Generalized Bayesian Learning

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Inria Lille - Nord Europe & UCL AI

2018–2019

[https://bguedj.github.io]

8h de cours (4 $\times$ 2h, 6 février & 5 mars 2019)

Evaluation : projet à rendre. Deadline : **19 mars 2019 à 23h59**.

Slides : [https://bguedj.github.io/teaching/bguedj.pdf]

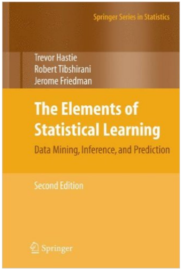
Projet : [https://bguedj.github.io/teaching/projet.pdf]

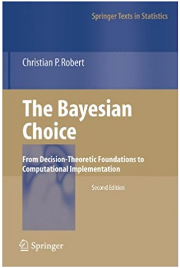
References

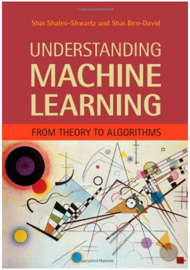
T. Hastie, R. Tibshirani and J. Friedman. *The Elements of Statistical Learning: Data Mining, Inference and Prediction*, Springer, 2009. [Link]

C. P. Robert. *The Bayesian Choice*, Springer, 2007. [Link]

S. Shalev-Shwartz and S. Ben-David. *Understanding Machine Learning: From Theory to Algorithms*, Cambridge University Press, 2014. [Link]





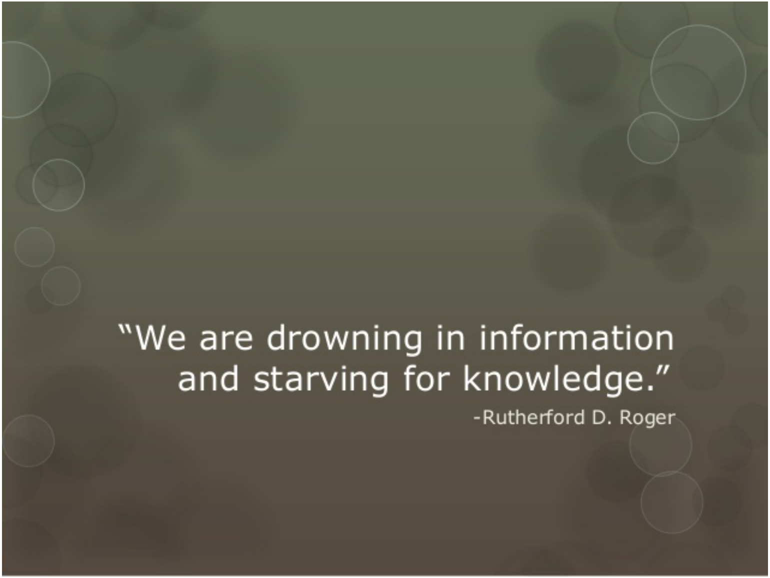


Outline

1. Introduction to statistical and machine learning
2. The Bayesian framework
3. Generalized Bayesian learning
4. Bayesian learning in practice: implementation

The rising of AI

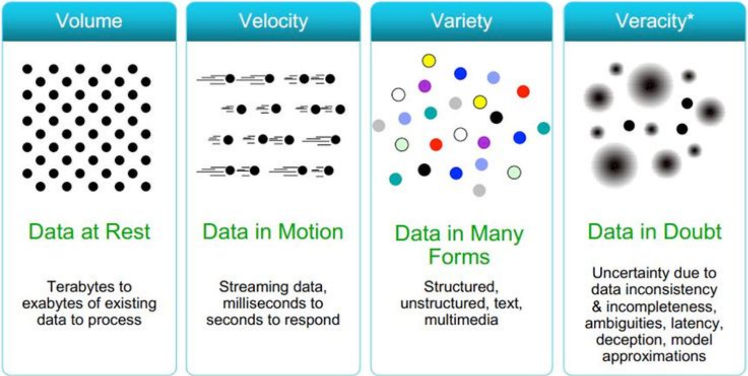
Introduction


"We are drowning in information
and starving for knowledge."
-Rutherford D. Roger

It is vital to remember that information - in the sense of raw data - is not knowledge, that knowledge is not wisdom, and that wisdom is not foresight. But information is the first essential step to all of these.

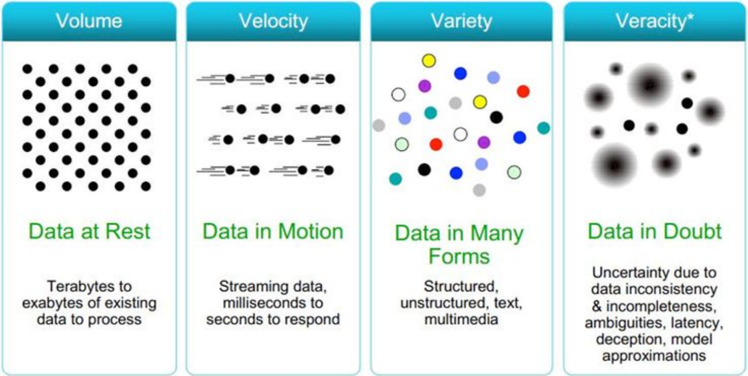
Arthur C Clarke

Big Data 4 V's



Volume
Data at Rest
Terabytes to exabytes of existing data to process
Velocity
Data in Motion
Streaming data, milliseconds to seconds to respond
Variety
Data in Many Forms
Structured, unstructured, text, multimedia
Veracity*
Data in Doubt
Uncertainty due to data inconsistency & incompleteness, ambiguities, latency, deception, model approximations

Big Data 4 V's



$\longrightarrow$ Value ($)

Data Scientists: voted 'most sexiest job' of the 21st century.
Demand is expected to exceed supply by 50 to 60% (McKinsey, 2015)

Volume / Velocity

i	3	6	9	12	15	18	21	24	
10^i	kilo	mega	giga	tera	peta	exa	zeta	yotta	bytes

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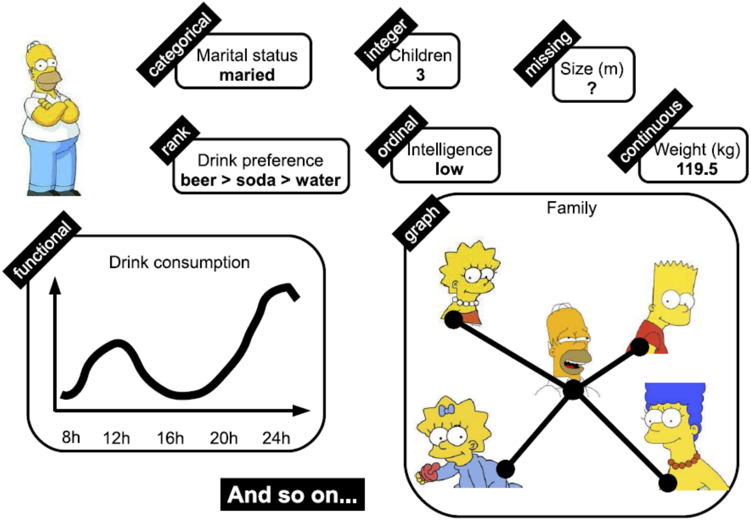
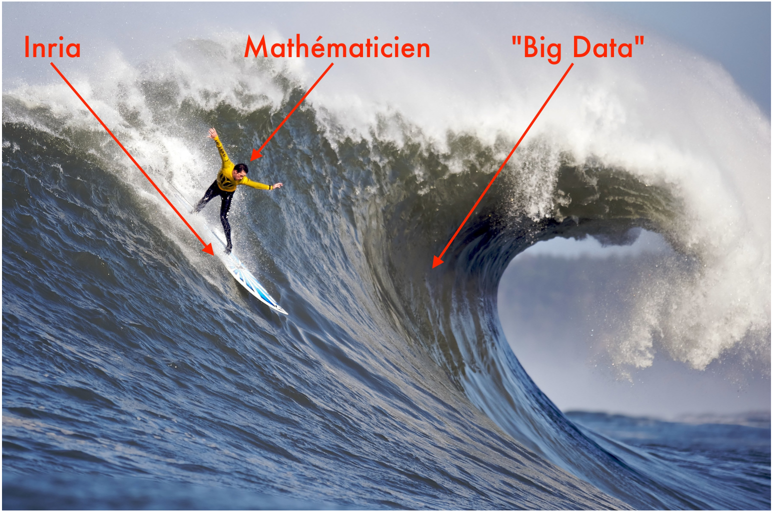
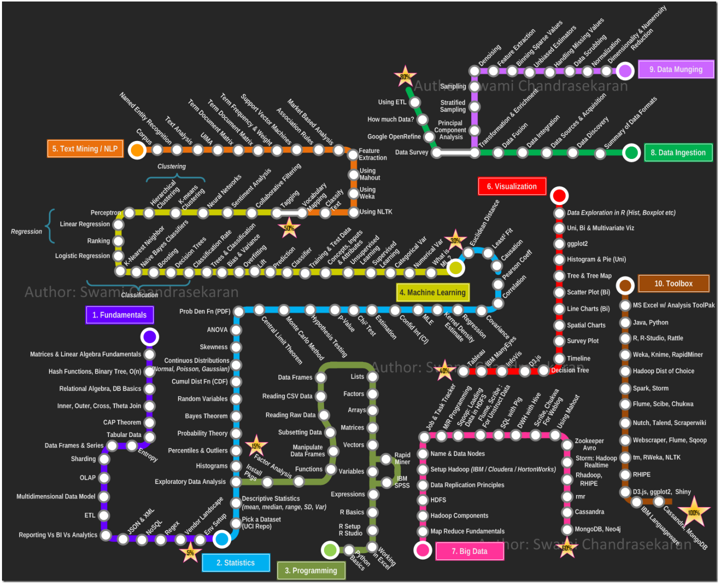
Variety / Veracity

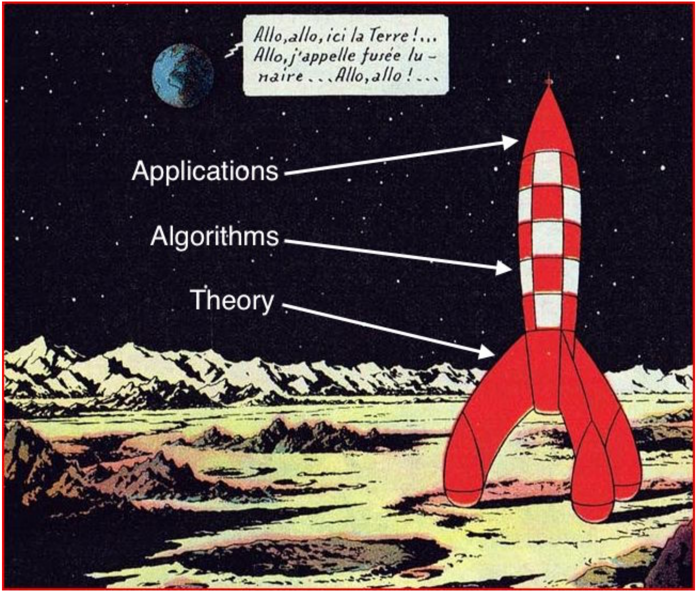


And so on...

My job (allegory)




1. Fundamentals
Matrices & Linear Algebra Fundamentals
Hash Functions, Binary Tree, O(n)
Relational Algebra, DB Basics
Inner, Outer, Cross, Theta Join
CAP Theorem
Tabular Data
Entropy
Data Frames & Series
Sharding
OLAP
Multidimensional Data Model
ETL
Reporting Vs BI Vs Analytics
JSON & XML
NoSQL
Regex
Vendor Landscape
Env Setup
5%
2. Statistics
Pick a Dataset (UCI Repo)
Descriptive Statistics (mean, median, range, SD, Var)
Exploratory Data Analysis
Histograms
Percentiles & Outliers
Probability Theory
Bayes Theorem
Random Variables
Cumul Dist Fn (CDF)
Continuos Distributions (Normal, Poisson, Gaussian)
Skewness
ANOVA
Prob Den Fn (PDF)
Central Limit Theorem
Monte Carlo Method
Hypothesis Testing
p-Value
Chi² Test
Estimation
Confid Int (CI)
MLE
Kernel Density Estimate
Regression
Covariance
Correlation
Pearson Coeff
Causation
Least² Fit
Euclidean Distance
3. Programming
Python Basics
Working in Excel
R Setup R Studio
R Basics
Expressions
Variables
IBM SPSS
Rapid Miner
Vectors
Matrices
Arrays
Factors
Lists
Functions
Manipulate Data Frames
Subsetting Data
Reading Raw Data
Reading CSV Data
Data Frames
Factor Analysis
Install Pkgs
15%
4. Machine Learning
What is ML?
Numerical Var
Categorical Var
Supervised Learning
Unsupervised Learning
Concepts, Inputs & Attributes
Training & Test Data
Classifier
Prediction
Lift
Overfitting
Bias & Variance
Trees & Classification
Classification Rate
Decision Trees
Boosting
Naive Bayes Classifiers
K-Nearest Neighbor
Classification
Logistic Regression
Ranking
Linear Regression
Perceptron
Regression
Hierarchical Clustering
K-means Clustering
Clustering
Neural Networks
Sentiment Analysis
Collaborative Filtering
Tagging
30%
5. Text Mining / NLP
Corpus
Named Entity Recognition
Text Analysis
UIMA
Term Document Matrix
Term Frequency & Weight
Support Vector Machines
Association Rules
Market Based Analysis
Feature Extraction
Using Mahout
Using Weka
Using NLTK
Classify Text
Vocabulary Mapping
50%
6. Visualization
Data Exploration in R (Hist, Boxplot etc)
Uni, Bi & Multivariate Viz
ggplot2
Histogram & Pie (Uni)
Tree & Tree Map
Scatter Plot (Bi)
Line Charts (Bi)
Spatial Charts
Survey Plot
Timeline
Decision Tree
D3.js
InfoVis
IBM ManyEyes
Tableau
40%
7. Big Data
Map Reduce Fundamentals
Hadoop Components
HDFS
Data Replication Principles
Setup Hadoop (IBM / Cloudera / HortonWorks)
Name & Data Nodes
Job & Task Tracker
M/R Programming
Sqoop: Loading Data in HDFS
Flume, Scribe: For Unstruct Data
SQL with Pig
DWH with Hive
Scribe, Chukwa For Weblog
Using Mahout
Zookeeper Avro
Storm: Hadoop Realtime
Rhadoop, RHIPE
rmr
Cassandra
MongoDB, Neo4j
60%
8. Data Ingestion
Summary of Data Formats
Data Discovery
Data Sources & Acquisition
Data Integration
Data Fusion
Transformation & Enrichment
Data Survey
Google OpenRefine
How much Data?
Using ETL
80%
9. Data Munging
Dimensionality & Numerosity Reduction
Normalization
Data Scrubbing
Handling Missing Values
Unbiased Estimators
Binning Sparse Values
Feature Extraction
Denoising
Sampling
Stratified Sampling
Principal Component Analysis
10. Toolbox
MS Excel w/ Analysis ToolPak
Java, Python
R, R-Studio, Rattle
Weka, Knime, RapidMiner
Hadoop Dist of Choice
Spark, Storm
Flume, Scibe, Chukwa
Nutch, Talend, Scraperwiki
Webscraper, Flume, Sqoop
tm, RWeka, NLTK
RHIPE
D3.js, ggplot2, Shiny
IBM Languageware
Cassandra, MongoDB
100%
Author: Swami Chandrasekaran


Allo, allo, ici la Terre !... Allo, j'appelle fusée lunaire ... Allo, allo ! ...
Applications
Algorithms
Theory

A foretaste of Learning Theory

{Statistical,Machine} Learning: building automatic procedures to infer general rules from examples.

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In the (~~rather~~ not so?) long term: mimic the inductive functioning of the humain brain to develop an artificial intelligence.

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In the Big Data Era, very dynamic field at the crossroads of Computer Science, Optimization and Statistics.

Probabilistic framework: n-sample $\mathcal{D}_n = (\mathbf{X}_i, \mathbf{Y}_i)_{i=1}^n$ of i.i.d. replications of some random variable

$$(\mathbf{X}, \mathbf{Y}) \in \mathcal{X} \times \mathcal{Y}, \quad \dim(\mathcal{X}) = d.$$

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We want to infer the link between the explanatory variable $\mathbf{X}$ and the response variable $\mathbf{Y}$, *i.e.*, use $\mathcal{D}_n$ to build up $\hat{\phi}$ such that $\hat{\phi}(\mathbf{X})$ is a "good" approximation of $\mathbf{Y}$.

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- Classification: $\mathcal{Y}$ is discrete.
- Regression: $\mathcal{Y}$ is a continuum.

- Online learning: observations are revealed over time.
- Batch learning: all observations are revealed at once.

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Big Data Era: easy/cheap to collect massive amounts of data, hence typically $\mathbf{X}_1, \dots, \mathbf{X}_n, \dots \in \mathbb{R}^{n \times d}$ where d and n may be (extremely) large.

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- Tall data: $n \gg d$
- Fat data: $d \gg n$
- Big/massive data: n and d huge

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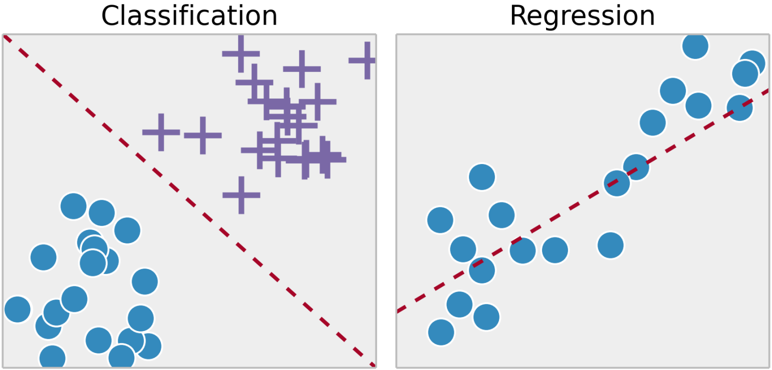

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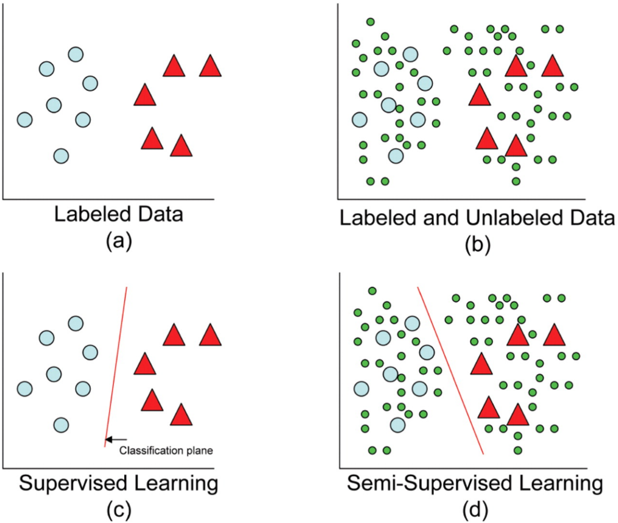

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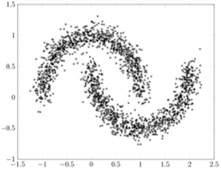

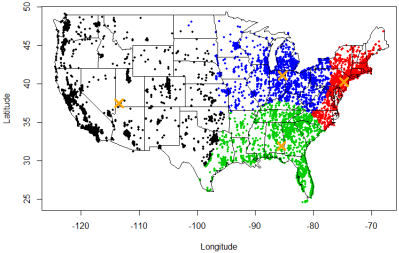

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Empirical risk

$$R_n(\hat{\phi}) = \frac{1}{n}\sum_{i=1}^{n}\left[\ell\left(\hat{\phi}(\mathbf{X}_i), Y_i\right)\right].$$

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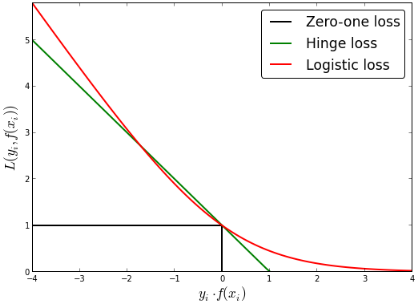

Convexity is (often) crucial

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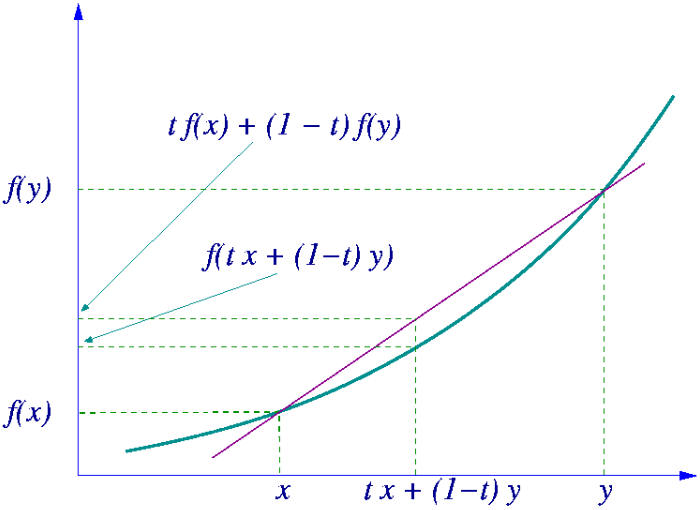

Statistical Learning vs. Machine Learning

Same task, different approaches:

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- In machine learning, given some deterministic sequence $(\mathbf{x}_i, y_i)$, solve

$$\widehat{\phi}(\cdot) = \arg\min_m \left\{ \sum_{i=1}^n \ell(y_i, m(\mathbf{x}_i)) \right\}.$$

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- In statistical learning, assume that the Y_is are realisations of some random variable Y (given $\mathbf{X}$) with distribution P. Solve

$$\widehat{\phi}(\cdot) = \arg\max_m \left\{ \sum_{i=1}^n \log \mathrm{d}P(Y_i; m(\mathbf{X}_i)) \right\}.$$

SL vs. ML in the simple parametric case

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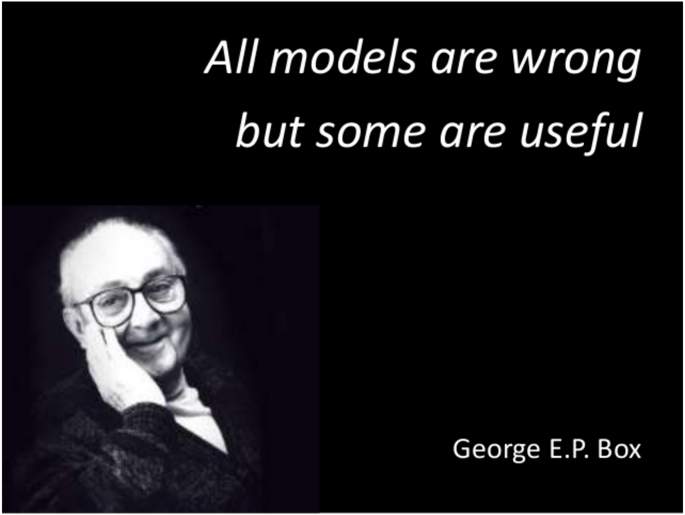
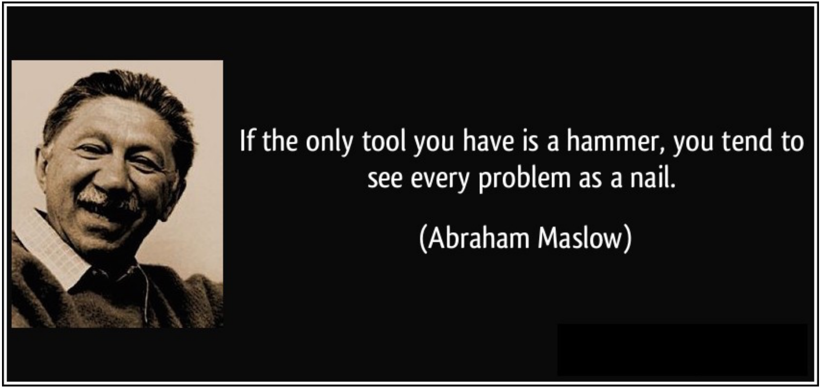
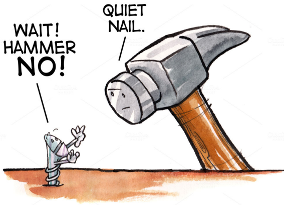

All models are wrong
but some are useful
George E.P. Box


If the only tool you have is a hammer, you tend to see every problem as a nail.
(Abraham Maslow)


WAIT! HAMMER NO!
QUIET NAIL.

A primer on probability distributions

All words are hyperlinks.

A primer on probability distributions

All words are hyperlinks.

- [Normal]

A primer on probability distributions

All words are hyperlinks.

- [Normal]
- [Inverse Gaussian (a.k.a Wald)]

A primer on probability distributions

All words are hyperlinks.

- [Normal]
- [Inverse Gaussian (a.k.a Wald)]
- [Beta]

A primer on probability distributions

All words are hyperlinks.

- [Normal]
- [Inverse Gaussian (a.k.a Wald)]
- [Beta]
- [Poisson]

A primer on probability distributions

All words are hyperlinks.

- [Normal]
- [Inverse Gaussian (a.k.a Wald)]
- [Beta]
- [Poisson]
- [Binomial]

A primer on probability distributions

All words are hyperlinks.

- [Normal]
- [Inverse Gaussian (a.k.a Wald)]
- [Beta]
- [Poisson]
- [Binomial]
- [Bernoulli]

A primer on probability distributions

All words are hyperlinks.

- [Normal]
- [Inverse Gaussian (a.k.a Wald)]
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A primer on probability distributions

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- [Student]
- ...

The Bayesian paradigm

Introductory example

Consider observations $\mathbf{x} = (x_1, \ldots, x_n)$ generated from a probability distribution with density $f(\cdot|\theta)$.

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The associated likelihood is the inverted density:

$$\mathcal{L}(\theta|x) = f(x|\theta).$$

Example $f(\cdot|\theta) = \mathcal{N}(\theta, 1)$.

Bayes' Theorem

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Inversion of probabilities a.k.a actualisation principle.

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If A and B are events such that $\mathbb{P}(B) \neq 0$,

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(B|A)\mathbb{P}(A)}{\mathbb{P}(B|A)\mathbb{P}(A) + \mathbb{P}(B|A^c)\mathbb{P}(A^c)}$$
$$= \frac{\mathbb{P}(B|A)\mathbb{P}(A)}{\mathbb{P}(B)}.$$

(due to Thomas Bayes, published in 1764)

Who was Thomas Bayes?

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Reverend Thomas Bayes (ca. 1702–1761) Presbyterian minister in Kent from 1731. Election to the Royal Society based on a tract of 1736 where he defended the views and philosophy of Newton. Sole probability paper, "Essay Towards Solving a Problem in the Doctrine of Chances", published posthumously in 1763 and containing the seeds of Bayes' Theorem.

A new paradigm

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- Uncertainty on the parameter θ, modeled through a probability distribution π, called *prior distribution*.
- Inference based on the distribution of θ conditional on $\mathbf{X}$ $\pi(\theta|\mathbf{x})$, called *posterior distribution*

$$\pi(\theta|\mathbf{x}) = \frac{f(\mathbf{x}|\theta)\pi(\theta)}{\int f(\mathbf{x}|\theta)\pi(\theta)\mathrm{d}\theta}.$$

A Bayesian model

. . . is made of a parametric (in this course) statistical model defined through its likelihood $f(\mathbf{x}|\theta)$ and a prior distribution on the parameter $\pi(\theta)$.

Consequences

- Semantic drift from unknown to random

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- Actualization of θ by extracting the information contained in the observation $\mathbf{x}$

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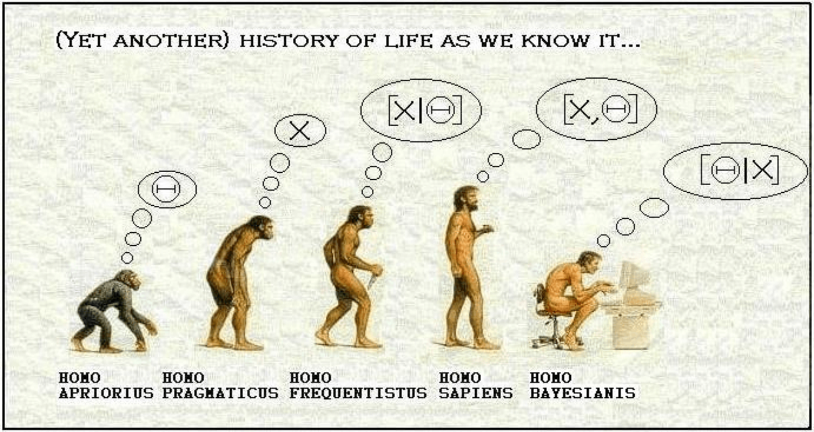
- Semantic drift from unknown to random
- Actualization of θ by extracting the information contained in the observation $\mathbf{x}$
- Allows incorporation of imperfect information in the decision process

The advantages of being a Bayesian



Distributions (1/2)

Given the likelihood $f(\mathbf{x}|\theta)$ and the prior $\pi(\theta)$, several distributions of interest:

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- The *joint distribution* of $(\theta, \mathbf{x})$

$$\varphi(\theta, \mathbf{x}) = f(\mathbf{x}|\theta)\pi(\theta).$$

- The *marginal distribution* of $\mathbf{x}$

$$m(\mathbf{x}) = \int \varphi(\theta, \mathbf{x})\mathrm{d}\theta = \int f(\mathbf{x}|\theta)\pi(\theta)\mathrm{d}\theta.$$

Distributions (2/2)

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- The *posterior distribution* of θ

$$\pi(\theta|\mathbf{x}) = \frac{f(\mathbf{x}|\theta)\pi(\theta)}{\int f(\mathbf{x}|\theta)\pi(\theta)\mathrm{d}\theta} = \frac{f(\mathbf{x}|\theta)\pi(\theta)}{m(\mathbf{x})}.$$

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- The *predictive distribution* of y when $y \sim g(\cdot|\theta, \mathbf{x})$

$$g(y|\mathbf{x}) = \int g(y|\theta, \mathbf{x})\pi(\theta|\mathbf{x})\mathrm{d}\theta.$$

A comprehensive example normal-normal

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&\propto \exp\left(-\frac{(\mathbf{x}-\theta)^2}{2} - \frac{(\theta-a)^2}{20}\right) \\
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$$

which means $\theta|\mathbf{x} \sim \mathcal{N}\left(\frac{10x+a}{11}, \frac{10}{11}\right)$.

A comprehensive example uniform-binomial

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A second ball O then rolls n times under the same assumptions. X denotes the number of times the ball O stopped on the left of W.

Bayes' question: given X, what inference can we make on p?

Mathematical translation

Derive the posterior distribution of p given X, when $p \sim \mathcal{U}(0, 1)$ and $X \sim \mathcal{B}(n, p)$.

Resolution 1/2

Since

$$\mathbb{P}(X = x|p) = \binom{n}{x} p^x (1-p)^{n-x},$$

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and

$$\mathbb{P}(X = x) = \int_0^1 \binom{n}{x} p^x (1-p)^{n-x} \mathrm{d}p,$$

Resolution 2/2

then

$$\mathbb{P}(a < p < b | X = x) = \frac{\int_a^b \binom{n}{x} p^x (1-p)^{n-x} \mathrm{d}p}{\int_0^1 \binom{n}{x} p^x (1-p)^{n-x} \mathrm{d}p} = \frac{\int_a^b \binom{n}{x} p^x (1-p)^{n-x} \mathrm{d}p}{\mathcal{B}(x+1, n-x+1)},$$

i.e., $p|x \sim \mathcal{B}(x+1, n-x+1)$.
(Beta distribution)

Pour se remettre dans le bain

Pour se remettre dans le bain

1. Quelle est la différence entre *statistical learning* et *machine learning* ?
2. Donner la définition d'un algorithme d'apprentissage.
3. Quels sont les quatre grands types d'apprentissage ?
4. Que définissent *fat data* et *tall data* ?
5. Comment compare-t-on les performances d'algorithmes d'apprentissage ?
6. Quelle notion est souvent cruciale au moment de choisir une bonne fonction de perte ? En donner la définition.
7. Donner quelques exemples de fonctions de perte.
8. Enoncer le théorème de Bayes.
9. Quel est le rôle de la distribution *a priori* ?
10. Donner la définition d'un modèle bayésien.
11. Quelles sont les quatre distributions importantes en bayésien ?

The posterior distribution

$$\pi(\theta|\mathbf{x}) \propto f(\mathbf{x}|\theta)\pi(\theta)$$

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- Operates conditional upon the observations.
- Integrates simultaneously prior knowledge and information brought by data.
- Coherent and complete inferential scope and unique motor of inference.
- Usually known up to a constant! $m(\mathbf{x})$ may be intractable.

Prior distributions

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A prior on θ may depend on additional parameters: those are called hyperparameters.

Conjugacy and explicit calculus of posteriors

Conjugate priors are a specific family of distributions with nice analytical properties.

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A family $\mathcal{F}$ of probability distributions is *conjugate* for a likelihood $f(x|\theta)$ if for every $\pi \in \mathcal{F}$, the posterior distribution $\pi(\theta|x)$ also belongs to $\mathcal{F}$.

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A family $\mathcal{F}$ of probability distributions is *conjugate* for a likelihood $f(x|\theta)$ if for every $\pi \in \mathcal{F}$, the posterior distribution $\pi(\theta|x)$ also belongs to $\mathcal{F}$.

Only of interest when $\mathcal{F}$ is parameterized: switching from the prior to the posterior is reduced to an update of parameters.

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- Limited/finite information conveyed by data x

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- Allows for generation of "virtual observations"
- Most importantly: tractability and simplicity

Exponential families

The family of distributions

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Main interest: allow for conjugate priors

$$\pi(\theta|\mu,\lambda) = K(\mu,\lambda)\exp(\theta\mu - \lambda\psi(\theta)), \quad \lambda > 0.$$

Classical exponential families and conjugate priors

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[Examples of exponential families]

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$f(x\|\theta)$	$\pi(\theta)$	$\pi(\theta\|x)$

Classical exponential families and conjugate priors

[Examples of exponential families]

$f(x\|\theta)$	$\pi(\theta)$	$\pi(\theta\|x)$
Normal	Normal	Normal
$\mathcal{N}(\theta, \sigma^2)$	$\mathcal{N}(\mu, \tau^2)$	$\mathcal{N}(\rho(\sigma^2\mu + \tau^2 x), \rho\sigma^2\tau^2)$
		$\rho^{-1} = \sigma^2 + \tau^2$

Classical exponential families and conjugate priors

[Examples of exponential families]

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Poisson $\mathcal{P}(\theta)$	Gamma $\mathcal{G}(\alpha, \beta)$	Gamma $\mathcal{G}(\alpha + x, \beta + 1)$

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Binomial $\mathcal{B}(n,\theta)$	Beta $\mathcal{B}e(\alpha,\beta)$	Beta $\mathcal{B}e(\alpha+x,\beta+n-x)$

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Binomial $\mathcal{B}(n, \theta)$	Beta $\mathcal{B}e(\alpha, \beta)$	Beta $\mathcal{B}e(\alpha + x, \beta + n - x)$
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Normal $\mathcal{N}(\mu, 1/\theta)$	Gamma $\mathcal{G}(\alpha, \beta)$	Gamma $\mathcal{G}(\alpha + 1/2, \beta + (\mu - x)^2/2)$

Non-informative priors: Jeffreys priors

Based on Fisher information:

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Pros & Cons:

- Relates to information theory
- Parameterization invariant
- Suffers from dimensionality curse
- Depends on data: incoherence with the likelihood principle

Example

If $x \sim \mathcal{B}(n, \theta)$, Jeffreys' prior is

$$\pi(\theta) \propto \mathcal{B}e(1/2, 1/2).$$

If $n \sim \mathrm{Neg}(x, \theta)$, Jeffreys' prior is

$$\pi(\theta) \propto \theta^{-1}(1-\theta)^{-1/2}$$

Non-informative priors: Laplace priors

With a finite set $\{\theta_1, \ldots, \theta_p\}$, uniform prior $\pi(\theta_i) = 1/p$.

Non-informative priors: Laplace priors

With a finite set $\{\theta_1, \dots, \theta_p\}$, uniform prior $\pi(\theta_i) = 1/p$.

Continuous extension: $\pi(\theta) \propto 1$. This is no longer a probability distribution yet if $\int f(x|\theta)\mathrm{d}\theta < +\infty$, the posterior is well-defined as a probability distribution. Modeling is crucial. Weakness: lack of reparameterization invariance.

Pour se remettre dans le bain

- Expliquer l'intérêt de la conjugaison, et en donner la définition.
- Quel est l'intérêt d'utiliser une vraisemblance issue d'une famille exponentielle naturelle ?
- Donner des exemples de lois conjuguées.
- Donner deux exemples de méthodes de construction de priors non-informatifs. Quelles sont les limites de ces méthodes ?

Bayesian estimators

Bayesian paradigm is based on the posterior distribution.

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Bayesian paradigm is based on the posterior distribution.

Many estimators may be derived from the posterior.

MAP

The maximum a posteriori estimator is defined as

$$\arg\max_{\theta} \; f(x|\theta)\pi(\theta)$$

(penalized likelihood estimator).

Binomial example

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Consider $x|\theta \sim \mathcal{B}(n, \theta)$.
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$$\pi(\theta) = \frac{1}{\mathcal{B}(1/2,1/2)}\theta^{-1/2}(1-\theta)^{-1/2} \; \Big| \; \hat{\theta} = \max\left(\frac{x-1/2}{n-1}, 0\right)$$

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Not always appropriate!

Consider $f(x|\theta) = \frac{1}{\pi}\left(1 + (x-\theta)^2\right)^{-1}$ and $\pi(\theta) = \frac{1}{2}\exp(-|\theta|)$.

Not always appropriate!

Consider $f(x|\theta) = \frac{1}{\pi}\left(1 + (x-\theta)^2\right)^{-1}$ and $\pi(\theta) = \frac{1}{2}\exp(-|\theta|)$.

The MAP is $\hat{\theta} = 0$!

Other possible estimators

- Mean: $\hat{\theta} = \mathbb{E}_{\theta \sim \pi(\cdot|x)} \theta = \int \theta \pi(\theta|x) \mathrm{d}\theta.$

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- Realization: $\hat{\theta} \sim \pi(\cdot|x)$.
- ...

Credible regions

Natural confidence region: highest posterior density (HPD).

$$\mathcal{C}^{\pi}_{\alpha} = \{\theta; \pi(\theta|x) > \alpha \}.$$

Prediction

Reminder: if $x \sim f(\cdot|\theta)$ and $z \sim g(\cdot|x,\theta)$, the *predictive* distribution is

$$g^{\pi}(z|x) = \int g(z|x,\theta)\pi(\theta|x)\mathrm{d}\theta.$$

Example: normal prediction

Assume that $(x_1, \ldots, x_n) \sim \mathcal{N}(\mu, \sigma^2)^{\otimes n}$ and

$$\pi(\mu, \sigma^2) \propto (\sigma^2)^{-\lambda_\sigma - 3/2} \exp\left(\frac{-\lambda_\mu(\mu - \xi)^2 + \alpha}{2\sigma^2} \right).$$

The posterior is

$$\mathcal{N}\left(\frac{\lambda_\mu \xi + n\bar{x}_n}{\lambda_\mu + n}, \frac{\sigma^2}{\lambda_\mu + n} \right) \times \mathcal{IG}\left(\lambda_\sigma + n/2, \frac{\alpha + s_x^2 + \frac{n\lambda_\mu(\bar{x}_n - \xi)^2}{\lambda_\mu + n}}{2} \right).$$

(where $s_x^2 = \frac{1}{n}\sum_{i=1}^n (x_i - \bar{x}_n)^2$)

$$
\begin{aligned}
g^\pi(z|x_1,\dots,x_n) \propto & \int (\sigma^2)^{-\lambda_\sigma-2-n/2} \exp(-(z-\mu)^2/2\sigma^2) \\
& \times \exp\left(-(\lambda_\mu+n)\left(\mu-\frac{\lambda_\mu\xi+n\bar{x}_n}{\lambda_\mu+n}\right)^2+\alpha+s_x^2+\frac{n\lambda_\mu(\bar{x}_n-\xi)^2}{\lambda_\mu+n}\right)/2\sigma^2 \\
& \quad \times \mathrm{d}(\mu,\sigma^2) \\
\propto & \left[\alpha+s_x^2+\frac{n\lambda_\mu(\bar{x}_n-\xi)^2}{\lambda_\mu+n}+\frac{\lambda_\mu+n+1}{\lambda_\mu+n}\left(z-\frac{\lambda_\mu\xi+n\bar{x}_n}{\lambda_\mu+n}\right)^2\right]^{-(2\lambda_\sigma+n+1)/2}
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\end{aligned}
$$

Student t distribution with mean $\frac{\lambda_\mu\xi+n\bar{x}_n}{\lambda_\mu+n}$ and $2\lambda_\sigma+n$ degrees of freedom.

Quasi-Bayesian learning, and a foretaste of PAC-Bayesian theory

The quasi-Bayesian approach

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Set of candidates $\mathcal{F}$ equipped with a probability measure π (prior).

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for some inverse temperature $\lambda > 0$.

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Key fact!

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for some inverse temperature $\lambda > 0$.

Key fact! In general, $\exp\left(-\lambda R_n(\cdot)\right)$ is not a likelihood, hence the term quasi-Bayesian.

A generalization of Bayesian learning

The pseudo-likelihood term $\exp(-\lambda R_n(\cdot))$ is to be seen as a data fit term. However no model is attached to this representation! Quasi-Bayesian learning natively is a model-free learning paradigm.

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The pseudo-likelihood term $\exp(-\lambda R_n(\cdot))$ is to be seen as a data fit term. However no model is attached to this representation! Quasi-Bayesian learning natively is a model-free learning paradigm.

Tradeoff between interpretability (Bayesian modeling) and performance (quasi-Bayesian prediction). Echoes the celebrated similar tradeoff between ML and SL!

The missing link between machine learning and statistical learning?

Reminder:

- In ML, deterministic sequence $(\mathbf{x}_i, y_i)$,

$$\widehat{\phi}(\cdot) = \arg\min_m \left\{ \sum_{i=1}^n \ell(y_i, m(\mathbf{x}_i)) \right\}.$$

- In SL, random variables,

$$\widehat{\phi}(\cdot) = \arg\max_m \left\{ \sum_{i=1}^n \log \mathrm{d}P(Y_i; m(\mathbf{X}_i)) \right\}.$$

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Quasi-Bayesian learning is a model-free approach yet relies on a stochastic assumption! Joining the best of two worlds.

A variational perspective

A variational perspective

With the classical quadratic loss $\ell\colon (a, b) \mapsto (a - b)^2$,

$$\widehat{\rho}_\lambda \in \operatorname*{arg\,inf}_{\rho \ll \pi} \left\{ \int_{\mathcal{F}} R_n(\phi)\rho(\mathrm{d}\phi) + \frac{\mathcal{K}(\rho, \pi)}{\lambda} \right\},$$

where $\mathcal{K}$ is the Kullback-Leibler divergence defined as

$$\mathcal{K}(\rho, \pi) = \begin{cases} \int_{\mathcal{F}} \log\left(\frac{\mathrm{d}\rho}{\mathrm{d}\pi}\right) \mathrm{d}\rho & \text{when } \rho \ll \pi, \\ +\infty & \text{otherwise.} \end{cases}$$

Typical quasi-Bayesian estimators

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MAQP

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Realization

$$\widehat{\phi}_\lambda \sim \widehat{\rho}_\lambda.$$

And so on.

Statistical aggregation revisited

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Assume that $\mathcal{F}$ is finite.

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The mean of the quasi-posterior $\widehat{\rho}_\lambda$ amounts to the celebrated exponentially weighted aggregate (EWA)

$$\widehat{\phi}_\lambda = \mathbb{E}_{\widehat{\rho}_\lambda} \phi = \sum_{i=1}^{\#\mathcal{F}} \omega_{\lambda,i} \phi_i$$

where

$$\omega_{\lambda,i} = \frac{\exp[-\lambda R_n(\phi_i)]\pi(\phi_i)}{\sum_{j=1}^{\#\mathcal{F}} \exp[-\lambda R_n(\phi_j)]\pi(\phi_j)}.$$

Guedj (2013). Agrégation d'estimateurs et de classificateurs : théorie et méthodes, *Ph.D. thesis, Université Pierre & Marie Curie*

Pour se remettre dans le bain

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1. Citer les quatre estimateurs bayésiens les plus couramment utilisés.
2. Qu'est-ce qu'une région de crédibilité ?
3. Comment prédire quand on est bayésien(ne) ?
4. Décrire l'approche quasi-bayésienne.
5. Pourquoi l'approche quasi-bayésienne peut-elle être vue comme une généralisation de l'apprentissage bayésien ?
6. Illustrer la provenance du quasi-posterior au moyen d'une formulation variationnelle.
7. Citer les quatre estimateurs quasi-bayésiens les plus couramment utilisés.
8. Rappeler le principe de l'ERM et de l'agrégation à poids exponentiels (EWA). Quel est le lien entre EWA et apprentissage quasi-bayésien ?

Assessing the performance: the oracle approach

Oracle:

$$\phi^\star \in \arg\min_{\phi \in \mathcal{Y}^{\mathcal{X}}} R(\phi).$$

Ultimate goal: do almost as well as the oracle.

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Excess risk:

$$\mathcal{E}(\cdot) = R(\cdot) - R^\star \geq 0, \qquad R^\star = R(\phi^\star).$$

PAC oracle inequalities

PAC oracle inequalities

Let $R^\star$ denote the oracle risk. For any $\epsilon > 0$,

$$\mathbb{P}\left(R\left(\widehat{\phi}_\lambda\right) - R^\star \leq \spadesuit \inf_{\phi \in \mathcal{F}} \left\{R(\phi) - R^\star + \frac{\Delta(\phi, \epsilon)}{n^\alpha}\right\}\right) \geq 1 - \epsilon,$$

where $\spadesuit \geq 1$ and $\lambda \propto n$. If $\spadesuit = 1$, the inequality is *exact* or *sharp*.

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Key argument: concentration inequalities (*e.g.*, Bernstein, Hoeffding) + Legendre transform of the Kullback-Leibler divergence.

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- $\alpha = \frac{1}{2}$ (slow rate)
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- $\Delta(\phi, \epsilon) \propto d + \log \frac{1}{\epsilon}$
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The remainder term grows with d and the size of $\mathcal{F}$. It decreases with n.

Hoeffding inequality

Let $V_1, \dots, V_n$ be independent real-valued random variables such that $a_i \leq V_i \leq b_i$ a.s. Let $\bar{V}_n = \frac{1}{n} \sum_{i=1}^{n} V_i$.

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$$\mathbb{P}(\bar{V}_n - \mathbb{E}\bar{V}_n > t) \leq \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right), \forall t > 0.$$

Lemma (Csiszar, 1975 ; Catoni, 2004)

Let $(A, \mathcal{A})$ *be a measurable space. For any probability* μ *on* $(A, \mathcal{A})$ *and any measurable function* $h : A \to \mathbb{R}$ *such that* $\int (\exp \circ h) \mathrm{d}\mu < \infty$,

$$\log \int (\exp \circ h) \mathrm{d}\mu = \sup_{m \in \mathcal{M}_\pi(A, \mathcal{A})} \left\{ \int h \mathrm{d}m - \mathcal{K}(m, \mu) \right\},$$

with the convention $\infty - \infty = -\infty$. *Moreover, as soon as* h *is upper-bounded on the support of* μ, *the supremum with respect to* m *on the right-hand side is reached for the Gibbs distribution* g *given by*

$$\frac{\mathrm{d}g}{\mathrm{d}\mu}(a) = \frac{\exp \circ h(a)}{\int (\exp \circ h) \mathrm{d}\mu}, \quad a \in A.$$

The PAC-Bayesian theory

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...consists in producing PAC inequalities of quasi-Bayesian estimators.

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Shawe-Taylor and Williamson (1997). A PAC analysis of a Bayes estimator, *COLT*

McAllester (1998). Some PAC-Bayesian theorems, *COLT*

McAllester (1999). PAC-Bayesian model averaging, *COLT*

Catoni (2004). Statistical Learning Theory and Stochastic Optimization, Springer

Audibert (2004). Une approche PAC-bayésienne de la théorie statistique de l'apprentissage, *Ph.D. thesis, Université Pierre & Marie Curie*

Catoni (2007). PAC-Bayesian Supervised Classification: The Thermodynamics of Statistical Learning, IMS

Dalalyan and Tsybakov (2008). Aggregation by exponential weighting, sharp PAC-Bayesian bounds and sparsity, *Machine Learning*

Alquier and Lounici (2011). PAC-Bayesian theorems for sparse regression estimation with exponential weights, *Electronic Journal of Statistics*

Guedj (2019). A Primer on PAC-Bayesian Learning, *arXiv preprint*

A flexible and powerful framework

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- Alquier and Wintenberger (2012). Model selection for weakly dependent time series forecasting, *Bernoulli*
- Seldin, Laviolette, Cesa-Bianchi, Shawe-Taylor and Auer (2012). PAC-Bayesian inequalities for martingales, *IEEE Transactions on Information Theory*
- Alquier and Biau (2013). Sparse Single-Index Model, *Journal of Machine Learning Research*
- Guedj and Alquier (2013). PAC-Bayesian Estimation and Prediction in Sparse Additive Models, *Electronic Journal of Statistics*
- Alquier and Guedj (2017). An Oracle Inequality for Quasi-Bayesian Non-Negative Matrix Factorization, *Mathematical Methods of Statistics*
- Guedj and Robbiano (2018). PAC-Bayesian High Dimensional Bipartite Ranking, *Journal of Statistical Planning and Inference*
- Li, Guedj and Loustau (2018). A Quasi-Bayesian Perspective to Online Clustering, *Electronic Journal of Statistics*

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Li, Guedj and Loustau (2018). A Quasi-Bayesian Perspective to Online Clustering, *Electronic Journal of Statistics*

Towards (almost) no assumptions to derive powerful results

Bégin, Germain, Laviolette and Roy (2016). PAC-Bayesian bounds based on the Rényi divergence, *AISTATS*

Alquier and Guedj (2018). Simpler PAC-Bayesian bounds for hostile data, *Machine Learning*

Sampling

Monte Carlo integration

Objective: approximation of an integral

$$\mathcal{J} = \int h(x)f(x)\mathrm{d}x.$$

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$$\mathcal{J} = \int h(x) f(x) \mathrm{d}x.$$

Key idea: exploit the fact that $\mathcal{J} = \mathbb{E}_{X \sim f}[h(X)]$.

Monte Carlo principle

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Sample a sequence $x_1, \ldots, x_m \sim f$.

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Justification: by the Strong Law of Large Numbers,

$$\hat{\mathcal{J}}_m \to \mathcal{J}.$$

Approximation evaluation

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Estimate the variance with

$$\nu_m = \frac{1}{m} \frac{1}{m-1} \sum_{i=1}^{m} (h(x_i) - \hat{\mathfrak{I}}_m)^2,$$

Approximation evaluation

Estimate the variance with

$$\nu_m = \frac{1}{m}\frac{1}{m-1}\sum_{i=1}^{m}(h(x_i) - \hat{\mathfrak{J}}_m)^2,$$

and recall that for m large,

$$\frac{\hat{\mathfrak{J}}_m - \mathbb{E}[h(X)]}{\sqrt{\nu_m}} \approx \mathcal{N}(0,1).$$

Importance sampling

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$$\begin{aligned}\mathbb{E}_{X\sim f}[h(X)] = \int h(x)f(x)\mathrm{d}x = \int h(x)\frac{f(x)}{g(x)}g(x)\mathrm{d}x \\ = \mathbb{E}_{X\sim g}\left[h(X)\frac{f(X)}{g(X)}\right],\end{aligned}$$

which allows us to use other distributions.

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$$\hat{\mathfrak{I}}_m = \frac{1}{m}\sum_{i=1}^{m} \frac{f(x_i)}{g(x_i)} h(x_i)$$

as an estimator of $\mathfrak{I}$.

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Justification

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2. Instrumental distribution g may be chosen among distributions easy to simulate.

3. The same sample generated from g can be used repeatedly, not only for different functions h but also for different densities f.

Choice of importance function

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The optimal choice is

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The instrumental function may be π (the prior). But often inefficient if data informative, and impossible is π is improper...

Sampling random variables

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If $U \sim \mathcal{U}(0, 1)$, let F denote a CDF, then $F^{-}(U)$ is a random variable with distribution $\mathrm{d}F$.

In practice, this theorem has a very limited scope since the pseudo-inverse F^{-} is usually unknown/not analytically tractable.

Accept-reject

Goal: sample $x \sim f$.

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Ingredients: a density g such that

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- sampling from g is easy

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The algorithm:

1. Sample $z \sim g$ and $u \sim \mathcal{U}(0, Mg(z))$
2. If $u \leq f(z)$, take $x = z$, otherwise go back to 1.

How should we choose g?

The mean number of samples to obtain 1 realization is M!
Efficient algorithm $= M$ close to 1.

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Nice fact: no need to know the normalizing constant of f!

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Examples: let (u_t) be a sequence of i.i.d variables

- $X_0 \sim \pi_0$ and $X_t = \rho X_{t-1} + u_t$
- More generally $X_t = g(X_{t-1}, u_t)$ for any measurable function g

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Burn-in period to reach convergence and stabilize the algorithm.

Construction and key properties

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A Markov chain is fully defined by

- The distribution of X_0
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Irreducible chain: every region of the state may be reached.

- Transient: the mean number of passages is finite
- Recurrent: coming back is assured

Invariant distribution: the chain admits an invariant distribution f is there exists a density f such that

$$x_t \sim f \implies x_{t+1} \sim f.$$

The chains built by MCMC algorithms admit a unique invariant distribution.

Convergence

Convergence

Given a density f, we are interested in transition dynamics such that

- The invariant distribution is unique (f)
- The distribution of x_t is "close" to the invariant density whenever t is large enough (total variation norm).
- Ergodic theorem

$$\frac{1}{T}\sum_{t=1}^{T} h(x_t) \xrightarrow[T\to\infty]{} \int h(x)f(x)\mathrm{d}x$$

Metropolis-Hastings (MH) algorithm

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Algorithm: at time $t+1$,

$$x_{t+1} = \begin{cases} z \sim q(\cdot|x_t) & \text{with probability } \rho, \\ x_t & \text{otherwise} \end{cases}$$

where

$$\rho = \min\left\{1, \frac{f(z)q(x_t|z)}{f(x_t)q(z|x_t)}\right\}.$$

Key properties

The chain produced by the MH algorithm

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The chain produced by the MH algorithm

1. is irreducible
2. is ergodic
3. admits f as an invariant distribution

Examples of instrumental / proposal distribution

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   This generalizes the accept-reject algorithm.

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   This generalizes the accept-reject algorithm.

2. Symmetric distributions

$$q(z|x_t) = h(|z - x_t|).$$

   The acceptation ratio does not depend on q:

$$\rho = \min\left(1, \frac{f(z)}{f(x_t)}\right).$$

Random walks

Given x_t, the transition dynamic writes

$$z = x_t + \epsilon$$

where (ϵ_t) is a sequence of i.i.d variables, independent from (x_t), and the distribution of ϵ is symmetric with respect to 0. Examples:

- normal distributions $\mathcal{N}(0, \sigma^2)$
- uniform distribution on symmetric intervals $\mathcal{U}(-a, a)$
- ...

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Key idea: decomposition of $x \in \mathbb{R}^p$ in blocks such that the conditional distributions $f_j(x_j | x_i, i \neq j)$, $j = 1, \ldots, p$ are easy to sample.

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1. ergodic
2. with f as invariant distribution

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Goal: minimize a differentiable function f (compute $\arg\min_x f(x)$).

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While $f'(x_k) \geq \epsilon$ $x_{k+1} = x_k - \alpha f'(x_k)$

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Instead of an infinite-dimensional functional space $\mathcal{F}$, we often resort to some projection onto $\mathbb{R}^d$.

Sampling from a d-dimensional non-standard distribution is still an algorithmic challenge.

Existing implementation

- (Transdimensional) MCMC

  Guedj and Alquier (2013). PAC-Bayesian Estimation and Prediction in Sparse Additive Models, *Electronic Journal of Statistics*

  Alquier and Biau (2013). Sparse Single-Index Model, *Journal of Machine Learning Research*

  Guedj and Robbiano (2018). PAC-Bayesian High Dimensional Bipartite Ranking, *Journal of Statistical Planning and Inference*

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Bridging the gap between theory and algorithms

Goal: PAC oracle inequalities for approximations of $\widehat{\rho}_\lambda$ (echoes the celebrated statistical / computational tradeoff).

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MCMC for online (sequential) quasi-Bayesian learning: the stationary distribution of the Markov Chain is indeed $\widehat{\rho}_\lambda$.

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Conclusion

Take-home messages

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- Algorithmic challenges: tractable methods which scale up to modern (massive and complex) data

Take-home messages

- Sound mathematical foundations for statistical learning (machine learning with a probabilistic perspective)
- Frequentist vs. Bayesian paradigms: uncertainty matters!
- Bayesian models vs. quasi-Bayesian prediction
- Algorithmic challenges: tractable methods which scale up to modern (massive and complex) data
- A very exciting field to work in!

Benjamin Guedj, Ph.D.

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