Introduction to Machine Learning

Formation ENSTA ParisTech
Conférence IA

Florent Chatelain[*] Olivier Michel[*]

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ENSTA, France

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

Olivier J.J. Michel

- Former student ENS-Cachan (ENS Paris-Saclay), aggrégation in applied physics, 1986
- Ph-D degree in signal processing from Univerisity paris 11-Orsay, 1991, Post-Doc at Univ. of Michigan, USA
- Associate prof at Lab. de Physique, ENS-Lyon 1991-1999
- Prof. at Univ. Nice Sophia-Antipolis, Astrophysics lab, 1999-2008
- Prof at GIPSA-Lab, University of Grenoble, France.
- Research interest : random processes, estimation, detection, AI for astro and geo-sciences.

Organization

Volume

- 4 × 7h lecture and practices sessions

	Tuesday	Wednesday	Thursday	Friday
09h30-12h45	Intro	Classif (Cont'd)	Clustering	Neural Nets: basics, deep
		Lunch		
14h15-17h30	PCA + Classif	Linear models	Random Forests	Recurrent Neural Nets

Objectives

- Understand the theoretical basis of data science/machine learning/AI
- Assess the quality of predictions and inferences
- Implement/apply data science algorithms and models using state-of-the-art frameworks

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 (see README.md)

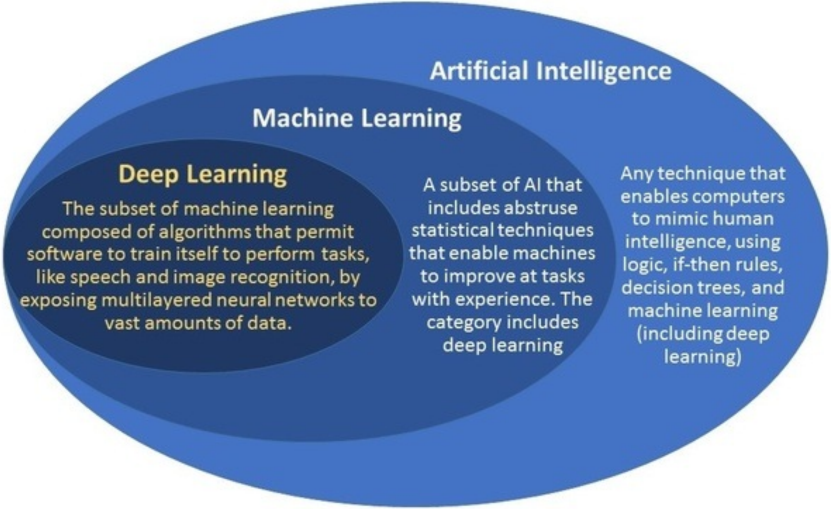
Reference books

- 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*

Machine Learning $\subset$ Artificial Intelligence



Artificial Intelligence

Machine Learning

Deep Learning

The subset of machine learning composed of algorithms that permit software to train itself to perform tasks, like speech and image recognition, by exposing multilayered neural networks to vast amounts of data.

A subset of AI that includes abstruse statistical techniques that enable machines to improve at tasks with experience. The category includes deep learning

Any technique that enables computers to mimic human intelligence, using logic, if-then rules, decision trees, and machine learning (including deep learning)

Data Science Objective

How to extract knowledge or insights from data ?

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

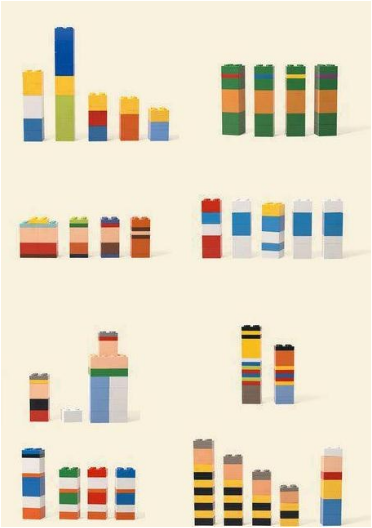
- *Machine learning* arose as a subfield of
  - Artificial Intelligence,
  - Computer Science.

  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

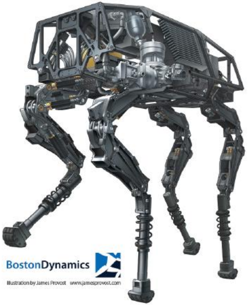
Learning problem

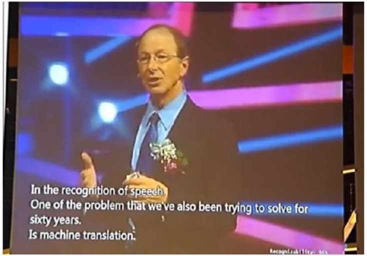


Learning: human vs machine

The learning of a child

- walking: 1 year
- speaking: 2 years
- reasoning: the rest of the time




In the recognition of speech
One of the problem that we've also been trying to solve for
sixty years.
Is machine translation.

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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Experience E: the data!

Type of data: qualitatives / ordinales / quantitatives variables

text	strings
speech	time series
ages/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

Objective and performance measures P

Generalize

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

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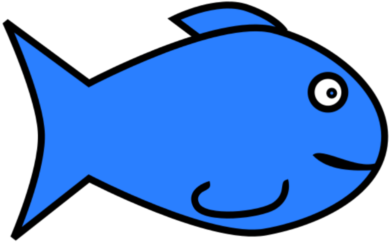
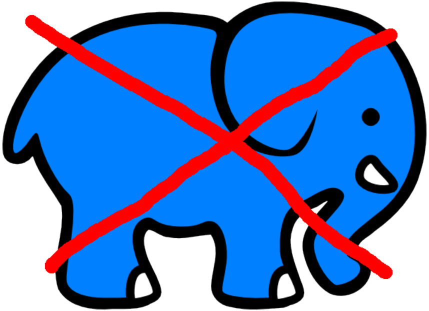


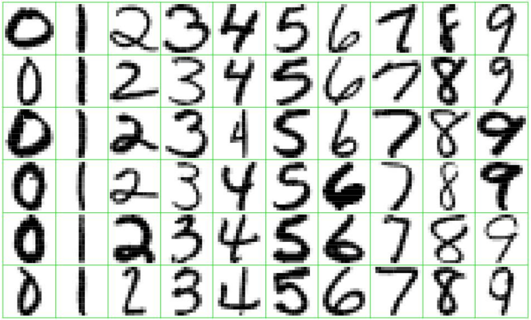
A fish



A fish

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

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

Regards,
Cathia
```

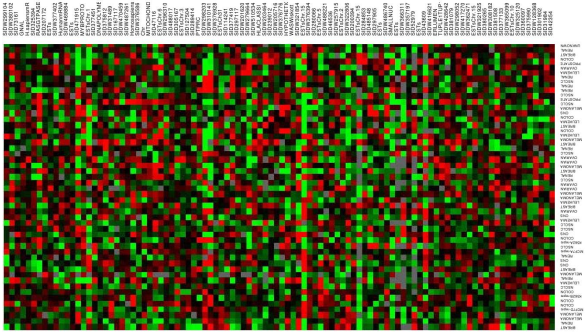
☞ Define a model to predict whether an email is spam or not

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

supervised classification

Examples of Tasks

DNA-microarrays



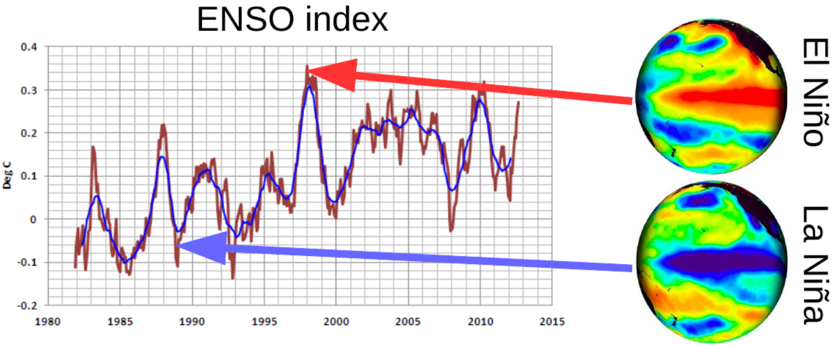
- Genes expression dataset fore several thousand individual genes (columns) and tens of samples (rows)

☞ Classification of genes (resp. samples) with similar expression profiles across samples (resp. genes)

unsupervised classification

Examples of Tasks in Geosciences

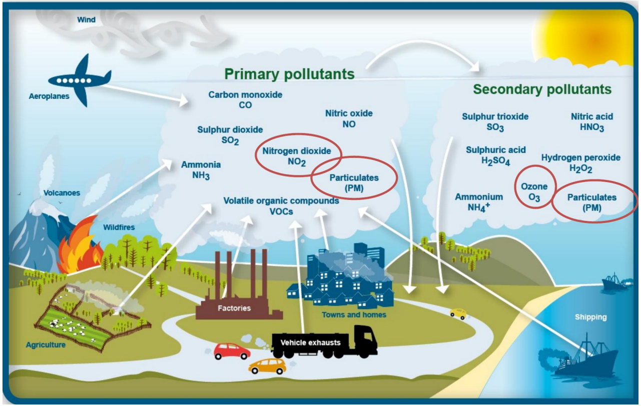
Prediction of El Niño southern oscillation



☞ 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

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 predicton) / classification (pollution alert or not)

Definitions

Variable terminology

- observed data referred to as *input* variables, *predictors* or *features* ← usually denoted as X
- data to predict referred to as *output* variables, or *responses* ← 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) ← regression
- when Y are categorical data (discrete qualitative variables, e.g. handwritten digits $Y \in \{0, \dots, 9\}$) ← classification

Two very close problems.

Prediction problem

Assumptions

- couples of input and output variables (X_i, Y_i) are i.i.d.
- 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)

Prediction rule

function of prediction / rule of classification $\equiv$ function $\widehat{f} : \mathcal{X} \rightarrow \mathcal{Y}$ that estimate the true link function f to get predictions of new elements Y given X

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

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)

During this course:

- most courses and labs devoted to supervised learning (more interpretable results, abundant literature)
- sessions on unsupervised learning: *dimension reduction (PCA)*, and *clustering*

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 β_k s.t.

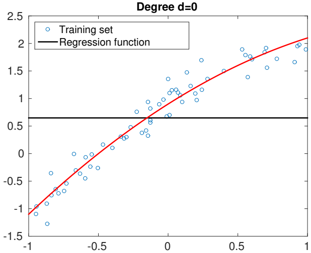
$$\begin{aligned} Y &= \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_d x^d + \epsilon, \\ &= \boldsymbol{X}_d \boldsymbol{\beta}_d + \epsilon, \end{aligned}$$

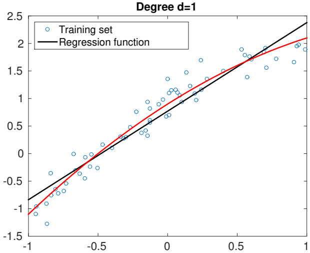
where

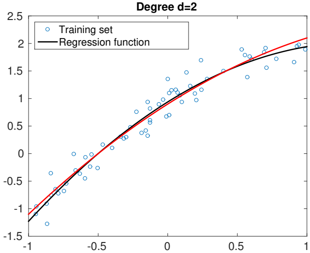
$$\begin{aligned} \boldsymbol{X}_d &= \left[1,\ x,\ x^2, \ldots, x^d\right], \\ \boldsymbol{\beta}_d &= [\beta_0, \beta_1, \beta_2, \ldots, \beta_d]^T. \end{aligned}$$

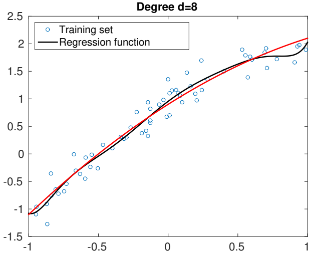
Linear regression: complexity vs stability

Polynomial degree *d* influence ← over-fitting issue









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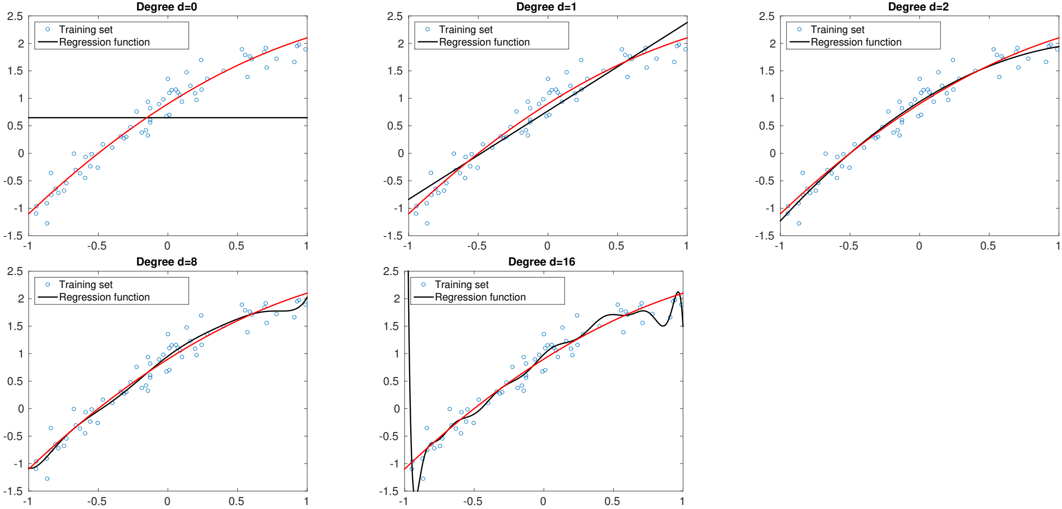

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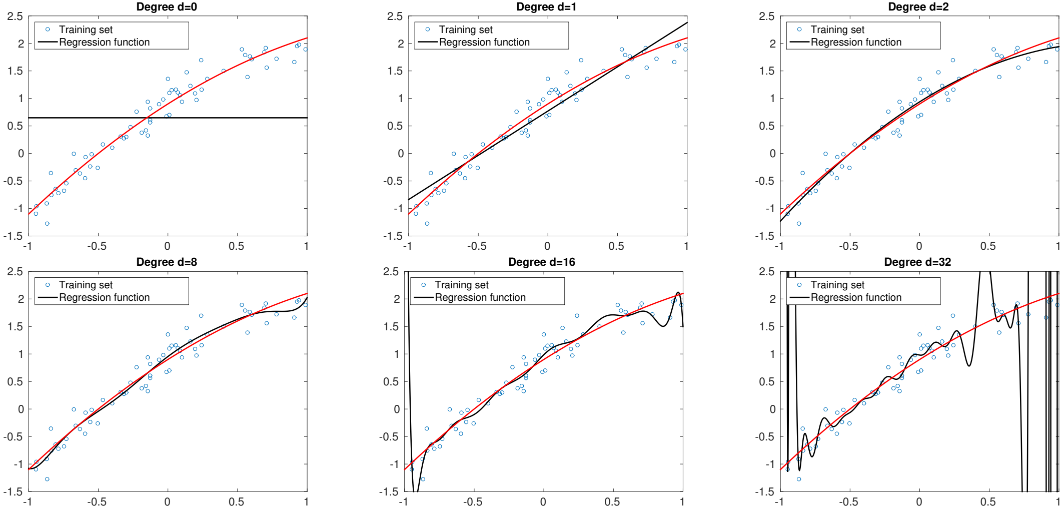
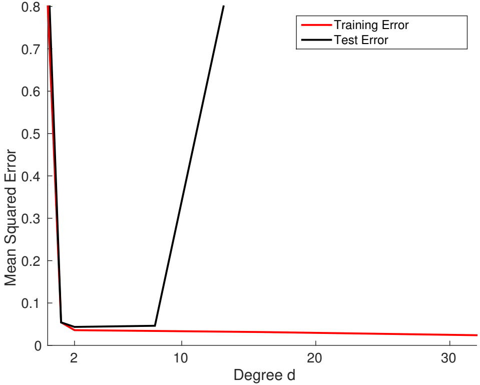


Linear Regression: Test error vs Train Error

Error rate vs polynomial order *d*



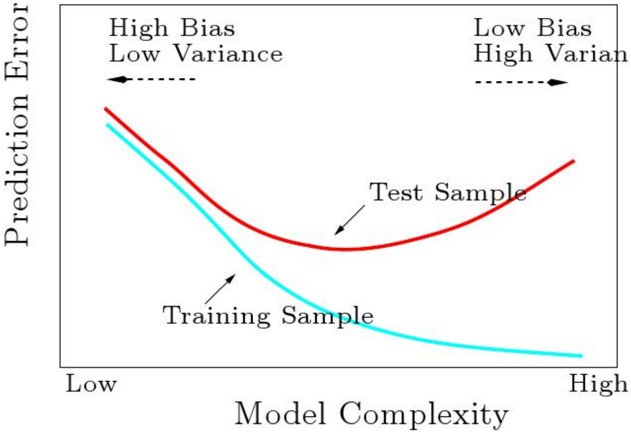
- True error rate (i.e. error rate for test data not used for learning) minimized when $d = 2$ ...
- ... true generative model: order $d = 2$ polynomial ($+$ white noise)

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

Model Selection

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

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

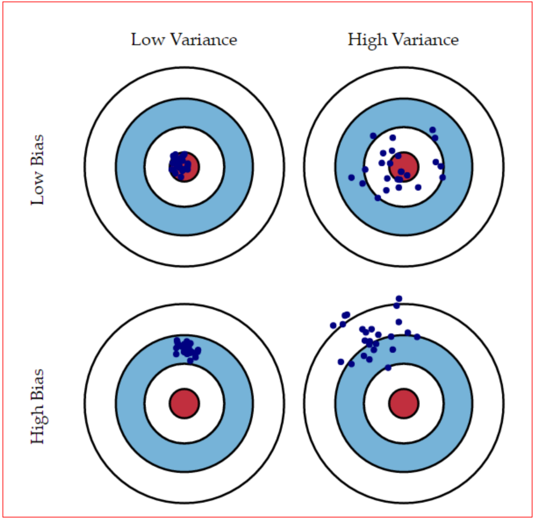
then for any prediction rule $\widehat{f}(X)$, Mean Squared Error (MSE) expresses as

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

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

☞ overfitting/underfitting trade-off

Overview of Bias-Variance


Low Variance
High Variance
Low Bias
High Bias