Statistical Learning with High-dimensional Data

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Preamble

"Ce qui est simple est toujours faux.
Ce qui ne l'est pas est inutilisable."

Paul Valéry

Outline

The AI revolution hasn't happened yet!

Artificial intelligence is a strategic field of research:

- with direct application in most scientific fields (Medicine, Biology, Astrophysics, Humanities)
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- deep learning has impressive results in a few specific cases and with a high-level supervision,
- use of DL techniques in various fields are promising but not well understood.

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"*Artificial Intelligence: the revolution hasn't happened yet*"
M. Jordan (UC Berkley)

Open problems of AI

Some open problems are critical:

- reliability of models and algorithms,
- handling data heterogeneity (categorical, functional, networks, images, texts, ...),
- unsupervised learning (clustering, dimension reduction),
- learning from HD and small data (n small / p large),

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Combination of statistical theory with deep learning techniques is certainly the future of AI!

AI in France

French policy for AI:

- C. Villani presented in March a recommendation report for AI,
- President Macron announced the creation of a network of AI institutes.

The 3IA institutes:

- 12 french research centers applied for the 3IA call in Sept.,
- 4 projects have been selected in the Spring 2019:
  - Paris, Toulouse, Grenoble
  - and Nice!

A few examples: Cervical cancer detection

Cervical cancer detection:

- it is an important public health field which is currently treated mostly manually,
- screening by human experts is complicated by the amount of cells (20 000/smear),
- and by the very small proportion of cancer cells (less than 1%).

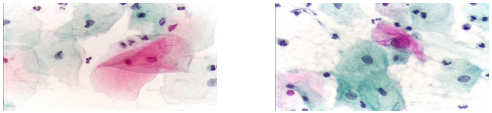
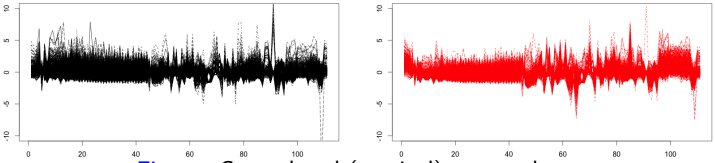


Figure: Normal (left) and abnormal (right) pap smears.

Classification is useful in this context:

- for building supervised classifiers which can select the most likely cancer cells,
- for helping experts in labeling the learning data through weakly-supervised classification,
- for selecting discriminative variables which can be used in a semi-automatic process.



A few examples: Sparse models in Medicine (HEGP)

Problem:

- overcome the curse of dimensionality that occurs in Metabolomics,
- for disease diagnostic and early-stage marker identification,
- metabolomic data fall into the "ultra-high dimensional data" case.

Our solution:

- a Bayesian variable selection technique for PCA,
- that identify the relevant variable for each stage of the disease.

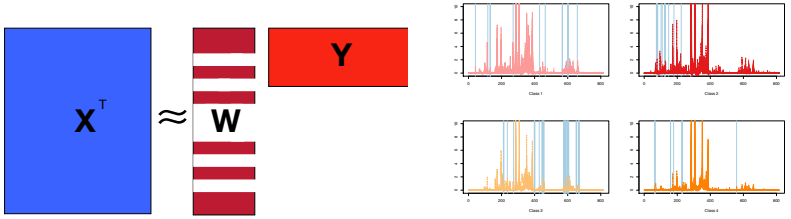


Figure: Functional co-clustering of Linky data (EDF).

Analysis of massive functional data (Linky / EDF)

Problem:

- Linky meters will allow EDF to have access to 27 million of Linky data,
- data are functional data and are measured every 30 minutes -> 17 520 obs./year,
- necessity to summarize those massive data before exploitation.

Our solution:

- a statistical co-clustering technique for functional data,
- that form homogeneous groups of both individuals and days.

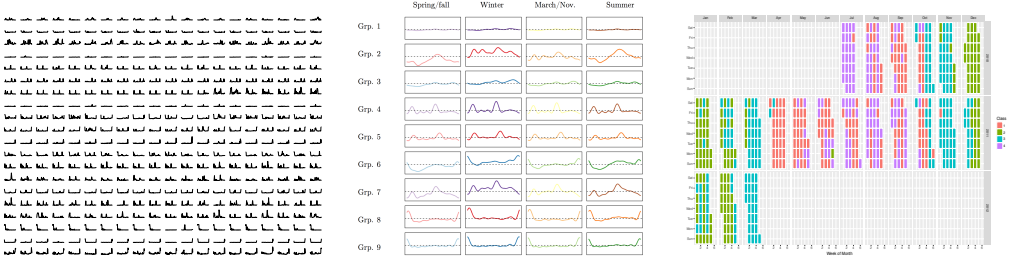


Figure: Functional co-clustering of Linky data (EDF).

Outline of the course

5 first sessions (C. Bouveyron):

- Introduction
- Dimension reduction: PCA, PPCA, FDA
- The GMM and EM algorithms
- Subspace methods for clustering and classification
- Analysis of functional data

5 following sessions (P.-A. Mattei):

- High-dimensional linear regression
- Sparse linear regression and the lasso
- Bayesian linear regression
- Sparsity beyond linear regression 1: classification, recommender systems
- Sparsity beyond linear regression 2: PCA, clustering

Outline

Learning from data...

One task, several families of approaches:

- Statistical learning
- Machine learning
- Deep learning
- ...

Learning from data...

Learning is a two-head problem:

Supervised	Unsupervised

Learning from data...

Methods are specific to each task:

Supervised	Unsupervised

Supervised learning

Supervised learning is also a field with different sub-tasks:

- classification:
- regression:
- time series analysis:
- ...

The supervised learning process

The material: a set of (complete) data

The goal: learn a predictor $f(.)$ from the (complete) data

Measuring the learning performance

One comfortable thing of working in the supervised context is:

- to be able to measure the performance of the learned predictor,

- compare several predictors and pick the most efficient one.

A minimal setup for supervised learning

The minimal setup for building a supervised predictor $f()$ from data is as follows:

Why such a minimal setup?

The goal is to avoid over-fitting when choosing the model or the model parameters:

An advanced setup for supervised learning

Resampling techniques:

- there are several methods (leave-one-out, V-fold cross-validation, bootstrap) depending on the context (sample size, computing time, ...),
- V-fold cross-validation:

Outline

Learning in high-dimensions

Learning in high-dimensions is one of the most important problems nowadays:

A motivating example: cytology

Cytology:

- it is the study of cells in terms of structure, function and chemistry,
- for the diagnosis of disease (we focused on cervical cancer).

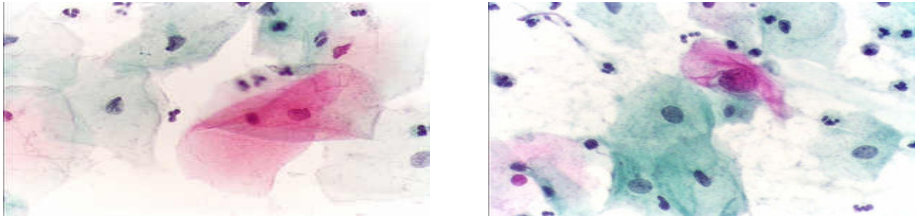


Figure: Normal (left) and abnormal (right) pap smears.

Cervical cancer detection:

- it is an important public health field which is currently treated mostly manually,
- pap smear screening by human experts is complicated by the amount of cells per smear (up to 20 000),
- and by the very small proportion of cancer cells (less than 1%).

A motivating example: cytology

Our data (BC Cancer Agency):

- 20 smears which contains between 4 000 and 10 000 cells,
- each nucleus is described by 111 features (morphological, photometric or texture features),
- only 0.52% of the cells are diseased cells.

Classification is useful in this context:

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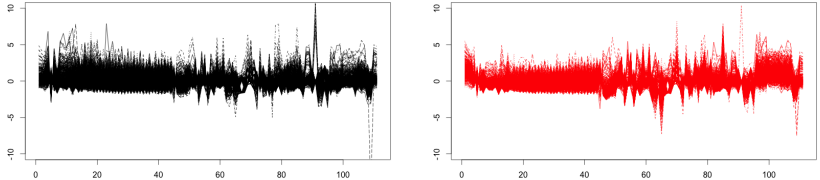
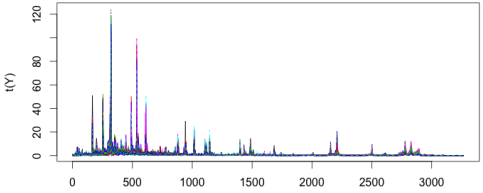


Figure: Control and (cervical) cancer data.

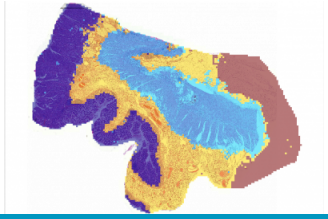
A motivating example: mass spectrometry

Mass spectrometry:

- it is a recent analytical technique that measures the mass-to-charge ratio of charged particles and which aims is to identify the elemental composition of a sample,
- It exist two types of mass spectrometry data:
  - multi-array data which aims to analyze serums or tissue fragments



  - MALDI images which are 2D or 3D MS images of tissues or organs



A motivating example: mass spectrometry

Classification is useful in this context:

- it is used in Medicine for disease diagnostic from blood samples:
  - a supervised classifier is learned from blood samples of healthy and sick patients,
  - the classifier is then used to classify new blood samples.
- a combination of supervised and unsupervised classification can be used to detect errors in the labels

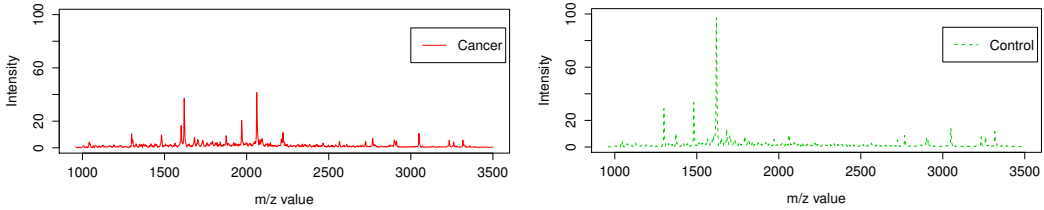


Figure: Control and cancer (colorectal) mass spectrometry spectra.

The curse of dimensionality

The curse of dimensionality:

- this term was first used by R. Bellman in the introduction of his book "Dynamic programming" in 1957:

  All [problems due to high dimension] *may be subsumed under the heading "the curse of dimensionality". Since this is a curse,* [...], *there is no need to feel discouraged about the possibility of obtaining significant results despite it.*

- he used this term to talk about the difficulties to find an optimum in a high-dimensional space using an exhaustive search,
- in order to promotate dynamic approaches in programming.

The curse of dimensionality

In the mixture model context:

- the building of the data partition mainly depends on:

$$H_k(x) = -2\log(\pi_k f(x, \theta_k)),$$

- model Full-GMM:

$$H_k(x) = (x - \mu_k)^t \Sigma_k^{-1}(x - \mu_k) + \log(\det \Sigma_k) - 2\log(\pi_k) + \gamma.$$

Consequently:

- it is necessary to invert Σ_k which have a number of parameters proportional to p^2,
- if n is small compared to p^2, the estimates of Σ_k are ill-conditionned or singular and it will be difficult or impossible to invert Σ_k.

The curse of dimensionality

From the estimation point of view:

- let us consider the normalized trace $\tau(\Sigma) = \mathrm{tr}(\Sigma^{-1})/p$ of the inverse covariance matrix Σ^{-1} of a multivariate Gaussian distribution $\mathcal{N}(0, \Sigma)$,
- the estimation of τ from a sample of n observations $\{x_1, ..., x_n\}$ conduces to:

$$\tau(\hat{\Sigma}) = \tau(\hat{\Sigma}) = \frac{1}{p}\mathrm{tr}(\hat{\Sigma}^{-1}),$$

$$E[\tau(\hat{\Sigma})] = \left(1 - \frac{p}{n-1}\right)^{-1} \tau(\Sigma).$$

- consequently, if the ratio $p/n \to 0$ when $n \to +\infty$, then $E[\tau(\hat{\Sigma})] \to \tau(\Sigma)$,
- however, if the dimension p is comparable with n, then $E[\tau(\hat{\Sigma})] \to c\tau(\Sigma)$ when $n \to +\infty$, where $c = \lim_{n\to+\infty} p/n$.

The blessings of dimensionality

As Bellman thought:

- all is not bad in high-dimensional spaces (hopefully!)
- there are interesting things which happen in high-dimensional spaces.

First example: volume of the unit sphere is $V(p) = \frac{\pi^{p/2}}{\Gamma(p/2+1)}$,

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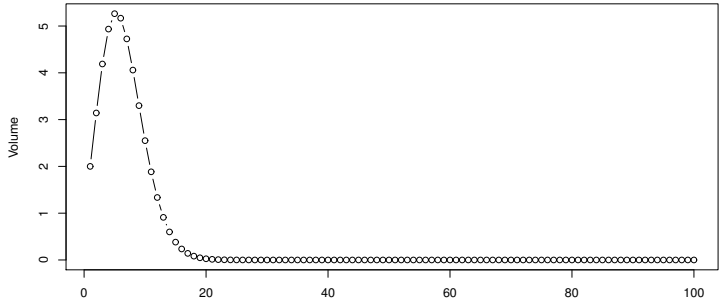

Fig. Volume of a sphere of radius 1 regarding to the dimension p.

The blessings of dimensionality

Second example: probability that a uniform variable on the unit sphere belongs to the shell between the spheres of radius 0.9 and 1 is

$$P(X \in S_{0.9}(p)) = 1 - 0.9^p \underset{p \to \infty}{\longrightarrow} 1$$

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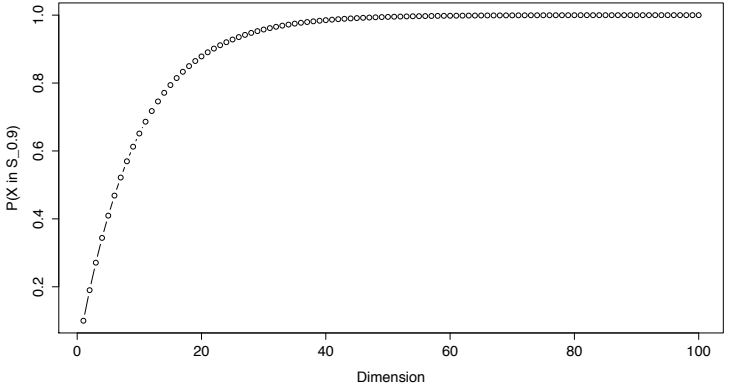

Fig. Probability that X belongs to the shell $S_{0.9}$ regarding to the dimension p.

The blessings of dimensionality

Third example:

- since high-dimensional spaces are almost empty,
- it should be easier to separate groups in high-dimensional space with an adapted classifier,
- a way to observe this is to look at the Bayes classifier behaviour.

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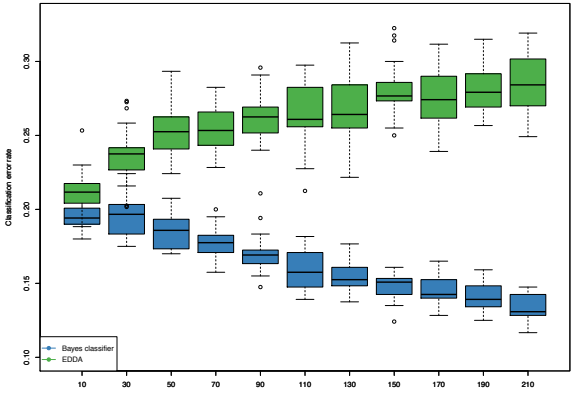


Fig. Classification error rate of the optimal classifier (blue) and EDDA (green) versus the data dimension on simulated data.

Classical ways to avoid the curse of dimensionality

Dimension reduction:

- the problem comes from that p is too large,
- therefore, reduce the data dimension to $d \ll p$,
- such that the curse of dimensionality vanishes!

Regularization:

- the problem comes from that parameter estimates are unstable,
- therefore, regularize these estimates,
- such that the parameter are correctly estimated!

Parsimonious models:

- the problem comes from that the number of parameters to estimate is too large,
- therefore, make restrictive assumptions on the model,
- such that the number of parameters to estimate becomes more "decent"!

Dimension reduction

A common phantasm about dimension reduction:

- believe that dimension reduction helps for classification,
- this is not true because, most of the time, dimension reduction implies an information loss which would be discriminative.

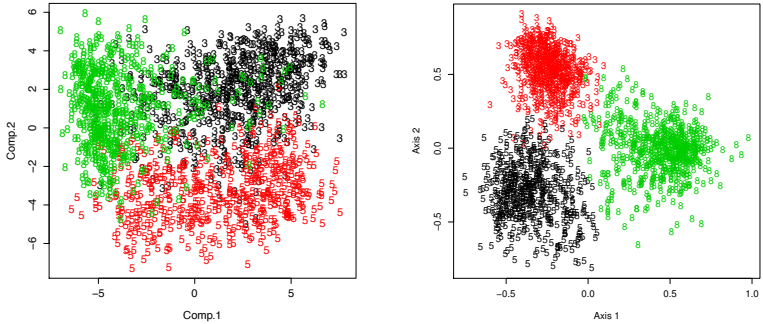


Figure: Projection of the 256-dimensional USPS data with PCA (left, unsupervised) and FDA (right, supervised).

Dimension reduction

Linear dimension reduction methods:

- feature combination: PCA,
- feature selection: ...

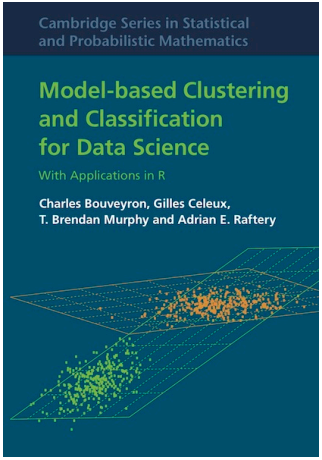
Non linear dimension reduction methods:

- Kohonen algorithms, Self Organising Maps,
- LLE, Isomap, ...
- Kernel PCA, principal curves, ...

Supervised dimension reduction methods:

- the old fashion method: Fisher Discriminant Analysis (FDA),
- many recent works on this topic... but useless in our context.

Want more?



Soon available at Cambridge University Press!