Data Science for Geosciences

Introduction

Florent Chatelain [1] Mathieu Fauvel [2]

27-31 January 2020
Toulouse, France

[1] MCF Grenoble INP, GIPSA-lab

[2] CR1 INRA, CESBIO

Florent Chatelain

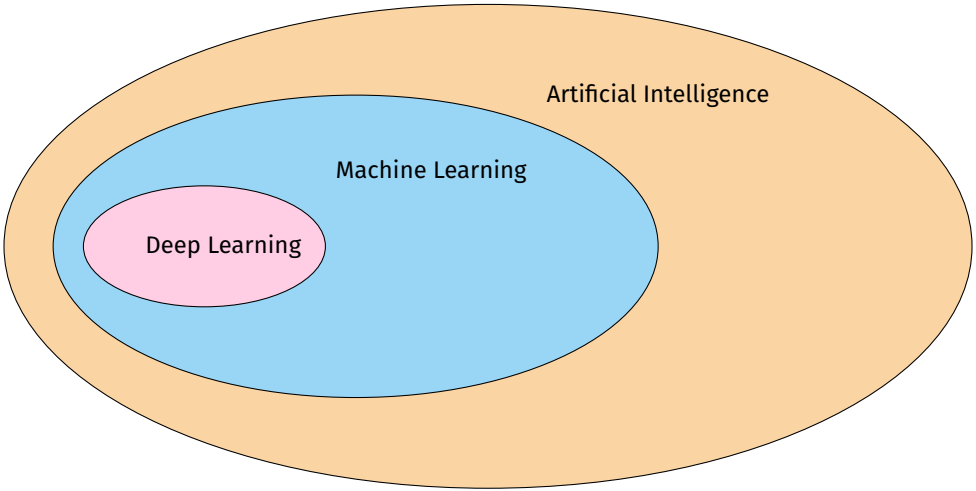
- Ph.D. degree in signal processing from the National Polytechnic Institute, Toulouse, France, in 2007
- Post-doc position at INRIA - ARIANA Team, 2007-2008
- Since 2008, Associate Professor at GIPSA-Lab, University of Grenoble, France.
- Research interests are centered around estimation, detection and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

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

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

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

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

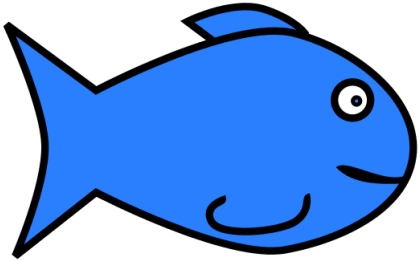
Generalize

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

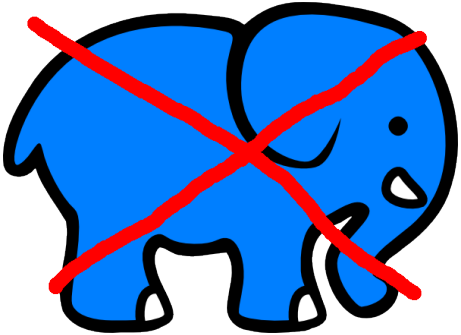
☞ Derive good (P/error rate) prediction functions

Generalize

- Perform well (minimize P) on new data (fresh data, i.e. unseen during learning)
- ☞ Derive good (P/error rate) prediction functions



A fish



A fish

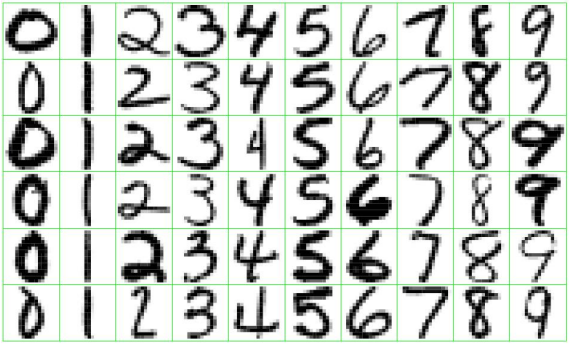
Reference books

- 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

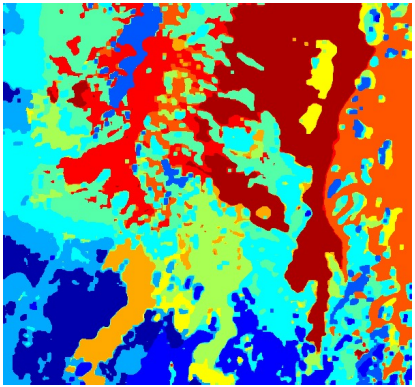
```
Dear George,
Could you please send me the report #1248 on
the project advancement?
Thanks in advance.

Regards,
Cathia
```

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

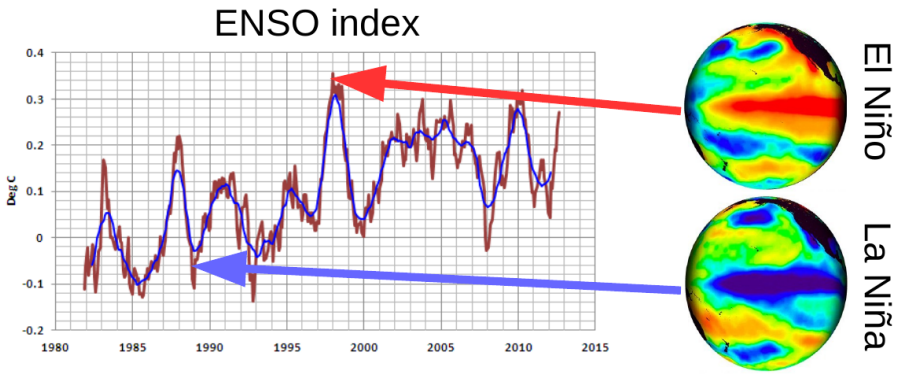
- Low error rate to avoid deleting useful messages, or filling the mailbox with useless emails

supervised classification



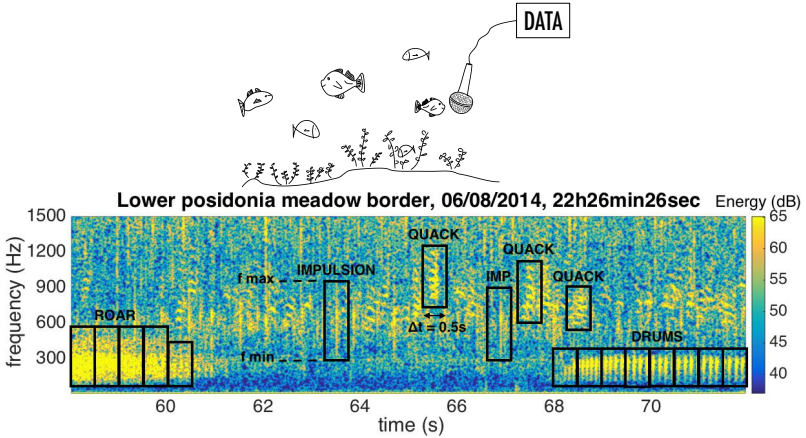
☞ Predict the class of landscape ∈ { Lava 1970, Lava 1980 I, Lava 1980 II, Lava 1991 I, Lava 1991 II, Lava moss cover, hyaloclastite formation, Tephra lava, Rhyolite, Scoria, Firn-glacier ice, Snow } from digital remote sensing images

supervised or unsupervised classification



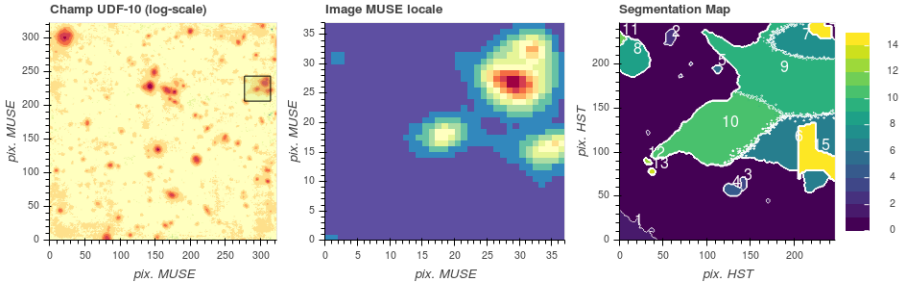
☞ Predict, 6 months in advance, the intensity of an El Niño Southern Oscillation (ENSO) event from ocean-atmosphere datasets (sea level pressure, surface wind components, sea surface temperature, surface air temperature, cloudiness...)

supervised regression



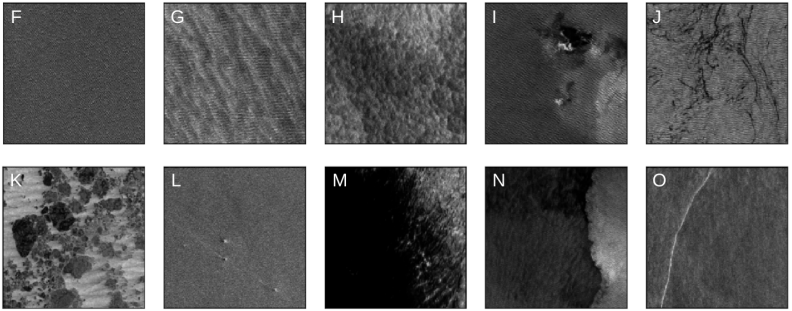
☞ Predict the class of underwater sounds (roar, quack, drums, impulsion) from times series recorded by hydrophones ($f_s = 156kHz$)

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 $Y \in \{0, \ldots, 9\}$): 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

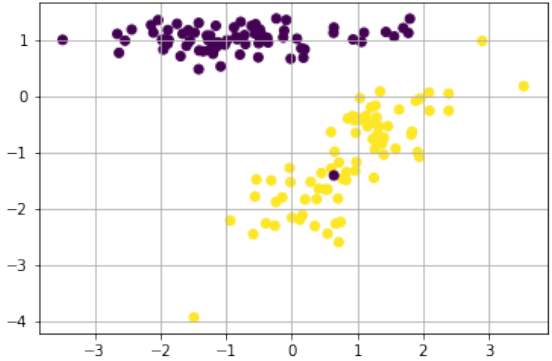
$$\widehat{Y} = \hat{f}(X)$$

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

For a sized n training set, different cases:

- Supervised learning: $\mathcal{T} \equiv \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ are available
- Unsupervised learning: $\mathcal{T} \equiv (X_1, \ldots, X_n)$ 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.

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

where

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

Notebook

Error rate vs polynomial order d

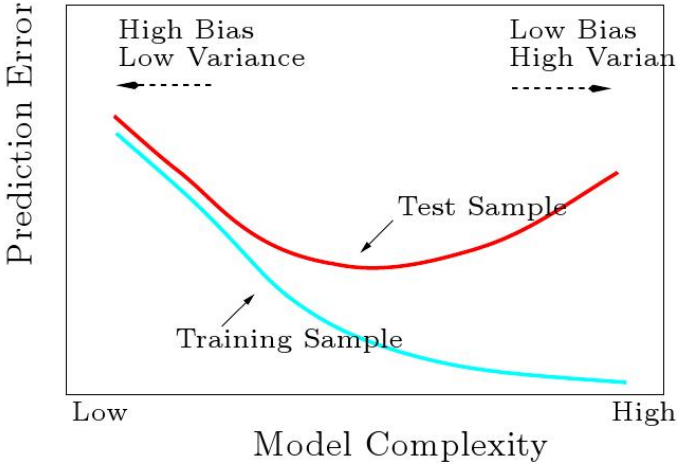
Notebook

- 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) → under-fitting
- Too complex model (high variance) → 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

This work is licensed under a Creative Commons “Attribution-ShareAlike 4.0 International” license.