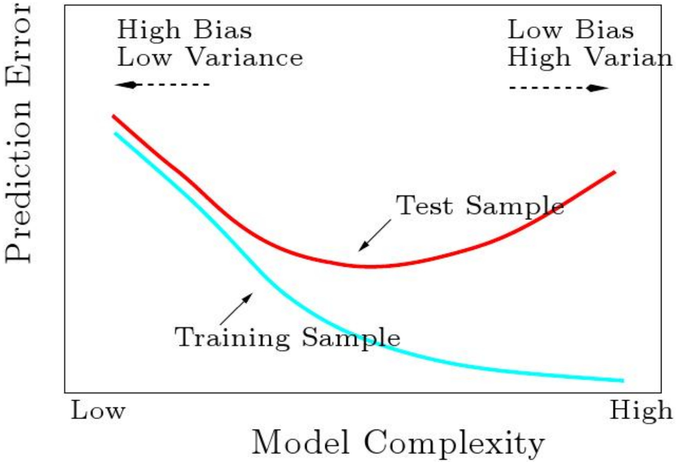
Notebook

- Training error rate (i.e. error rate for train data used for learning) minimized when $d = 19$
- True error rate (i.e. error rate for test data not used for learning) minimized when $d = 5$ ...

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

Fundamental trade-off

- Too simple model (high bias) $\rightarrow$ under-fitting
- Too complex model (high variance) $\rightarrow$ over-fitting



If the true model is

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

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

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

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

☞ overfitting/underfitting trade-off

Thank you for your attention