Forschungszentrum Jülich
Jülich Supercomputing Centre (JSC)

Training Course # 107/2017

Introduction to descriptive and parametric statistic with R

The Thursday 9th of March 2017 from 9:00 to 16:00 in Besprechungsraum 2 (room 315), Building 16.3

Antoine Tordeux — Forschungszentrum Jülich and Wuppertal University

PHONE: 0049 2461 61 96553 — EMAIL: a.tordeux@fz-juelich.de

Content

Introduction to descriptive and parametric statistic with R

The objectives are both to propose useful **statistical methods** allowing to analyze data, or to develop and calibrate models (Master level), as well as to learn how to **use R**.

The course is organized in three sessions of two hours :

- Session 1 : **Introduction to statistic and R package**
- Session 2 : **Statistic for multivariate dataset**
- Session 3 : **Parametric statistic and statistical inference**

Git : `gitlab.version.fz-juelich.de`
Download R : `cran.r-project.org`

History

The term ‘Statistic’ initially refers to the **collection of information by states**

- Etymology from the New Latin *statisticum* and the German words *Statistik* and *Staatskunde* (18th century)
- **Counting** of demographic and economic data

Statistic in the modern sense refers to the **collection, analysis, modelling and interpretation of information of all types**

- **Statistical inference** : Statistical activity associated with the probability theory
- Development of statistical **models for understanding** Physic, biology, social science, ...
  Parameter estimation and interpretation
- Development of statistical **models for prediction** Engineering, social science, ...
  Knowledge discovery, data mining and machine learning

Context

Data : n **independent** observations of **characteristics** (of individuals, systems...) or **results of experiments**

⚠ Sample is **not a time series** (order of the observations has no importance)

⇝ Stochastic processes for dynamical systems

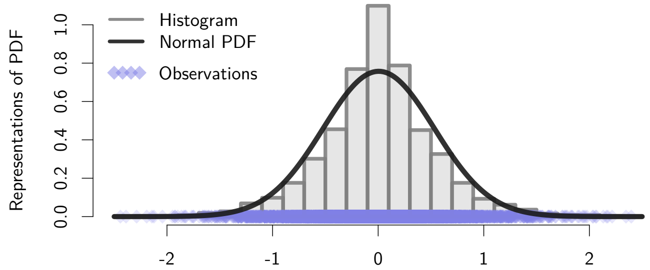
Statistic : Mathematical tools allowing to **present, resume, explain or predict some data**, and to **develop and calibrate models**

- **Loose of information** (data too big to individually analyze each observation)
- Focus on **phenomena of interest, tendencies, global performances**

Descriptive statistic : Tools describing data with no probabilist assumptions

Parametric statistic : Probabilist assumptions on the distributions of the data

Illustrative example



Representations of PDF by

Histogram :	**Descriptive estimation**
Normal PDF :	**Parametric estimation**

Statistical packages

Product	Description	Creation Date	Open Source	Written in Scripting	Support
MatLab `mathworks.com`	Platform for numerical computing	1970's		C++, java MatLab	Windows, Mac OS, Linux
SAS `sas.com`	Statistical analysis system	1974		C SAS language	Windows, Linux
SPSS `ibm.com`	Software package for statistical analysis	1968		java R, Python	Windows, Mac OS, Linux
Stata `stata.com`	General-purpose statistical software	1985		C ado, Mata	—
Statistica `dell.com`	Advanced analytics software package	1991		C++ R, SVB	Windows
R `r-project.org`	Software environment for statistical computing	1993	×	C, Fortran R language	Windows, Mac OS, Linux
SciLab `scilab.org`	Open-source alternative to MatLab	1990	×	C, C++, java SciLab	—
PSPP `gnu.org`	Open-source alternative to SPSS	1998	×	C Pearl	—
SciPy `scipy.org`	Python library for scientific computing	1992	×	C, Fortran Python	—

And many others ... (see for instance `Wikipedia : Statistical packages`)

R software environment[1]

R is a **open source programming language**
and environment for **statistical computing** and graphics

> Implementation of S language — **Functional programming**
> Computation in R consists of **sequentially evaluating statements**
> separated by semi-colon or new line, and that can be grouped using braces

Windows :	**The terminal** — **The script** (eventual) — **The plots** (eventual)
Help with R :	`?`*name_of_a_function* or `help(`*name_of_a_function*`)`

 # Variable, vector, operations

```
pi*sqrt(10)+exp(4)
2:7
seq(0,1,0.1)
x=c(1,2,3);y=c(4,5)
z=c(x,y)
z∧2;log(z)
```

 # Main control structures

```
x=7
if(x>0) y=0
for(i in 1:7)
  x=x+i
while(y>1)
  y=y/2
```

 # Functions

```
exp(2)
?exp
exp_app=function(x,n)
  sum(x∧n/factorial(n))
exp_app(2,1:5)
```

[1] 1993, GNU General Public License, `r-project.org`

Overview

Part 1 Descriptive statistics for univariate and bivariate data

Repartition of the data (histogram, kernel density, empirical cumulative distribution function), order statistic and quantile, statistics for location and variability, boxplot, scatter plot, covariance and correlation, QQplot

Part 2 Descriptive statistics for multivariate data

Least squares and linear and non-linear regression models, principal component analysis, principal component regression, clustering methods (K-means, hierarchical, density-based), linear discriminant analysis, bootstrap technique

Part 3 Parametric statistic

Likelihood, estimator definition and main properties (bias, convergence), punctual estimate (maximum likelihood estimation, Bayesian estimation), confidence and credible intervals, information criteria, test of hypothesis, parametric clustering

Appendix LaTeX plots with R and Tikz

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Appendix LaTeX plots with R and Tikz

Data used

Experiments with pedestrians on a ring

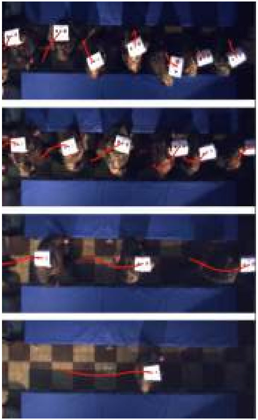
→ 11 experiments done for different density levels

Measurement of :

Spacing
(position difference with predecessor)

Speed
(position time-difference)

Acceleration rate
(speed time-difference)



Descriptive statistics for univariate data

$$(x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$$

Histogram — R : hist(x)

Counting of the observations on a regular **partition** $(I_j)_j$ with **window** δ

$$\forall j, x \in I_j, \quad \tilde{h}(x) = \sum_{i=1}^{n} \mathbb{1}_{I_j}(x_i) \qquad \text{with} \quad \mathbb{1}_I(x) = \begin{cases} 1 & \text{if } x \in I \\ 0 & \text{otherwise} \end{cases}$$

$\rightarrow$ **Normalized histogram** $h(x) = \frac{1}{\delta n}\,\tilde{h}(x)$ is used for the estimation of the PDF

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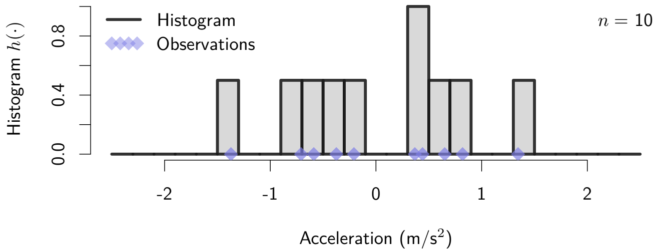

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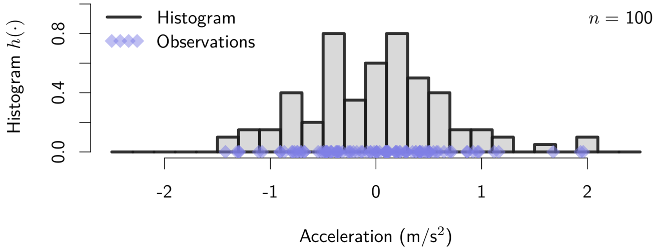

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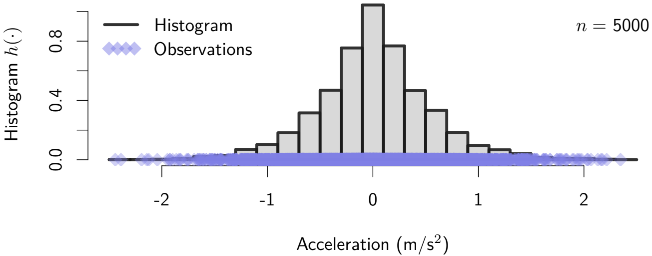

Kernel density — `R : density(x)`

Kernel continuous estimation of the PDF

$$d(x) = \frac{1}{nb}\sum_{i=1}^{n} k((x - x_i)/b) \qquad \text{with } b > 0 \textbf{ the bandwidth}$$

→ **kernel** $k(.)$ such that $\int k(x)\,\mathrm{d}x = 1$ and $k(x) = k(-x)$

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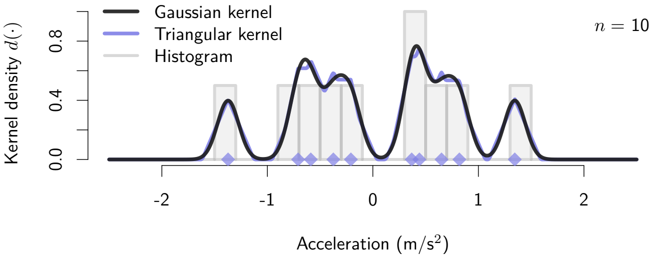

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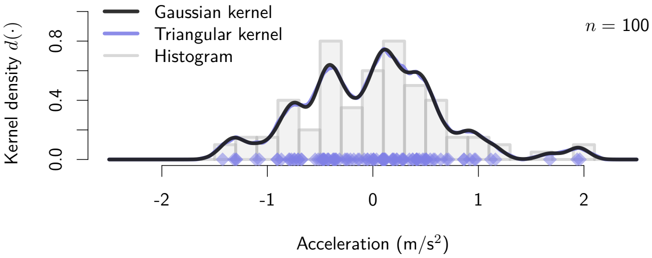

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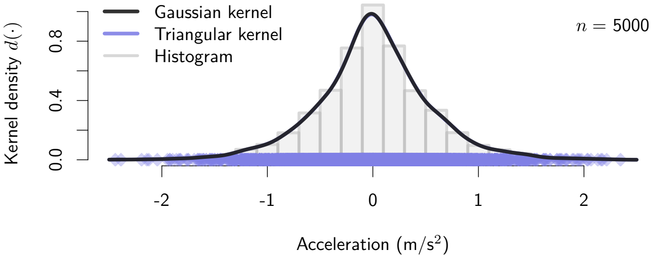

Cumulative distribution function — `R : ecdf(x)`

Empirical cumulative distribution function (ECDF)

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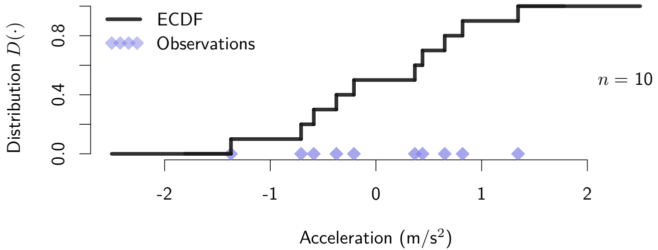

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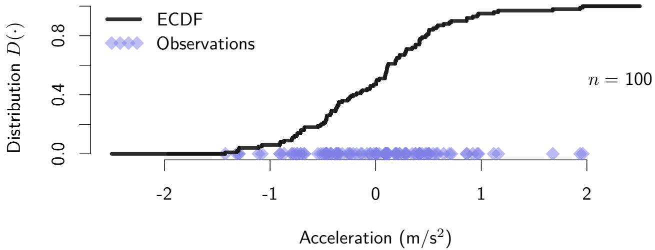

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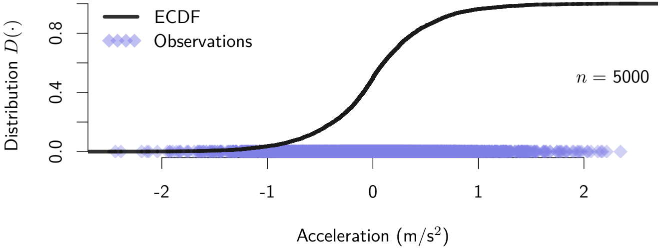

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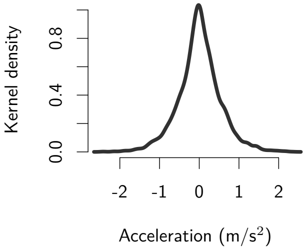

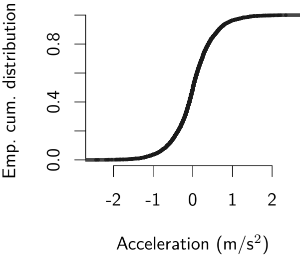

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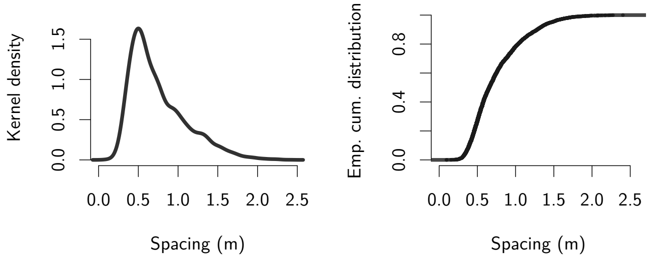

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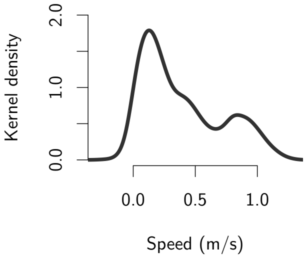
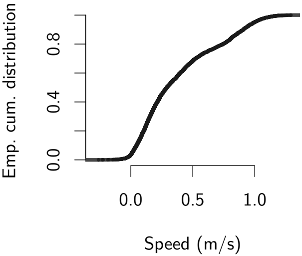
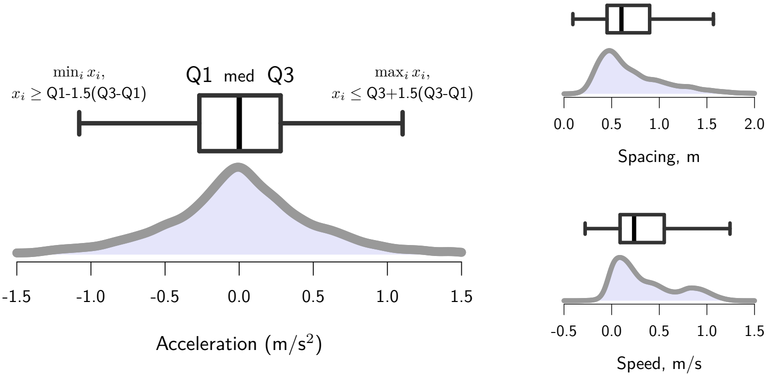




Boxplot — R : boxplot(x)



50% of the data **into the box** — 50% **right (resp. left) to the median**
Normal distribution : $\geq 95\%$ of the data **into the whiskers**
Different definitions for the whiskers exit (0.01/0.99-quantiles, minimum/ maximum, ...)

Order statistic and quantile — R : `sort(x)`, `quantile(x,·)`

Univariate data : $x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$

$(i_1, \ldots, i_n)$ is a permutation of the ID $(1, \ldots, n)$ such that $x_{i_1} \leq x_{i_2} \leq \ldots \leq x_{i_n}$

- The k**-th order statistic** is $x^{(k)} = x_{i_k}, \quad k = 1, \ldots, n$
  - $\rightarrow$ k is the **rank variable** : $k-1$ observations smaller, $n-k+1$ bigger
- The α**-quantile** is $q_x(\alpha) = x^{([\alpha n])}, \quad \alpha \in [0,1]$
  - $\rightarrow$ α % of the data smaller, $1-\alpha$ % bigger

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Unique values if $x_{i_1} < x_{i_2} < \ldots < x_{i_n}$

Minimum and maximum values are : $\min_i x_i = q_x(0) = x^{(1)}$, $\max_i x_i = q_x(1) = x^{(n)}$

Statistics stable by monotone transformation f :

$$(f(x))^{(k)} = \begin{cases} f\left(x^{(k)}\right) \\ f\left(x^{(n-1-k)}\right) \end{cases} \quad \text{and} \quad q_{f(x)}(\alpha) = \begin{cases} f\left(q_x(\alpha)\right) & \text{if } f \nearrow \\ f\left(q_{fx}(1-\alpha)\right) & \text{if } f \searrow \end{cases}$$

Statistic for the location — `R : mean(x), median(x)`

Three main statistics for the **central position** of univariate data $x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$

- **Arithmetic mean** value (or mean value) $\bar{x} = \frac{1}{n} \sum_i x_i$ `R : mean(x)`
- **Median** (central observation) $med_x = x^{([n/2])} = q_x(0.5)$ `median(x)`
- **Mode** (most probable value) $mod_x = sup_z \, \mathrm{PDF}_x(z)$ `x[pdf(x)==max(pdf(x))]`

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$\bar{x} = med_x = mod_x$ **for uni-modal symmetric repartition of the data**

Mean and median solution of : $\bar{x} = \arg\min_a \sum_i (x_i - a)^2$ and $med_x = \arg\min_a \sum_i |x_i - a|$

Mean sensible to extreme values, median or mode not (if $x_i \to \infty$ then $\bar{x} \to \infty$ but med_x, $mod_x \not\to \infty$)

Median and mode stable by monotone transform $med_{f(x)} = f(med_x)$, $mod_{f(x)} = f(mod_x)$
But the mean is not :

$$\frac{1}{n} \sum_i f(x_i) \quad \begin{matrix} \leq \\ = \\ \geq \end{matrix} \quad f(\bar{x}) \quad \begin{matrix} \text{if } f \text{ is concave} \\ \text{if } f \text{ is affine} \\ \text{if } f \text{ is convex} \end{matrix}$$

(Jensen inequality)

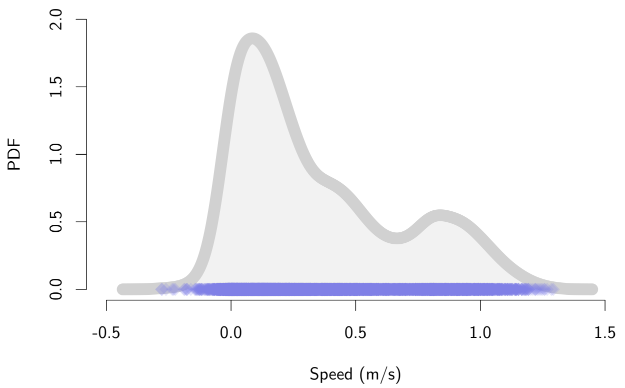
Other statistics for the location

Average		Example (1, 2, 3)	R
Harmonic	$\bar{x}_H = \left(\frac{1}{n}\sum_i 1/x_i\right)^{-1}$	$1.\underline{64}$	`1/mean(1/x)`
Geometric	$\bar{x}_G = \sqrt[n^{-1}]{\prod_i x_i}$	1.82	`prod(x)^{1/length(x)}`
Arithmetic	$\bar{x}_A = \frac{1}{n}\sum_i x_i$	2	`mean(x)`
Quadratic	$\bar{x}_Q = \sqrt{\frac{1}{n}\sum_i x_i^2}$	2.16	`sqrt(mean(x^2))`
Temporal	$\bar{x}_T = \sum_i x_i^2 / \sum_i x_i$	$2.\underline{3}$	`mean(x^2)/mean(x)`

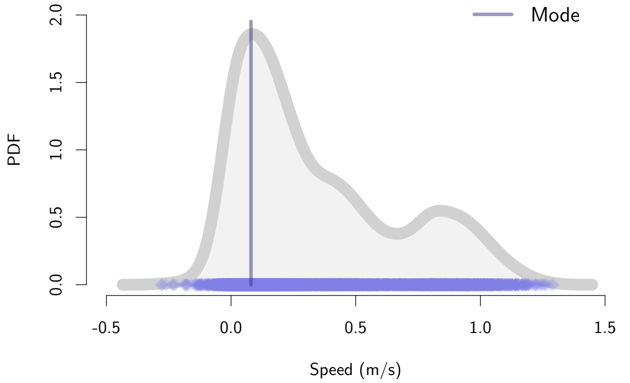
→ If $x_i > 0$ for all i, then we have[2]: $\bar{x}_H \leq \bar{x}_G \leq \bar{x}_A \leq \bar{x}_Q \leq \bar{x}_T$

[2] We have more generally for $x_i > 0$ and $\bar{X}_m = \sqrt[m^{-1}]{\frac{1}{N}\sum_i x_i^m}$ $\bar{X}_m \leq \bar{X}_{m'}$ for all $m \leq m'$

Example



Example



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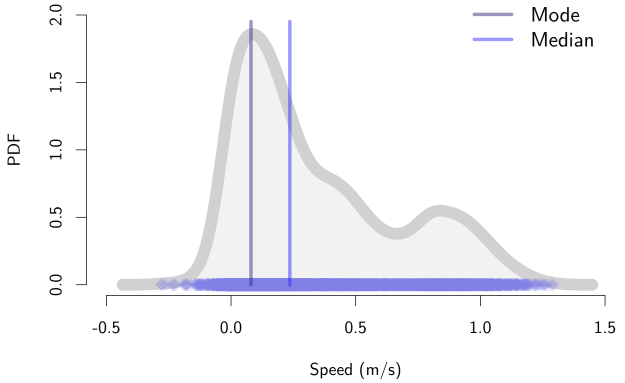

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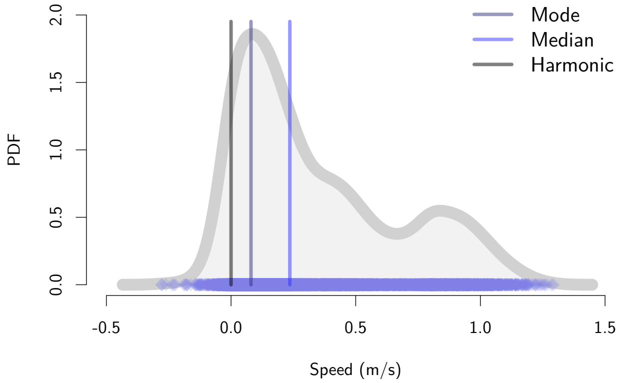

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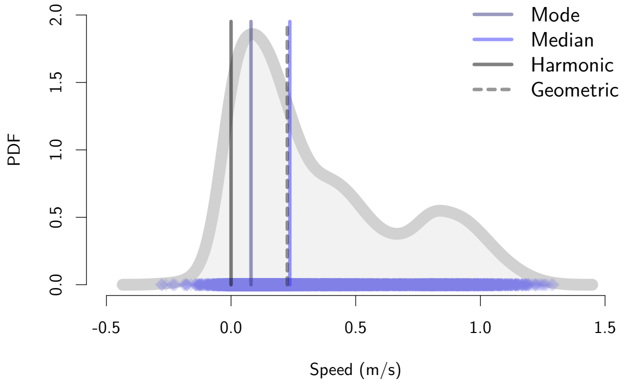
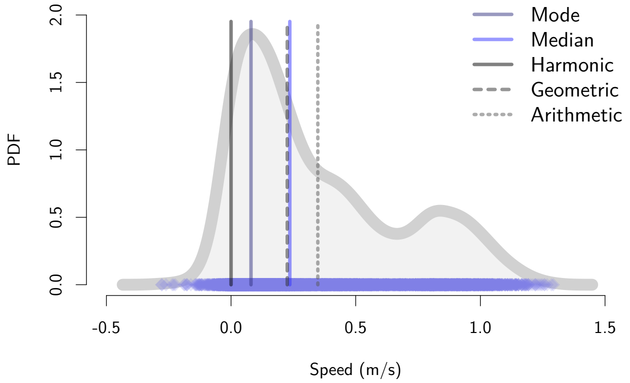


Mode
Median
Harmonic
Geometric
PDF
0.0
0.5
1.0
1.5
2.0
-0.5
0.0
0.5
1.0
1.5
Speed (m/s)

Example



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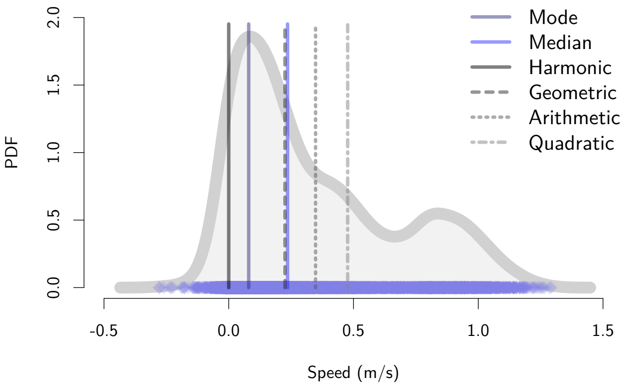

Mode
Median
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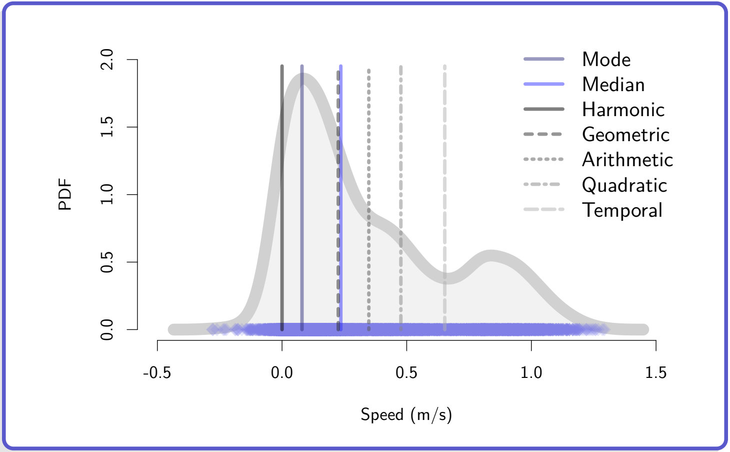
Geometric
Arithmetic
Quadratic
PDF
0.0
0.5
1.0
1.5
2.0
-0.5
0.0
0.5
1.0
1.5
Speed (m/s)

Example



PDF
2.0
1.5
1.0
0.5
0.0
-0.5
0.0
0.5
1.0
1.5
Speed (m/s)
Mode
Median
Harmonic
Geometric
Arithmetic
Quadratic
Temporal

Scattering statistics — `R : var(x), sqrt(var(x)), ...`

Main statistics used to **measure the variability** of $x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$

- **Variance** $var_x = \frac{1}{n} \sum_i (x_i - \bar{x})^2$ — `R : var(x)`
- **Standard-deviation** $s_x = \sqrt{var_x}$ — `sqrt(var(x))`
- **Mean absolute error** $abs\,dev_x = \frac{1}{n} \sum_i |x_i - \bar{x}|$ — `mean(abs(x-mean(x)))`
- **Inter-quartile range** $IQR_x = q_x(0.75) - q_x(0.25)$ — `quantile(x,.75)-quantile(x,.25)`
- **Max–min difference** $max\,min_x = \max_i x_i - \min_i x_i$ — `max(x)-min(x)`

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All these statistics are **positive** and **all the units are the one of the** (x_i), excepted the variance

We have $s_x \geq abs\,dev_x$ and $\max_i x_i - \min_i x_i \geq IQR_x$

Statistics stable by affine transformation

$$s_{ax+b} = |a|\,s_x, \quad IQR_{ax+b} = |a| IQR_x, \quad var_{ax+b} = a^2 var_x$$
$$abs\,dev_{ax+b} = |a|\,abs\,dev_x, \quad max\,min_{ax+b} = |a| max\,min_x,$$

Other statistics for the shape of a distribution

The **Skewness** quantifies the **symmetry** of the distribution

`R : skewness(x)`

$$S_x = \frac{1}{n s_x^3} \sum_i (x_i - \bar{x})^3$$

- $S < 0$: Left asymmetry — Large left tail
- $S = 0$: Symmetric distribution — Similar left and right tails
- $S > 0$: Right asymmetry — Large right tail

Other statistics for the shape of a distribution

The **Skewness** quantifies the **symmetry** of the distribution

R : `skewness(x)`

$$S_x = \frac{1}{ns_x^3} \sum_i (x_i - \bar{x})^3$$

- $S < 0$: Left asymmetry — Large left tail
- $S = 0$: Symmetric distribution — Similar left and right tails
- $S > 0$: Right asymmetry — Large right tail

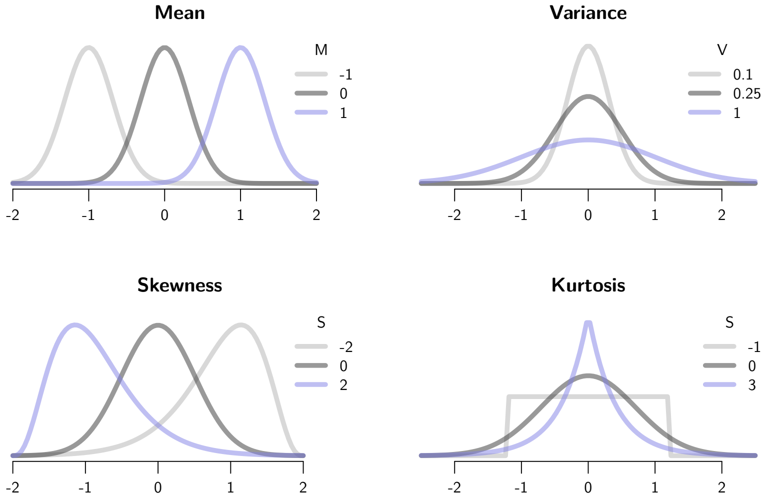
The **Kurtosis** quantifies whether a distribution is **straight or concentrated**

R : `kurtosis(x)`

$$K_x = \frac{1}{ns_x^4} \sum_i (x_i - \bar{x})^4$$

- $K < 0$: Tailness distribution — Straight distribution
- $K > 0$: Distribution with tails — Concentrated distribution

Statistics for the shape of a distribution : Summary

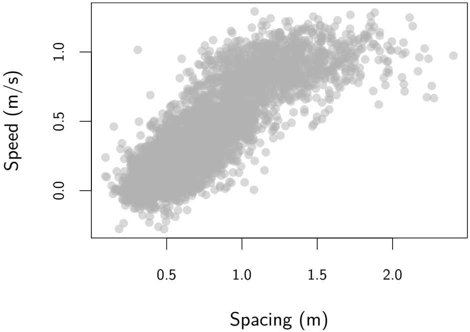


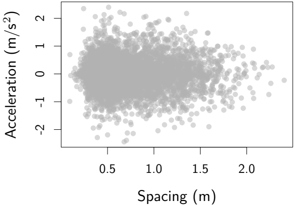
Descriptive statistics for bivariate data

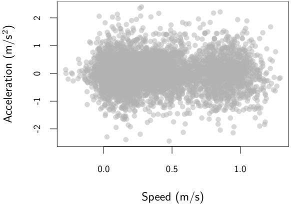
$$\big((x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\big) \in \mathbb{R}^{2n}$$

Scatter plot — R : `plot(x,y)`, `plot(db)`

Scatter plot : The plot of **bivariate data**







Covariance and correlation — R : `cov(x,y)`, `cor(x,y)`

One considers $(x, y) = ((x_1, y_1), \ldots, (x_n, y_n))$ some bivariate data

- **The covariance** $covar$ quantifies how two variables **fluctuate together**

$$covar_{x,y} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) \in \mathbb{R}$$

- **The correlation** cor (or linear or Pearson correlation coefficient) quantifies how two variables **linearly** fluctuate together

$$cor_{x,y} = \frac{covar_{x,y}}{\sqrt{var_x var_y}} \in [-1, 1]$$

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Covariance and correlation **tend to zero as** $n \to \infty$ if x and y are **independent**

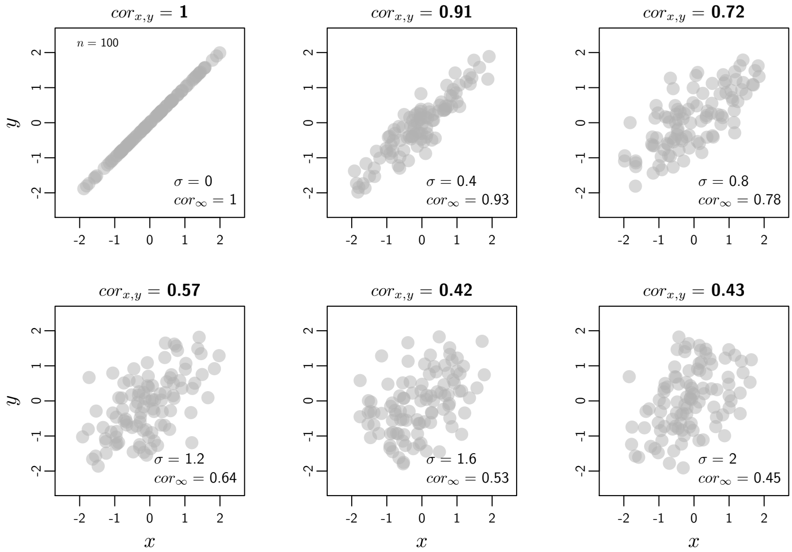
The correlation $cor_{x,y} = |1|$ if and only if x and y are linked by an affine relation

Symmetric, $covar_{x,x} = var_x$, $covar_{ax+b,cy+d} = ac\ covar_{x,y}$, $cor_{ax+b,cy+d} = \pm cor_{x,y}$

Correlation : Illustrative example

$$y_i = (x_i + \sigma z_i)(1+\sigma^2)^{-1/2}$$

$cor_{x,y} \to (1+\sigma^2)^{-1/2}$ as $n \to \infty$



Spearman correlation coefficient — `R : cor(x,y,method='spearman')`

Pearson correlation coefficient allows to assess **linear relationships**

→ The **Spearman correlation coefficient** extends the assessment to **monotonic relationships**

We denote by (rg_x) and (rg_y) the ranks of the variables $(x, y) = ((x_1, y_1), \ldots, (x_n, y_n))$

- **The Spearman correlation coefficient** is

$$cor^s_{x,y} = cor_{r_x, r_y} = \frac{covar_{r_x, r_y}}{\sqrt{var_{r_x} var_{r_y}}} \in [-1, 1]$$

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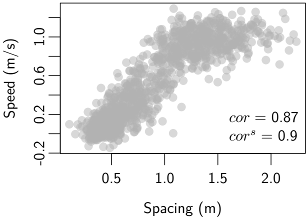
Stable by any monotonic transformation of the data

Insensitive to extreme values

$cor^s_{x,y} = \frac{6\sum_i d_i^2}{n(n^2-1)}$ with $d_i = r_{x_i} - r_{y_i}$ if all n ranks are distinct integers

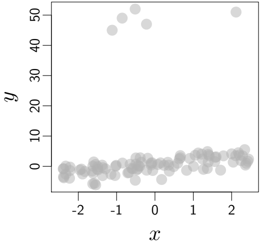


Correlation : Remark 1 — *Low correlation $\not\Rightarrow$ independent variables !*

⚠ **Extreme values annihilate Pearson correlation**

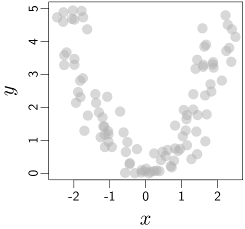
If $y_i = x_i \ \forall i \neq i'$ and $y_{i'} = \gamma$, then $covar_{x,y} \to 0$ as $\gamma \to \pm\infty$

$cor_{x,y} =$ **0.15 / 0.63**



⚠ **Symmetric non-linear** relations can have **correlations nil**

$cor_{x,y} =$ **-0.07 / -0.03**



see also `Wikipedia : Correlation`

Correlation : Remark 2 — *Correlation is not causality !*

Simple cause/consequence relationships have high correlation coefficients

⚠ However, **high correlation coefficient** $\not\Rightarrow$ **Cause/consequence relationship**

$\rightarrow$ Both variables can be the consequence of the same cause without being linked, or can have just by chance similar trends

Correlation : Remark 2 — *Correlation is not causality !*

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Illustrative examples

1. Researchers initially believed that electrical towers impact the health because life expectation and living distance to electrical towers are significantly negatively correlated

   $\rightsquigarrow$ Further analysis shown that this due to the fact that people living around electrical towers are generally poor, with fewer access to healthcare

2. *Shadoks* scientist found significant correlations between the number of times someone eats his birthday cake and having a long life ...

   $\rightsquigarrow$ He deduced that eating his birthday cake is very healthy !

Some useful properties

Mean value

- Mean of a sum is the sum of the means $\overline{x+y} = \bar{x} + \bar{y}$
- Stable for the product if the variables are linearly independent $\overline{xy} = \bar{x}\bar{y}$, if x and y ind.

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Variance and covariance

- Variance stable by sum when the variables are linearly independent
  In general $var(x+y) = var(x) + var(y) + 2covar(x,y)$
- Variance of a product is always bigger than the product of the variances
  $$var(xy) = var(x)var(y) + var(x)\bar{y} + var(y)\bar{x}$$
- In general $var(x) = \overline{x^2} - \bar{x}^2$ and $covar(x,y) = \overline{xy} - \bar{x}\bar{y}$

QQplot — R : `qqplot(x,y)`

Correlations quantify existence of linear or monotonic relationship

More generally, **QQplots** (quantile/quantile plots) allow to qualitatively compare two distributions

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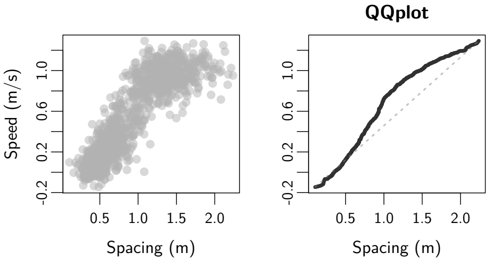
- Variables **linked by an affine relationship** if the curve is a **straight line**
- **Distributions are the same** if the curve is $x \mapsto x$
- **Different distributions in the other cases**



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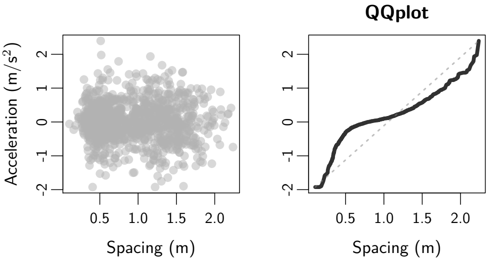

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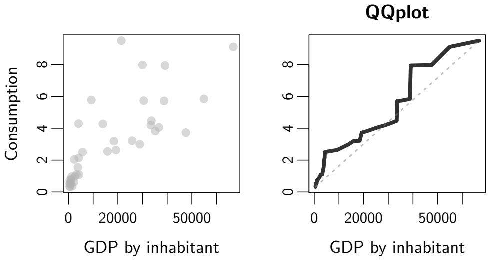

QQplot — R : qqplot(x,y)

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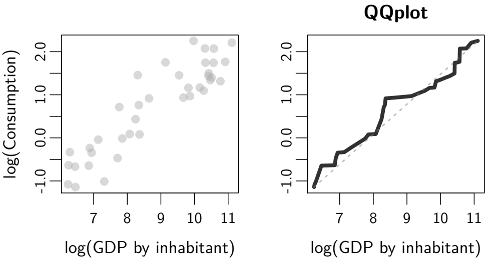

Summary with R

Univariate data

```
# Histogram
hist(x)

# Kernel density
density(x)

# Cumulative distribution function
ecdf(x)

# Quantile, order statistic
quantile(x,0.5);sort(x)

# Mean value, Median
mean(x);median(x)

# Variance, standard deviation
var(x);sqrt(var(x))

# Boxplot
boxplot(x)
```

Bivariate data

```
# Scatter plot
plot(x,y)

# Covariance
cov(x,y)

# Correlation
cor(x,y)

# QQplot
qqplot(y,x)
```

Overview

Part 1 Descriptive statistics for univariate and bivariate data

Repartition of the data (histogram, kernel density, empirical cumulative distribution function), order statistic and quantile, statistics for location and variability, boxplot, scatter plot, covariance and correlation, QQplot

Part 2 Descriptive statistics for multivariate data

Least squares and linear and non-linear regression models, principal component analysis, principal component regression, clustering methods (K-means, hierarchical, density-based), linear discriminant analysis, bootstrap technique

Part 3 Parametric statistic

Likelihood, estimator definition and main properties (bias, convergence), punctual estimate (maximum likelihood estimation, Bayesian estimation), confidence and credible intervals, information criteria, test of hypothesis, parametric clustering

Appendix LaTeX plots with R and Tikz

Regression models

Introduction

Multivariate data $(y_i, x_i^1, \ldots, x_i^p),\ i = 1, \ldots, n$

- n observations of $p+1$ **characteristics**

> y is the **variable to explain** (output or regressant) Continuous
> $x^1, \ldots, x^p$ are the p **explanatory variables** (inputs or regressors) Discrete or continuous

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Model $M_\alpha : \mathbb{R}^p \mapsto \mathbb{R}$ for y as a function of the $(x^1, \ldots, x^p)$

$$y = M_\alpha(x^1, \ldots, x^p) + \sigma\mathcal{E}$$

- α are the parameters and $\sigma\mathcal{E}$ is a *noise* (or an error) with amplitude σ (unexplained part)

Example : Multiple linear model $M_\alpha(x^1, \ldots, x^p) = \alpha_0 + \alpha_1 x^1 + \ldots + \alpha_p x^p$

$\rightarrow$ $p + 2$ parameters : $(\alpha_0, \alpha_1, \ldots, \alpha_p)$ and σ — Simple linear regression for $p = 1$

Estimation of the parameters by least squares

Non-parametric estimation of the parameters by least squares

(or ordinary least squares (OLS), or regression model)

$$\tilde{\alpha} = \arg\min_{\alpha} \sum_{i=1}^{n} \Big(y_i - M_\alpha \big(x_i^1, \ldots, x_i^j \big) \Big)^2$$

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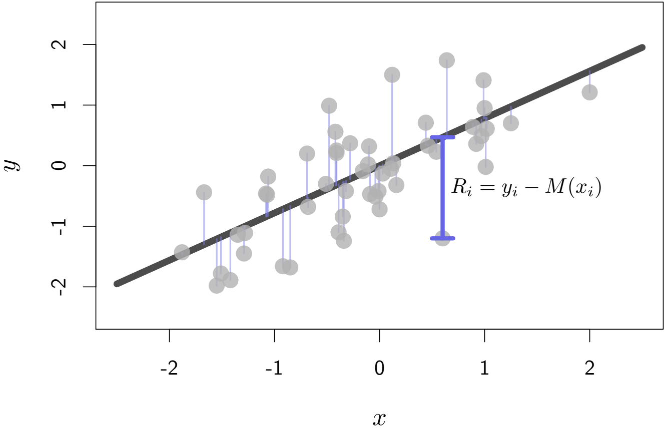
The residuals are the quantities $R_\alpha(y, x^1, \dots, x^p) = y - M_\alpha(x^1, \dots, x^p)$

- OLS : **Minimisation of the variance of the residuals** / **Sensible to extreme values**
- Estimation of the **amplitude** of the noise using the empirical residual variance

$$\tilde{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} R_{\tilde{\alpha}}^2 (y_i, x_i^1, \dots, x_i^p)$$

Estimation of the parameters by least squares



Goodness of the fit

Evaluation of the goodness through **the repartition of the variability**

- $SST = \sum_{i=1}^{n} (y_i - \bar{y})^2$ **Total Sum of Squares**
- $SSM = \sum_{i=1}^{n} (\bar{M} - M_{\tilde{\alpha}}(x_i))^2$ **Sum of Squares of the Model**
- $SSR = \sum_{i=1}^{n} (y_i - M_{\tilde{\alpha}}(x_i))^2$ **Sum of Squared Residuals**

Residuals centred and linearly independent : $SST = SSM + SSR$

$\rightarrow$ Minimizing the variance of residuals maximizes variance explained by the model

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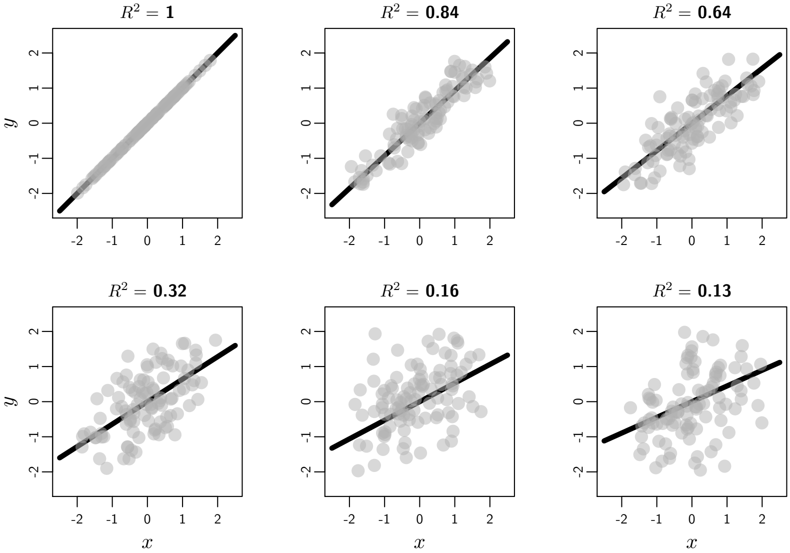
$\rightarrow$ Minimizing the variance of residuals maximizes variance explained by the model

Coefficient of determination *Explained proportion of the variance*

$$R^2 = \frac{SSM}{SST} = 1 - \frac{SSR}{SST} \leq 1$$

$\rightarrow$ Good fit if $R^2 \approx 1$ — OLS estimation maximizes the R^2 — If $p = 1$ then $R^2 = cor^2_{x,y}$

R^2 : Example



Linear regression — `R : lm(y ∽ x)`

Matrix notations of the multiple linear model :

$$y = X\alpha, \qquad \left| \begin{array}{lcll} y & = & (y_1, \ldots, y_n)^t & \text{the variable to explain} \\ X & = & (1_n, x^1, \ldots, x^p) & \text{the matrix of the regressors} \\ \alpha & = & (\alpha_0, \ldots, \alpha_p)^t & \text{the parameters} \end{array} \right.$$

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OLS estimation of the parameters α : $\tilde{\alpha} = (X^t X)^{-1} X^t y$

Formal proof : $\forall j = 1, \ldots, p, \ \frac{\partial}{\partial \tilde{\alpha}_j} \sum_i (y_i - \tilde{\alpha}_0 - \tilde{\alpha}_1 x_i^1 - \ldots - \tilde{\alpha}_p x_i^p)^2 = 0$

$\Leftrightarrow \quad \forall j = 1, \ldots, p, \ \sum_i x_i^j (y_i - \tilde{\alpha}_0 - \tilde{\alpha}_1 x_i^1 - \ldots - \tilde{\alpha}_p x_i^p) = 0$

$\Leftrightarrow \quad X^t (y - X\tilde{\alpha}) = 0 \quad \Leftrightarrow \quad \tilde{\alpha} = (X^t X)^{-1} X^t y$

Generalized Least Squares (GLS) estimation $\tilde{\alpha}^G = (X^t \Omega^{-1} X)^{-1} X^t \Omega^{-1} y$

→ Variance/Covariance matrix Ω for the residuals

Simple linear regression

Bivariate data $(x, y) = ((x_1, y_1), \ldots, (x_n, y_n)) \in \mathbb{R}^2$

The linear regression of y on x is the straight line $y = a_{\mathsf{OLS}} x + b_{\mathsf{OLS}}$

$$(a_{\mathsf{OLS}}, b_{\mathsf{OLS}}) = \arg\min_{a,b} \sum_i (y_i - (ax_i + b))^2 \quad \Rightarrow \quad \left\{ \begin{array}{lcl} a_{\mathsf{OLS}} & = & \frac{covar_{x,y}}{var_x} \\ b_{\mathsf{OLS}} & = & \bar{y} - a_{\mathsf{OLS}} \bar{x} \end{array} \right.$$

Formal proof : We denote as $F(a, b) = \sum_i (y_i - (ax_i + b))^2$

$\partial F / \partial a = 0$ and $\partial F / \partial b = 0$ is $\left\{ \begin{array}{lcl} \sum_i (-x_i y_i + x_i b + x_i^2 a) & = & 0 \\ \sum_i (y_i + x_i a + b) & = & 0 \end{array} \right.$

This gives $a = \frac{\frac{1}{n} \sum_i x_i yi - \frac{1}{n} \sum_i x_i \frac{1}{n} \sum_i y_i}{\frac{1}{n} \sum_i x_i^2 - \left(\frac{1}{n} \sum_i x_i\right)^2} = \frac{cov_{x,y}}{var_x}$ and $b = \frac{1}{n} \sum_i y_i + ax_i = \bar{y} - a\bar{x}$

$\rightarrow$ Regressions y/x and x/y are not the same as soon as $var_x \neq var_y$ but both cross $(\bar{x}_n, \bar{y}_n)$

Linear and non-linear regression

Non-linear regression by invertible (monotone) non-linear transformation of the data

- Linear regression with the variables x and $f(y)$, $f(x)$ and y or $f(x)$ and $f(y)$

Example : Exponential model $M_\alpha = e^{\alpha_0} \cdot (x^1)^{\alpha_1} \dots (x^p)^{\alpha_p}$

$\rightarrow$ Linear model with $\tilde{x} = \log(x)$ and $\tilde{y} = \log(y)$

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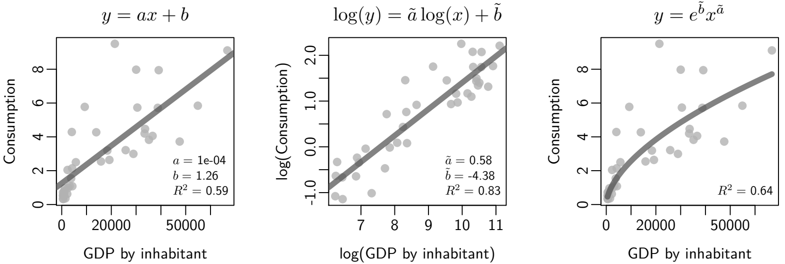
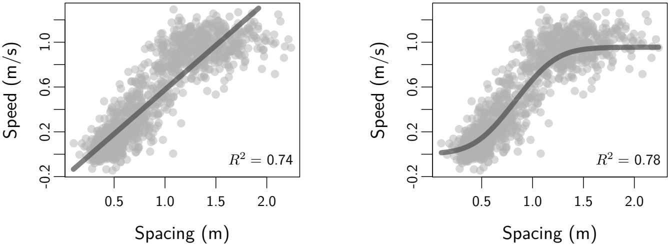


Linear and non-linear regression

Non-invertible model : Linearisation of the problem and numerical solution

- Iterative algorithms based on the partial derivatives of the model (Jacobian matrix)
- R : `nls(model,data)` Gauss-Newton or Golub-Pereyra algorithms
- Local minima and divergence problems possible



Multiple linear and non-linear regression with R

y, x1, x2 and x3 are vectors with the same size

Linear least squares estimate

```
lm(y ∽ x1 + x2 + x3)
```

- Linear regression of y on x1, x2 and x3
- Linear model (with intercept nil) : `lm(y ∽ 0 + x1 + x2 + x3)`

Non-linear least squares estimate

```
nls(y ∽ mod(x,p1,p2,p3,...))
```

- The model must be at least derivable — Default method : Gauss–Newton
- Partial derivative can be given as input or are estimated numerically

Regression models : Summary

- Regression models allow to describe relationships between a **variable to explain** and **explanatory factors**
  - Parameter estimations by **least squares method** (sensitivity to extreme values)
  - **Linear** (explicit solution) and **non-linear** (invertible transformation or numerical approximation) models

- The **variability of the variable to explain** can be decomposed as
  - **Variability explained by the model**
  - **Variability of the residuals** (non-explained part)

  $\rightarrow$ The $R^2 \in [0, 1]$ is the **proportion of variable explained by the model**
  R^2 allows to **compare models** and to **evaluate the quality of the fit**

- Linear and non-linear regression are **very easy to implement** in R
  $\rightarrow$ `lm(·)` and `nls(·)` functions — `coef(·)` to get the estimations of the coefficients

Principal Component Analysis

Introduction

Multivariate data : observations of p **characteristics** of n **individuals**

$$X = \begin{bmatrix} x_1^1 & x_1^2 & \dots & x_1^p \\ x_2^1 & x_2^2 & \dots & x_2^p \\ \vdots & \vdots & & \vdots \\ x_n^1 & x_n^2 & \dots & x_n^p \end{bmatrix} \in (\mathbb{R}^p)^n, \quad \left| \begin{array}{ll} x_i = (x_i^1, \dots, x_i^p), & i = 1, \dots, n \\ x^j = (x_1^j, \dots, x_n^j)^t, & j = 1, \dots, p \end{array} \right.$$

$\rightarrow$ **Variables** $(x^1, \dots, x^p)$ are **correlated** (inter-dependence of the characteristics)

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$\rightarrow$ **Variables** $(x^1, \dots, x^p)$ are **correlated** (inter-dependence of the characteristics)

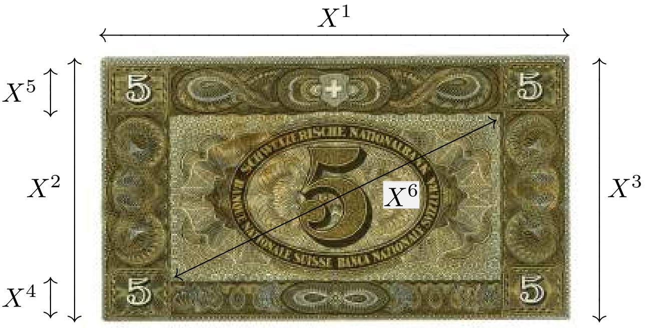
Specific tools for the **visualisation and description of multivariate data**

- **Scatterplots** — By coupling the variables — $p(p-1)$ plots
- **Parallel plots**, **Andrews plot**, **radar charts** — Different geometrical representations
- **Chernoff faces** — Human face representation
- **Principal component analysis** — Decomposition in principal components

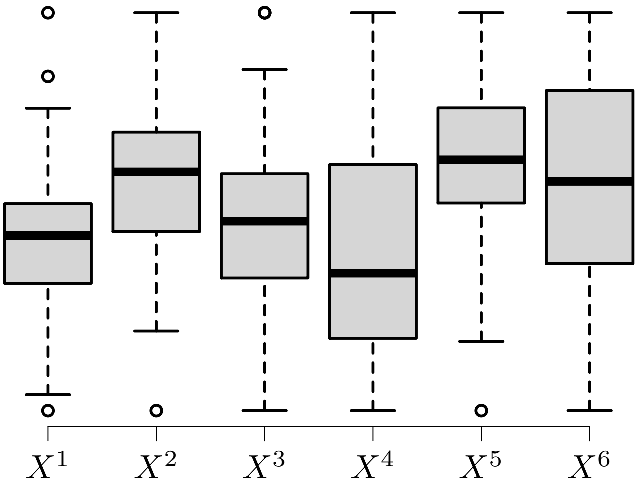
Example

Six measurements of Swiss banknotes ($n = 200$ observations, $p = 6$)

$\rightarrow$ Some are **authentic**, some are **counterfeit**



Boxplot — `R : boxplot(database)` Normed data

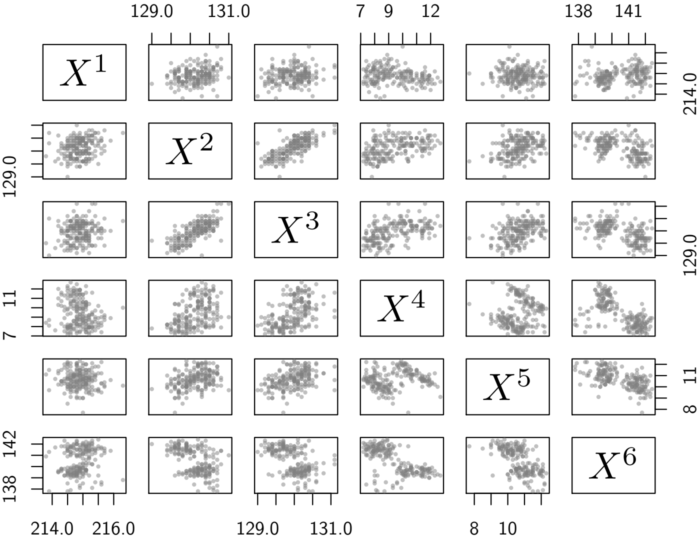


Correlation coefficients

	X^1	X^2	X^3	X^4	X^5	X^6
X^1	1.00	0.23	0.15	-0.19	-0.06	0.19
X^2	0.23	1.00	**0.74**	0.41	0.36	**-0.50**
X^3	0.15	**0.74**	1.00	**0.49**	0.40	**-0.52**
X^4	-0.19	0.41	**0.49**	1.00	0.14	**-0.62**
X^5	-0.06	0.36	0.40	0.14	1.00	**-0.59**
X^6	0.19	**-0.50**	**-0.52**	**-0.62**	**-0.59**	1.00

- X^2 and X^3 are highly correlated
- X^4 and X^5 are highly correlated to X^3
- X^6 is highly correlated to all the variables excepted X^1

Scatterplot — `R : plot(database)`



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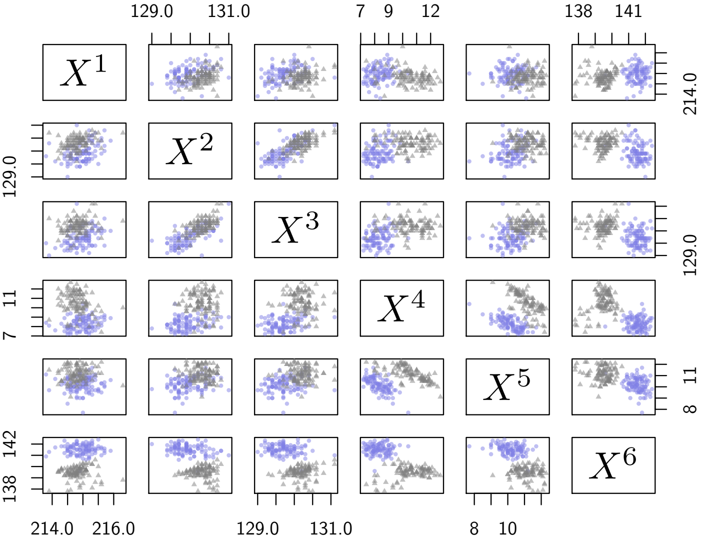
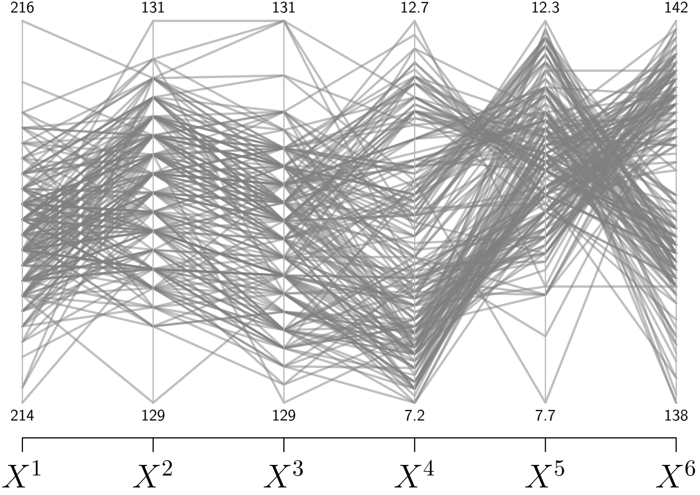


Parallel plots — R : `parcoord(database)` Package : MASS



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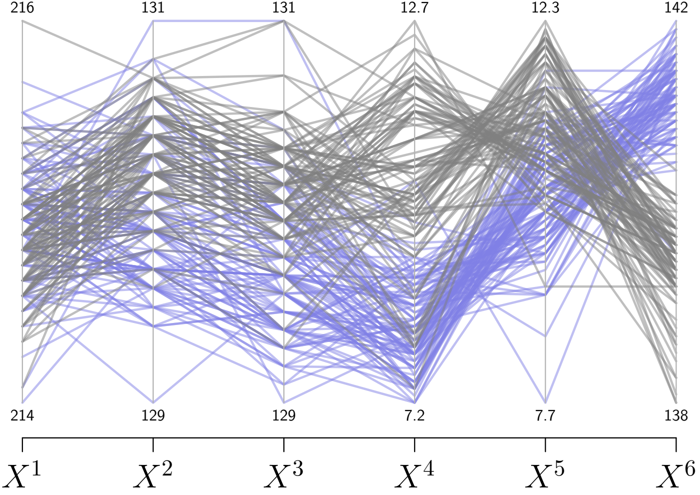
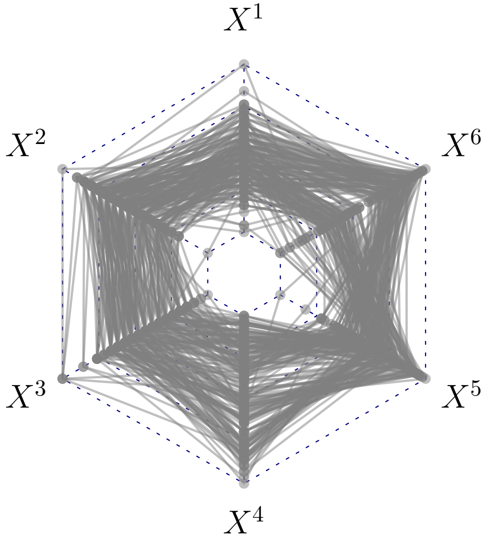


Radar charts — `R : radarchart(database)` Package : `fmsb`



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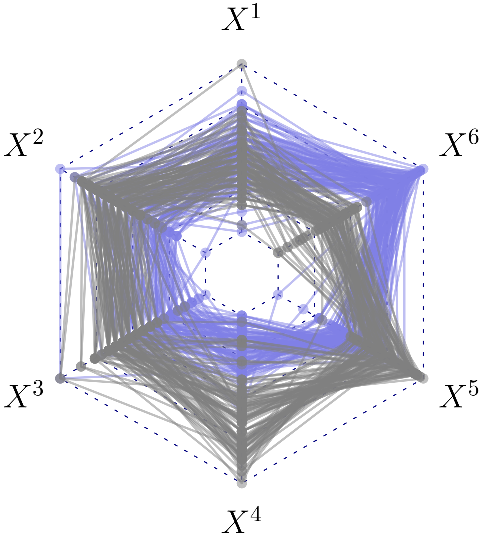
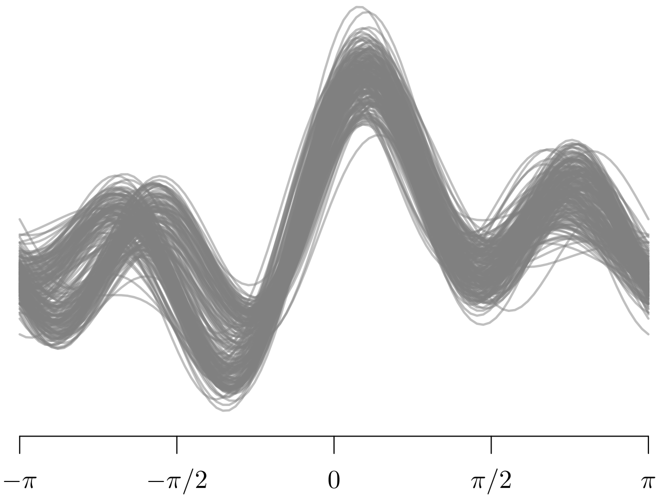


Andrews plots — `R : andrews(database)` Package : `andrews`

$X^1 \cos(t) + X^2 \sin(t) + X^3 \cos(2t) + X^4 \sin(2t) + X^5 \cos(3t) + X^6 \sin(3t)$



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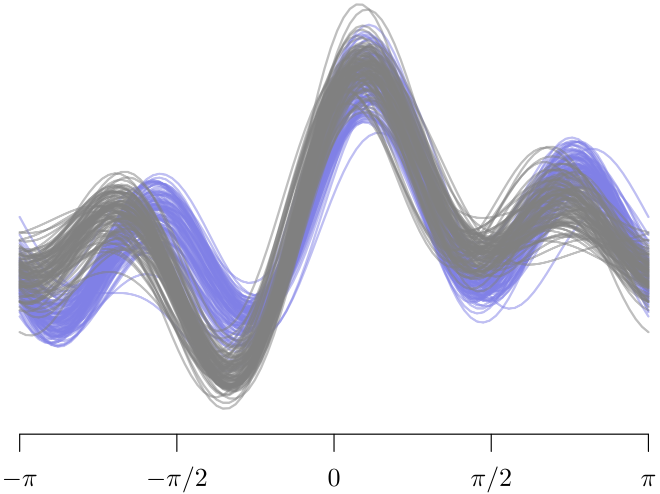
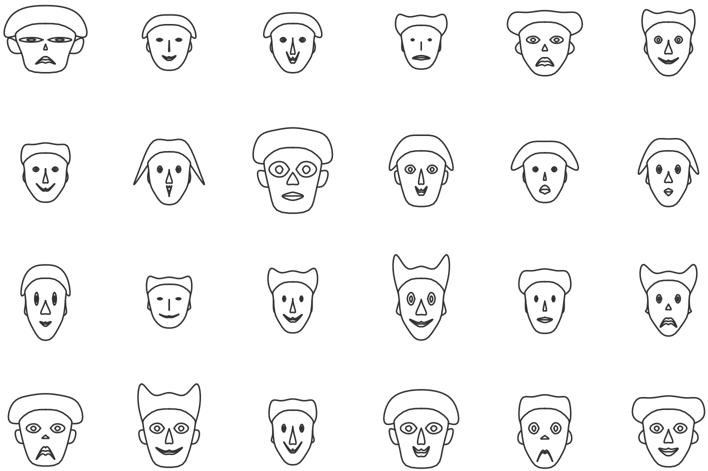


Chernoff faces — R : faces(database) Package : aplpack

$i = 1, \ldots, 24$



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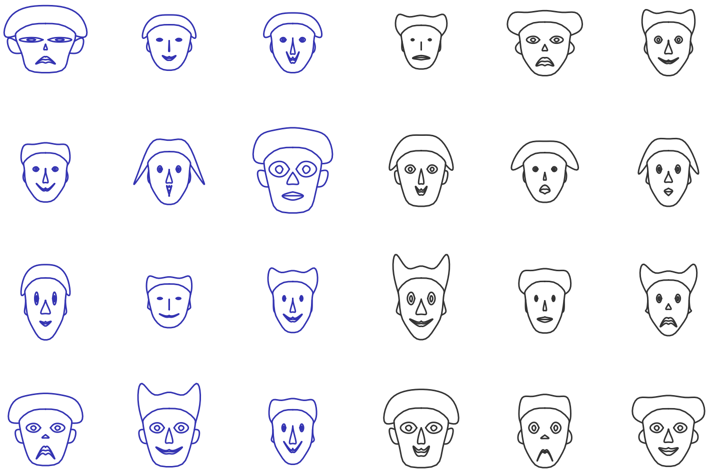

Chernoff faces — R : faces(database) Package : aplpack

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Principal component analysis (PCA)

PCA allows to explore large **multivariate data** $X = (x_i^1, \ldots, x_i^p)$, $i = 1, \ldots, n$

- The variable $(x^1, \ldots, x^p)$ are dependent (otherwise individual analyse !) and continuous (PCA for categorical data : *Multiple correspondence analysis*)
- The dimension p is high and the visualisation of the global structure of the data is difficult
- Correlated variable bring same information and could be resumed as linear combinations (i.e. principal factors) to reduce the dimension of the database

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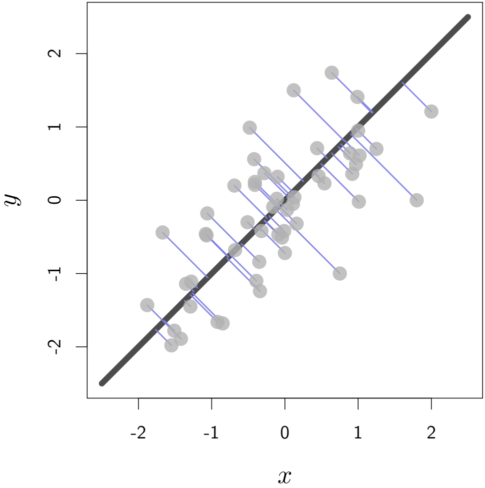
Principle : Reduction of the dimension with **uncorrelated linear combinations** of $(x^1, \dots, x^p)$ **maximising the variability**

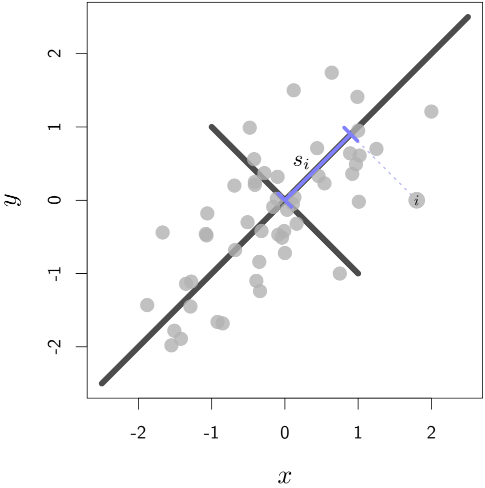
- Geometric interpretation : Projection of the data in orthogonal basis maximising the variance (i.e. the information – other criteria may be used)
- The 1st component is an optimal representation of the data in one dimension, 1st and 2nd components optimal representation of the data in two dimensions, and so on

PCA : Maximisation of the variance



- **Orthogonal projection**

PCA : Maximisation of the variance



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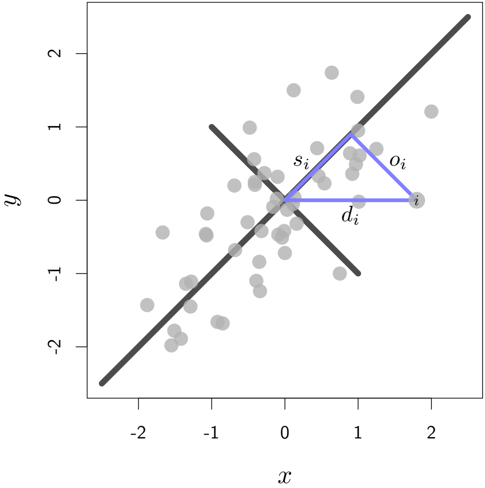
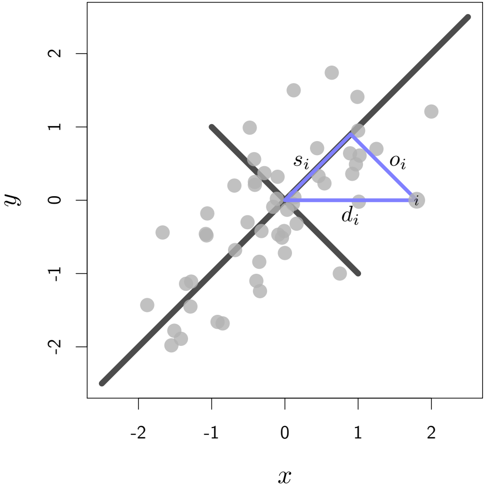


- **Orthogonal projection**
- **Maximisation of the variance** $\sum_i s_i^2$
- $\forall i,\ d_i^2 = o_i^2 + s_i^2$ **constant** in any direction (distance to the center)

  $\Rightarrow \sum_i o_i^2 + \sum_i s_i^2 = C$

PCA : Maximisation of the variance



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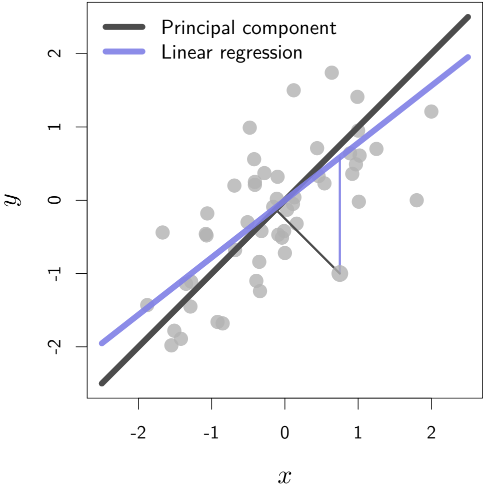

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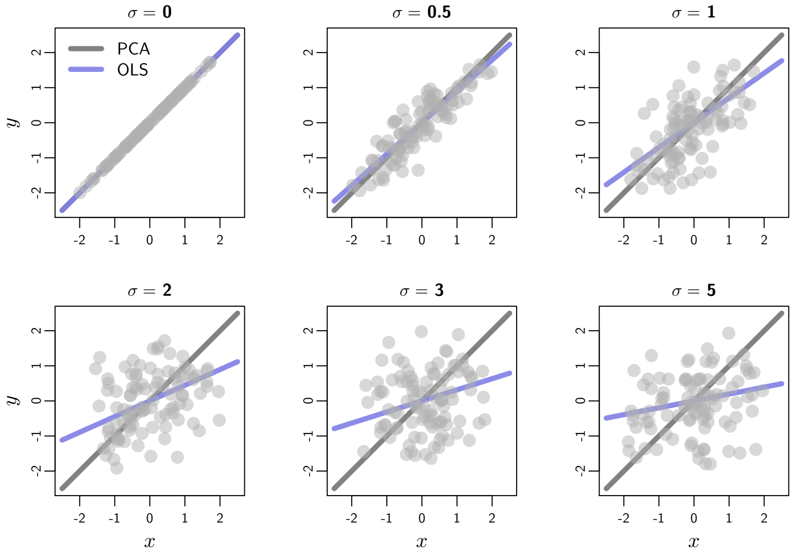
  Maximising the variance $\Leftrightarrow$ Minimising orthogonal squared distances
- Principal component $\neq$ linear regression

Example

$$y_i = (x_i + \sigma z_i)(1+\sigma^2)^{-1/2}$$

$a_{\text{PCA}} \to 1$ while $a_{\text{OLS}} \to (1+\sigma^2)^{-1/2}$ as $n \to \infty$



Construction of the components

Standard score transformations of the data

$$x_i^j \to \tilde{x}_i^j = \frac{x_i^j - \bar{x}^j}{s_{x^j}}$$

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The total variance of the dataset is

$$var_{\tilde{X}} = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{p} \left(\tilde{x}_i^j\right)^2 = \sum_{j=1}^{p} s^2_{\tilde{x}^j} \qquad (= p \text{ if std. score})$$

$P_H \tilde{X}$ is the **orthogonal projection** of the data on subset H and $\tilde{X} - P_H \tilde{X}$ is the projection on a subset orthogonal to H, then (Pythagore)

$$var_{\tilde{X}} = var_{P_H \tilde{X}} + var_{\tilde{X} - P_H \tilde{X}}$$

$\rightarrow$ **PCA :** Iterative calculation of orthogonal 1D subsets **maximizing the variance**

Construction of the components

Iterative construction of the components $(PC1, PC2, \ldots, PCp)$ as linear combinations of the centred data :

- $PC1 = \tilde{X}u_1$, u_1 such that var_{PC1} maximal
- $PC2 = \tilde{X}u_2$, $u_2 \perp u_1$ and var_{PC2} maximal
- $PC3 = \tilde{X}u_3$, $u_3 \perp (u_1, u_2)$ and var_{PC3} maximal

  $\vdots$
- $PCp = \tilde{X}u_p$, $u_p \perp (u_1, \ldots, u_{p-1})$ (unique)

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The unit vectors $(u_1, u_2, \ldots, u_p)$ form an **orthonormal basis** of R^p — The last component is fixed

By construction $var_{PC1} \geq var_{PC2} \geq \ldots \geq var_{PCp}$ and $\sum_j var_{PCj} = var_X$

The **first components contain most of the variability** of the data when the initial variables are correlated

Construction with multivariate data

Variance/covariance matrix of the data Γ (diagonalizable $p \times p$ real and symmetric matrix)

$$\Gamma = \frac{1}{n} X^t X \qquad \left| \begin{array}{l} \Gamma_{j,j} = var_{\tilde{x}^j} = \frac{1}{n}\sum_i (\tilde{x}_i^j)^2, \\ \Gamma_{j,j'} = covar_{\tilde{x}^j, \tilde{x}^{j'}} = \frac{1}{n}\sum_i \tilde{x}_i^j \tilde{x}_i^{j'}, \end{array} \right. \qquad \forall j, j' \in \{1, \ldots, p\}$$

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Principal components $PCj = \tilde{X} u_j$ described by **eigenvectors and eigenvalues** of Γ

Proof $\tilde{X}_v$ is the projection of the data X on axis subset $v \in \mathbb{R}^p$

$$\begin{aligned} var_{\tilde{X}_v} &= \tfrac{1}{n} \textstyle\sum_j \sum_{j'} v_j v_{j'} \sum_i \tilde{x}_i^j \tilde{x}_i^{j'} = v^t \Gamma v \\ &= \textstyle\sum_j \lambda_j \langle v, u_j \rangle^2 \leq \lambda_1 \sum_j \langle v, u_j \rangle^2 \leq \lambda_1 = var_{PC1} \end{aligned}$$

The axis v for which the variance is maximal is u_1 (and the variance is var_{PC1})

$\rightarrow$ Then for all $v \perp u_1$ (i.e. $\langle v, u_1 \rangle = 0$), the axis maximizing the variance is u_2 etc...

Construction with bivariate data

The **first component** $PC1 = u\tilde{x} + \sqrt{1-u^2}\tilde{y}$ is the **straight line** $y = a_{\mathsf{PCA}}x$ with $a_{\mathsf{PCA}} = \frac{\sqrt{1-u^2}}{u}$ where u is such that

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The slope for linear regression is $a_{\mathsf{OLS}} = \frac{covar_{x,y}}{var_x}$

If $y_i = ax_i$ for all i, then $a_{\mathsf{PCA}} = a_{\mathsf{OLS}} = a$ (since $covar_{xy} = a\,var_x$ and $var_y = a^2 var_x$)

If $s_x = s_y$ then $a_{\mathsf{PCA}} = \pm 1$, according to the sign of $covar_{x,y}$ (and $a_{\mathsf{OLS}} = cor_{x,y}$)

The second component has the slope $-1/a_{\mathsf{PCA}}$

Properties of the components

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Only the linear relations are resumed : Observation of non-linear phenomena

- **Interpretation of the components** with **the correlations to the initial variables**

$$\forall j, j' \in \{1, \ldots, p\}, \quad cor_{x^j, PCj'} = u^j_{j'}\sqrt{\lambda_{j'}}/s_{x^j}$$

Practical use of PCA

In practice, the PCA consists in :

1. Calculus of **the variances of the principal components** (eigenvalues) to **select the number of new variables** to take in consideration

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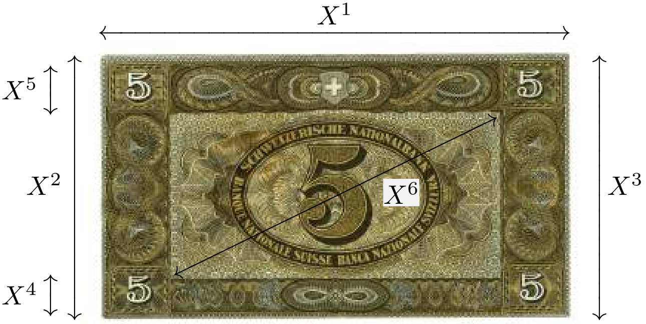
   → **Circle of the correlations plot**

3. **Analysis of the components** (linear and non-linear phenomena)

   → **Boxplot, scatter plots or clustering analysis of the new variables**

Example of the notes

Six measurements for the notes



Principal components — R : `prcomp(database)`

Rotations (eigenvectors u_j)

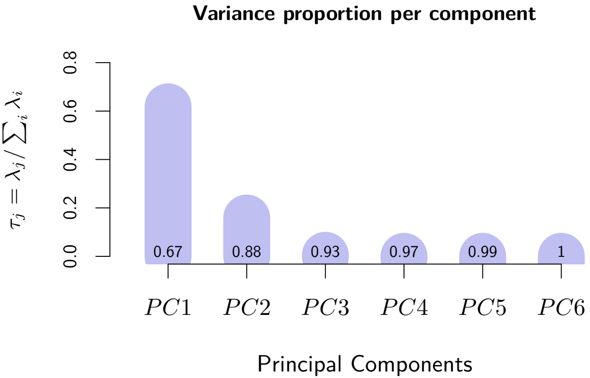
	$PC1$	$PC2$	$PC3$	$PC4$	$PC5$	$PC6$
X^1	0.04	-0.01	0.33	-0.56	-0.75	0.10
X^2	-0.11	-0.07	0.26	-0.46	0.35	-0.77
X^3	-0.14	-0.07	0.34	-0.42	0.53	0.63
X^4	-0.77	0.56	0.22	0.19	-0.10	-0.02
X^5	-0.20	-0.66	0.56	0.45	-0.10	-0.03
X^6	0.58	0.49	0.59	0.26	0.08	-0.05

Component variance (eigenvalues λ_j)

	$PC1$	$PC2$	$PC3$	$PC4$	$PC5$	$PC6$
λ	3.00	0.94	0.24	0.19	0.09	0.04
τ	0.67	0.21	0.05	0.04	0.02	0.01

Plot of the proportions of variance per component

Selection of the component number



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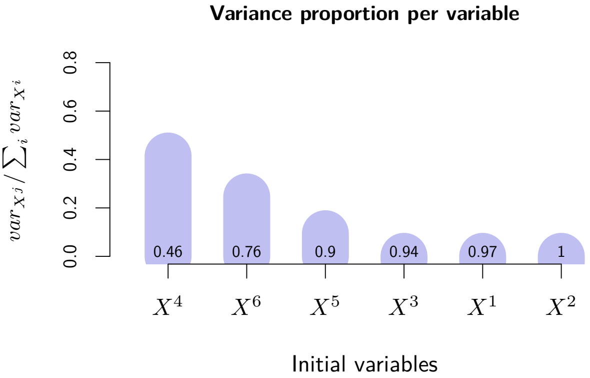
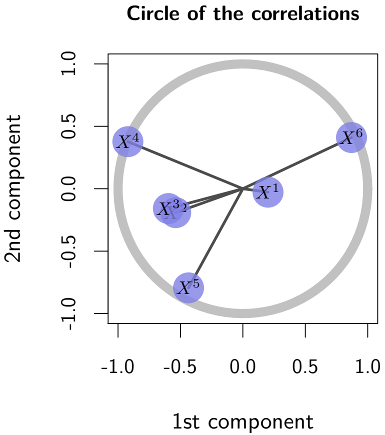
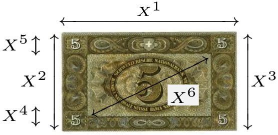


Plot of the circle of the correlations

Interpretation of the components

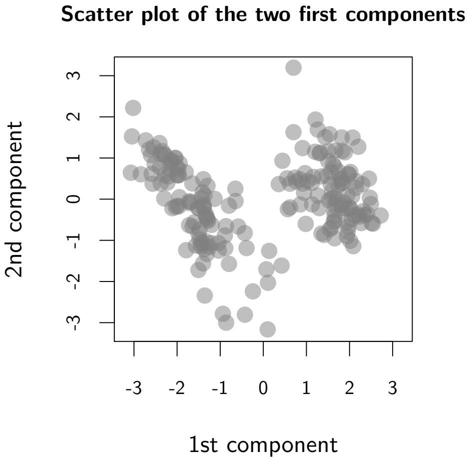


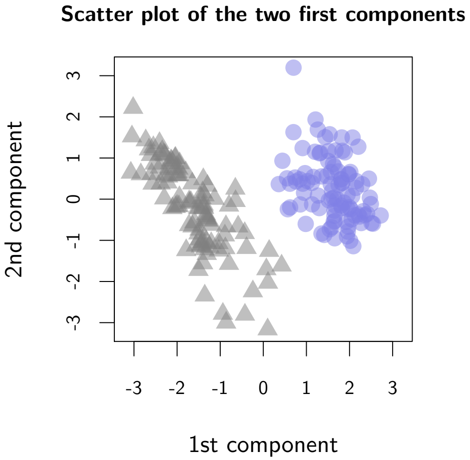


- **PC1** Large flag / Short border — Long / not large note
- **PC2** Large flag and down border / Short up border

Scatter plot of the components

Analysis of the results





Scatter plot of the two first components
2nd component
1st component
-3
-2
-1
0
1
2
3

PCA with R

Read of the data `data=read.table('C/...')`

- **Principal component analysis with R** `prcomp(M)`

  No standard score transformation of the data by default
  `prcomp(M,scale=T)` for PCA on standard scores

- **Basic example :**

```
pca=prcomp(data)
pca$rotations
pca$stddev
summary(pca)
```

Principal component regression

OLS estimation has **interesting properties** if **regressors are linearly independent**

→ **Regression on the principal components**

- **Principal components**: $p \times n$ matrix $PC = \hat{X} S U$

  $\hat{X}$ is the **centred data** ($\hat{x}_i^j \to x_i^j - \bar{x}^j$ for all i, j)
  $S = Diag(1/s_{x^1}, \ldots, 1/s_{x^p})$ is the diagonal $p \times p$ **normalization matrix**
  $U = (u_1, \ldots, u_p)$ is the $p \times p$ matrix of **unit and orthogonal** eigenvectors

- **Regression on the components**: $\hat{y} = \alpha_1^{PC} PC1 + \ldots + \alpha_p^{PC} PCp$

$$\tilde{\alpha}^{PC} = (PC^t PC) PC^t y = (SU)^{-1} (X^t X) X^t y = (SU)^{-1} \tilde{\alpha}$$

Principal component regression

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$$\tilde{\alpha}^{PC} = (PC^t PC) PC^t y = (SU)^{-1} (X^t X) X^t y = (SU)^{-1} \tilde{\alpha}$$

The **estimation using initial parameters** is $\tilde{\alpha} = SU \tilde{\alpha}^{PC}$ and $\tilde{\alpha}_0 = \bar{y} - \frac{1}{n} \hat{X} \tilde{\alpha}$
By shorting the regressors to the first principal components the model still depends on **all the initial variables**

Principal component analysis : Summary

PCA is a **descriptive tool** allowing to **reduce the dimension of multivariate data**
$\rightarrow$ Then use of tools for low dimension data (uni- or bivariate)

The principal components are

- **Linear combinations of the initial variables**
- **Linearly independent**
- **Ordered by maximizing the variability**

Practical use of PCA :

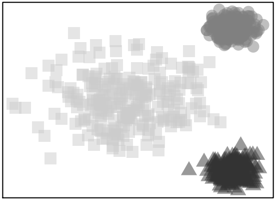
- **Number of components used** — Proportion of variance per component
- **Interpretation of the new variables** — Circle of the correlations
- **Analysis of the components** — Scatter plot of the components

Clustering methods

Introduction

Clustering : Division of **heterogeneous data** in subsets (clusters)

→ **Observations in the same cluster are more similar** (in some sense) to each other than to those in other subsets



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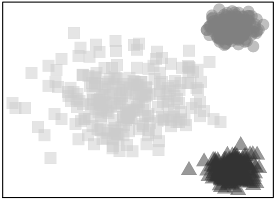

Possible distinctions

Supervised / unsupervised :	Clusters and cluster number are known / unknown
Strict clustering :	Each observation belongs to exactly one cluster
Strict clustering with outliers :	Observations can also belong to no cluster (outliers)
Overlapping clustering :	Observations may belong to more than one cluster
Fuzzy clustering :	Each observation belongs to each cluster according to a certain degree
Hierarchical clustering :	Observations of a child cluster also belong to the parent cluster
Centroid clustering :	Cluster represented by a centroid (mean value)
Density-based clustering :	Clustering based on empirical PDF estimation

K-means clustering — `R : kmeans(database,K)`

Observation $(x_1, \ldots, x_n)$, partition $S = \{S_1, \ldots, S_K\}$, mean by cluster $(u_1, \ldots, u_K)$

Unsupervised clustering method based on mean by cluster (*k-medoid* based on median)

→ Number of clusters K **to be given**

Minimization of the intra-cluster variability

$$S = \arg\min_S \sum_{j=1}^{K} \sum_{i \in S_j} \|x_i - u_j\|^2$$

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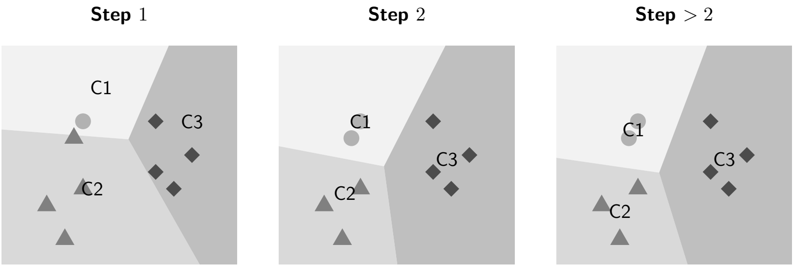
Minimizing the intra-variability ⇔ **Maximizing the inter-variability** (Pythagore)

Partition based on the **Voronoi diagram for the means**

Calculation of the global minimum is a **NP-complex problem**

→ Iterative numerical algorithms (Hartigan-Wong, Lloyd-Forgy, ...) with **convergence to local minima**

K-means : Illustrative example with 3 clusters



Convergence to steady state in 3 steps (the step's number depends on the initial partition / mean values)

In this example the reached **local optimum** is the **global** one

Agglomerative hierarchical method (AHM) — R : `hclust(dist(data))`

Hierarchical method : Unsupervised clustering based on tree representations

- Top of the tree : One cluster with all the observations
- Bottom of the tree : each observation is a cluster

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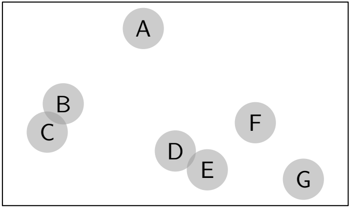
Agglomerative iterative method (bottom up approach, by opposition to divisive methods)

1. **Initialization** : Each observation is a cluster
2. **Definition** of the metric (Euclidean, Manhattan, Mahalanobis, maximum, ...)
3. **Definition** of a distance between two clusters – Linkage (max, min, mean, centroid, ...)
4. **Repeat while** `Cluster_number > 1` {`Merge_two_closest_clusters`}

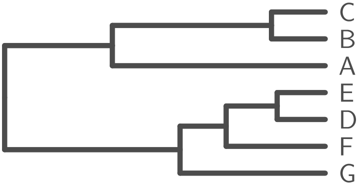
Dendrogram : Tree with observation in x-coordinate and distances in y-coordinate
$\rightarrow$ Cut of the dendrogram determinates the number of clusters

AHM : Illustrative example

Observations

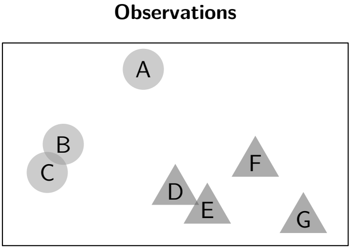


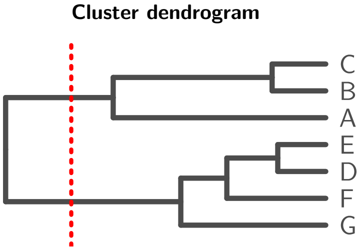
Cluster dendrogram



> The dendrogram allows to summarize/represent the hierarchical clustering
> Cut of the dendrogram when the branches are long (cut at height h give groups having distance higher than h)

AHM : Illustrative example





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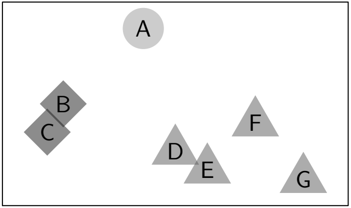
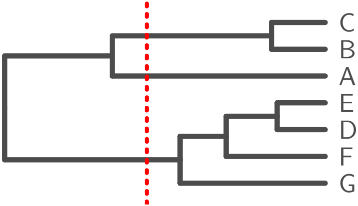


Cluster dendrogram



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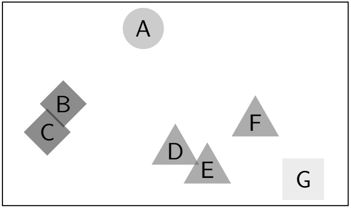
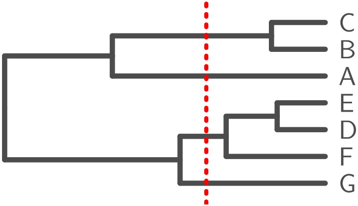
AHM : Illustrative example

Observations



Cluster dendrogram



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Mean-shift clustering — `ms(database)` Package LPMC

K-means and AHM based on distances to quantify the similarities

Mean-shift clustering : Gradient-method based on kernel density estimate

- **Iterative method** allowing to detect local maximum of the kernel density
- Method calibrated by a **bandwidth** (to be given)
- **Clustering** : threshold for local maxima (cluster number), kernel density gradient (cluster belonging)

→ See also DBSCAN or OPTICS algorithms

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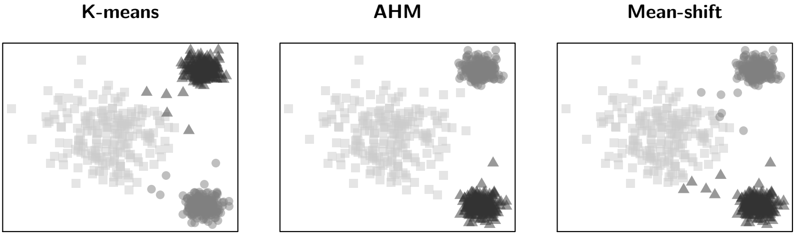
→ See also DBSCAN or OPTICS algorithms

More flexible method than K-means or AHM, suitable for any type of clusters
Bandwidth not easy to calibrate, adaptive bandwidth often required

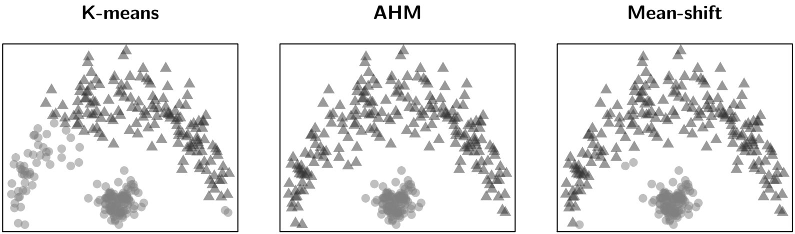
Illustrative examples



Circular clusters : K-means, AHM and mean-shift methods give satisfying results

→ Distance between observations in each clusters smaller than distance between cluster's means

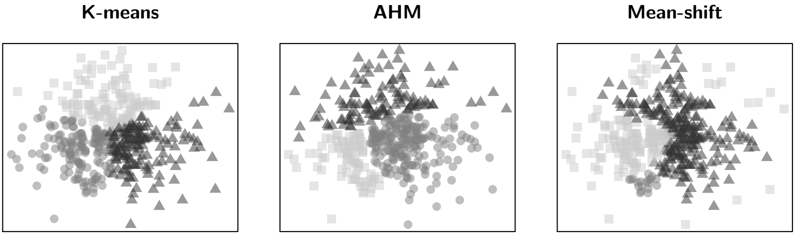
Illustrative examples



Non-circular clusters : K-means not adapted / AHM and mean-shift more robust

→ Distance between observations in each clusters bigger than distance between cluster's means

Illustrative examples

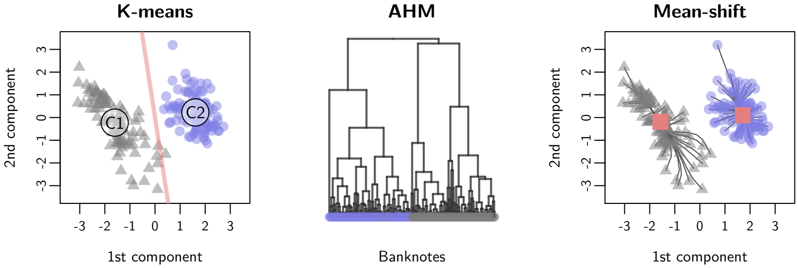


⚠ Clustering methods find clusters **even if there is no significant dissimilarities**

→ Criteria for significance of inter/intra-variability, dendrogram branch size, bandwidth size, ...

Example of the notes

Detection of the counterfeit notes	Method		
Miss-classification error	K-means	AHM	Mean-shift
Complete sample	0.005%	0	0.005%
Two first components (PCA)	0.005%	0	0%



Linear discriminant analysis — `lda(data,cluster)` `Package MASS`

Clustering : Observations (continuous variables) → Clusters (discrete variable)
Discriminant analysis : Clusters (discrete variable) → Observations (discriminant)

Linear discriminant analysis

- Data :
  - **Continuous explanatory variables** (regressors) $X^1, \ldots, X^p$
  - **Discrete variable to explain** (clusters) $Y = 1, \ldots, K$
- **Discriminant variable** D as **linear combination of the regressors** minimizing the variance by cluster $Y = 1, \ldots, K$:

$$D(\alpha_0, \ldots, \alpha_p) = \alpha_0 + \alpha_1 X^1 + \ldots + \alpha_p X^p$$

$$\text{with} \quad (\alpha_0, \ldots, \alpha_p) = \arg\min_\alpha \sum_{j=1}^{K} \sum_{Y_i=j} \left(D_i - \bar{D}_j\right)^2$$

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Clustering : Observations (continuous variables) $\rightarrow$ Clusters (discrete variable)
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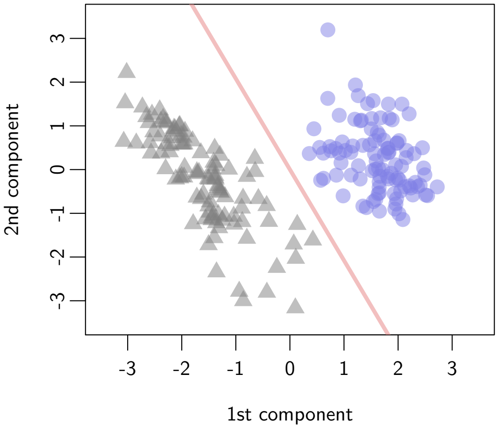
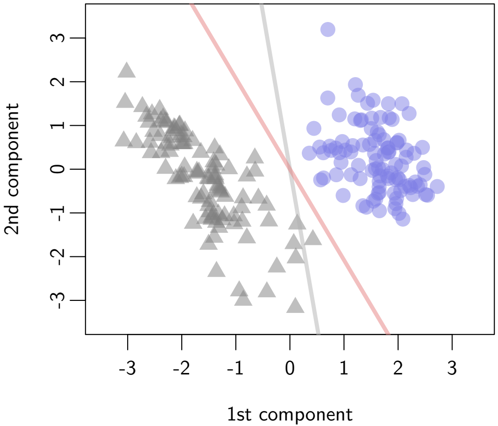
The discriminant D in the linear combination of the (X^j) **minimizing the intra-variability**
Best linear combination of the regressors (X^j) for the **clustering given by** Y

LDA : Example of the notes



LDA : Example of the notes



$\rightarrow$ The linear discriminant and the K-means only match when the given clustering in LDA is the one minimizing the intra-variability for $\alpha_0 = 0$ and $\alpha_j = 1$ for all $j = 1, \ldots, p$

Clustering and LDA with R

Clustering methods

- **K-means** `kmean(database,k)`

  with `database` the data (vector or matrix) and `k` the number of clusters

- **AHM** `hclust(dist(X))`

  - Specification of the metric `dist()` (see option `methods`)
  - Specification of the linkage with option `methods` in `hclust()` function
  - Cutting of the dendrogram with `cutree(H,k)`, with `H` a `hclust()`-object and `k` the number of clusters

- **Mean-shift** `ms(X,h)`

  with `h` the bandwidth — Package `LPMC` to install

Linear discriminant analysis `lda(X)` or `fda(X)`

Packages `MASS` or `MDA` to install

Clustering : Summary

Clustering methods allow to partition **heterogeneous data in homogeneous clusters**

- Optimisation of intra/inter-variability **K-means**
  $\rightarrow$ **Fixed number of clusters**
- Hierarchy between the observations **Hierarchical method**
  $\rightarrow$ Representation with **dendrogram**
- $\rightarrow$ Cluster based on empirical PDF **Mean-shift**
  Specification of the **bandwidth**

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  Specification of the **bandwidth**

⚠ **Significance of a clustering has to be tested** : Intra/inter-variability difference, branch size of dendrogram, bandwidth size over observation number, ...

Bootstrap technique

Introduction

Regression, PCA and clustering allow to define and **calibrate models**

$\rightarrow$ **Single (punctual) estimates** of the parameters

Would the estimations be the same for another sample of observations?

In other worlds : How does the estimation depend on the specific values of the sample

Introduction

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Bootstrap technique allows to answer these questions by

1. **Resampling** the observations (independent urn sampling)
2. Analysing the **distribution of the estimates on the (bootstrap) subsamples**

> Numerical technique allowing to evaluate the precision of estimation of model parameters
> Approaching initially used in end of the 1970's when computer capacity became important

An illustrative example

A machine produces some components

→ Some of them are **operational**, some others are **defective**

→ Estimation the **probability** p **that a component is defective**

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→ Some of them are **operational**, some others are **defective**

→ Estimation the **probability** p **that a component is defective**

Two sets of observations

1. **Sample 1** : Among 10 observed components, two are defective
2. **Sample 2** : Among 100 observed components twenty two are defective

→ **Respective estimates** : $\tilde{p}_1 = 0.2$ and $\tilde{p}_2 = 0.22$

Are these estimations precise?

Bootstraping — R : `sample(data,n,replace=T)`

Sample 1 $(n = 10)$ $\{0, 0, 1, 0, 1, 0, 0, 0, 0, 0\}$, $\tilde{p}_1 = 0.2$

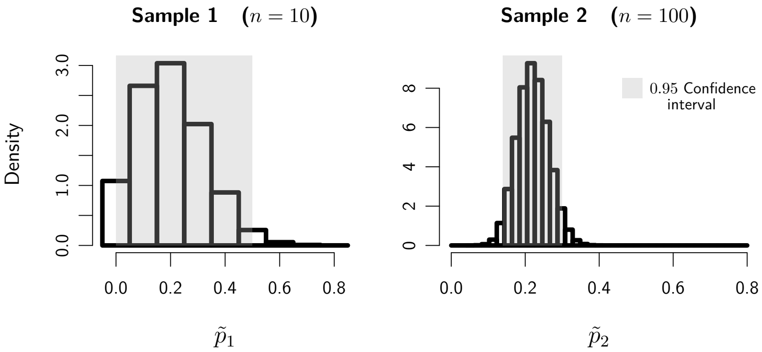
- **Bootstrap Sample 1** $\{0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}$, $\tilde{p}_1^1 = 0$
- **Bootstrap Sample 2** $\{0, 0, 0, 0, 1, 0, 0, 0, 1, 0\}$, $\tilde{p}_1^2 = 0.2$
- **Bootstrap Sample 3** $\{0, 0, 0, 0, 0, 0, 1, 0, 0, 0\}$, $\tilde{p}_1^3 = 0.1$
- ...

Sample 2 $(n = 100)$ $\{0, 0, 0, 0, \ldots, 1, 0, 0, 0\}$, $\tilde{p}_2 = 0.22$

- **Bootstrap Sample 1** $\{0, 0, 0, 1, \ldots, 1, 0, 0, 0\}$, $\tilde{p}_2^1 = 0.26$
- **Bootstrap Sample 2** $\{0, 0, 0, 0, \ldots, 0, 1, 0, 0\}$, $\tilde{p}_2^2 = 0.25$
- **Bootstrap Sample 3** $\{1, 0, 0, 0, \ldots, 0, 1, 1, 0\}$, $\tilde{p}_2^3 = 0.17$
- ...

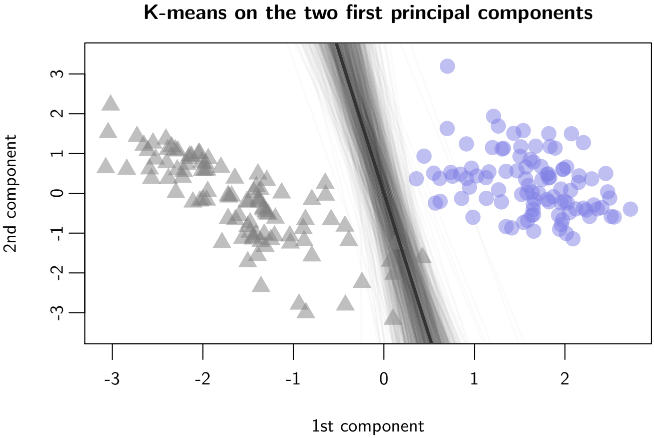
Bootstraping

Histogram of the estimations of probability p for 1e5 bootstrap subsamples



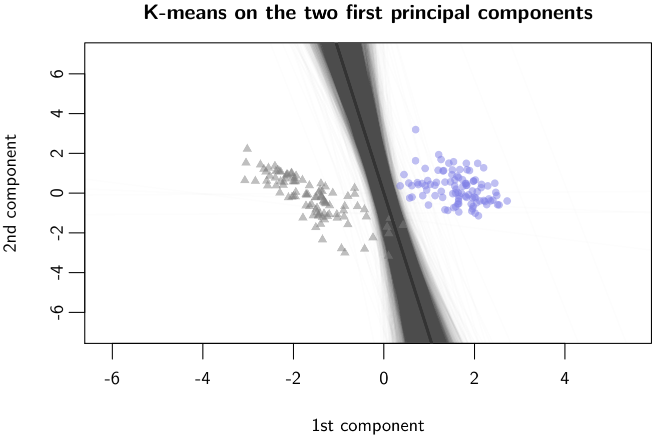
Example of the notes

1e3 bootstrap subsamples



Example of the notes

1e4 bootstrap subsamples



Bootstrap : Summary

- The Bootstrap method is strictly descriptive, **with no assumption on the data and their distribution**
- The method is **purely numerical** and can be **computationally costly**
- Bootstrap **does not improve punctual estimate** but give information on its **variability** (i.e. the precision of estimation)
- The approach can be used for **any type of estimates** (mean, quantil, etc...)
- **Smooth bootstrap** by adding noise onto each resampled observation (equivalent to sampling from a kernel density estimate of the data).
- Time series : **Moving block bootstrap**
- Bootstrap with random variable generator : **Monte Carlo simulation**

Overview

Part 1 Descriptive statistics for univariate and bivariate data

Repartition of the data (histogram, kernel density, empirical cumulative distribution function), order statistic and quantile, statistics for location and variability, boxplot, scatter plot, covariance and correlation, QQplot

Part 2 Descriptive statistics for multivariate data

Least squares and linear and non-linear regression models, principal component analysis, principal component regression, clustering methods (K-means, hierarchical, density-based), linear discriminant analysis, bootstrap technique

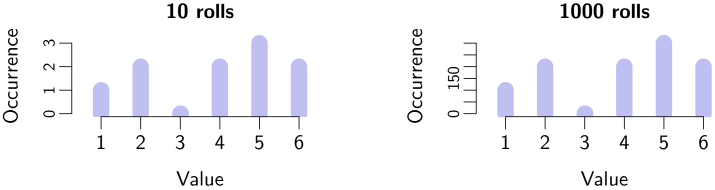
Part 3 Parametric statistic

Likelihood, estimator definition and main properties (bias, convergence), punctual estimate (maximum likelihood estimation, Bayesian estimation), confidence and credible intervals, information criteria, test of hypothesis, parametric clustering

Appendix LaTeX plots with R and Tikz

The example of the dice

Are my dices biased ??



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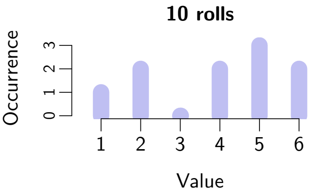

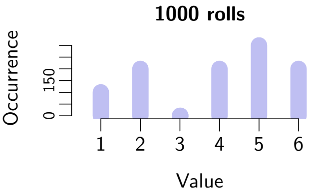

No

Observed differences
may be random

Yes

Observed differences
can not be random

The example of the machine

A machine produces some components that can be operational or defective

- **Estimation of the probability p that a component is defective** by **mean value**

$$\tilde{p}_n = \frac{1}{n}\sum_{i=1}^{n} X_i, \qquad \text{with} \quad X_i = \begin{cases} 0 & \text{if the component } i \text{ is operational} \\ 1 & \text{if the component } i \text{ is defective} \end{cases}$$

The estimation from a sample with **100 observations** is **more precise** than the estimation with **10 observations** (cf. bootstrap)

Why ? Because the variability of the mean decreases as the observation number increases

- Implicitly this reasoning supposes **probabilist assumptions** on the convergence of the mean, its distribution or again existence of expected values

$\rightarrow$ **Parametric statistic**

Introduction

Fundamental assumption in parametric (or inference or mathematical) statistic :

> **The observations $i = 1, \ldots, n$ are independent random variables with probability distribution function P_θ, $\theta \in \mathbb{R}^k$**
>
> $\rightarrow$ **Independent and identically distributed (iid) model**

- P_θ **is general** (but can have to satisfy properties) — θ are the **parameters of the models**
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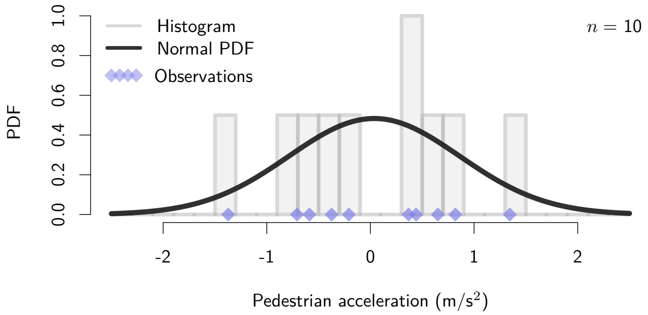
The parametric statistic allows to :

- **Fit the parameters** θ of a model and evaluate the **precision of estimation**
- Obtain **properties on usual estimators** or **posterior distribution** (Bayesian approach)
- **Testing modelling assumptions and compare models**

Example 1

Assumption : Normal distribution $\mathcal{N}(\mu, \sigma^2)$ $f(x) = e^{-\frac{(x-\mu)^2}{2\sigma^2}} \sqrt{2\pi\sigma^2}^{-1}$

$\rightarrow$ Estimation of μ and σ by $\tilde{\mu}_n = \bar{x}$ and $\tilde{\sigma}_n = s_x$



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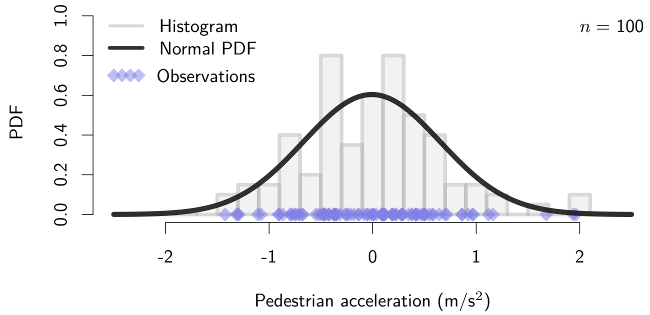

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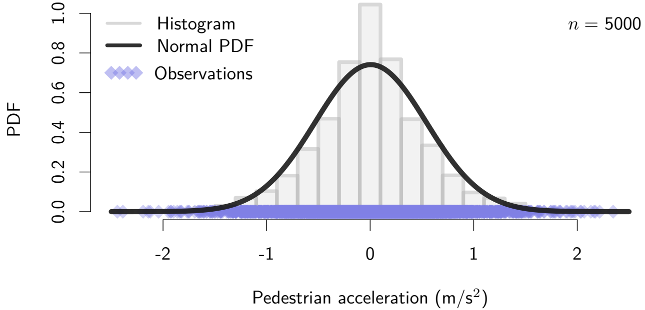
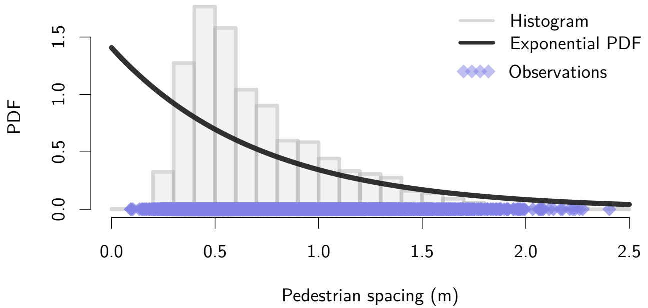


Example 2

Assumption: Exponential distribution $\mathcal{E}(\lambda)$ $f(x) = \lambda e^{-\lambda x}$

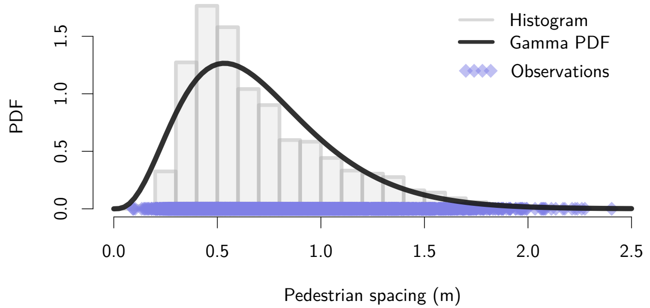
$\rightarrow$ Estimation of expected value λ by $\tilde{\lambda}_n = \bar{x}$



Example 2

Assumption : Gamma distribution $\mathcal{G}(k,\alpha)$ $f(x) = \frac{x^{k-1}e^{-x/\alpha}}{\Gamma(k)\alpha^k}$

$\rightarrow$ Estimation of k and α by $\tilde{k}_n = \bar{x}^2/var_x$ and $\tilde{\alpha}_n = var_x/\bar{x}$



Convergence of random variables

- **Convergence in distribution** denoted D

  A sequence $X_1, X_2, \ldots$ of real-valued random variables is said to **converge in distribution**, or **converge weakly**, or **converge in law** to a random variable X if

  $$D_n(x) \to D(x) \quad \text{as} \quad n \to \infty \quad \text{for all } x \in \mathbb{R} \text{ at which } F \text{ is continuous}$$

  Here D_n and D are the **cumulative distribution functions** of X_n and X, respectively.

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- **Almost sure convergence** denoted a.s.

  $X_1, X_2, \ldots$ **converges almost surely**, or **almost everywhere**, or **with probability 1**, or **strongly** towards X if

  $$P\left(X_n \to X \text{ as } n \to \infty\right) = 1$$

Main theorems

Law of large number (LLN)

$(X_1, \ldots, X_n)$ is a iid sample with expected value $E(X_i) = \mu < \infty$. Then

$$\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i \overset{\text{a.s.}}{\to} E(X_i) = \mu \quad \text{as} \quad n \to \infty$$

$\rightarrow$ **Mean value converges to expected value**

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Central limit theorem (CLT)

$(X_1, \dots, X_n)$ is a iid sample with $E(X_i) = \mu < \infty$ and $var_{X_i} = \sigma^2 < \infty$. Then

$$\sqrt{n}\frac{\bar{X}_n - \mu}{\sigma} \overset{\text{D}}{\to} Z \quad \text{as} \quad n \to \infty, \qquad \text{with } Z \text{ a normal random variable}$$

$\rightarrow$ **Mean value has a normal asymptotic distribution**

Example of the Bernoulli distribution

In the example machine, the state of a component has a Bernoulli distribution with expected value $\mu = p < \infty$ and variance $\sigma^2 = p(1-p) < \infty$

$\rightarrow$ **Assumptions of LLN and CLT hold**

The estimation $\tilde{p}$ of the probability p that a component is defective is the **mean value** estimate

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- **LLN** allows to show that the mean $\tilde{p}$ converges to p as $n \to \infty$
- **CLT** allows to describe the distribution of this estimator and to quantify the precision of estimation of p by $\tilde{p}$ for fixed n

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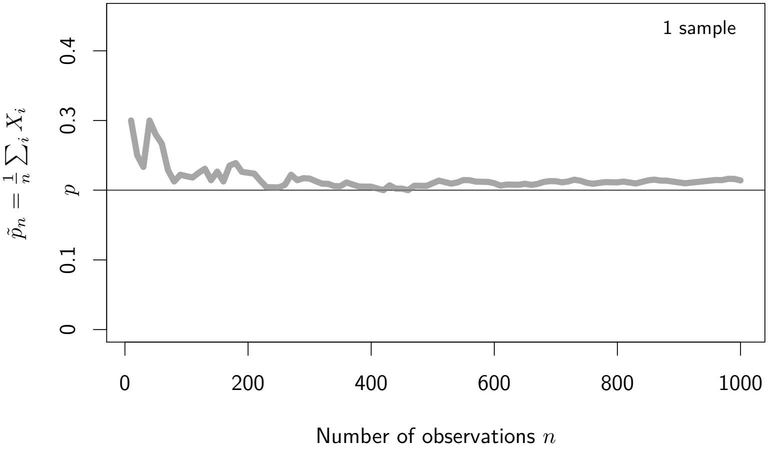

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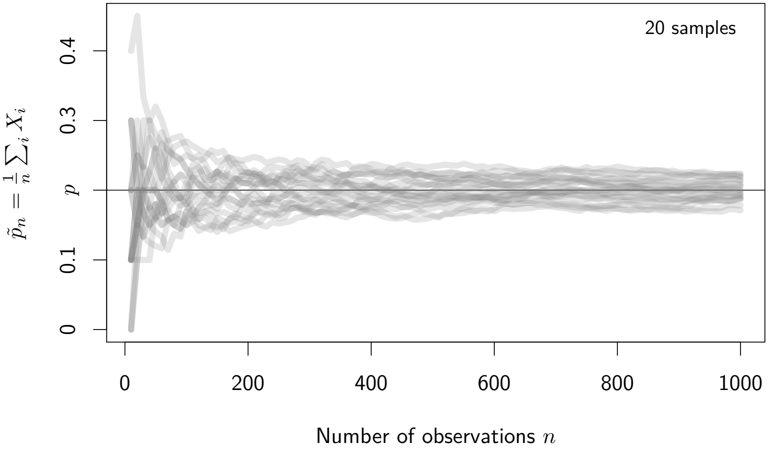
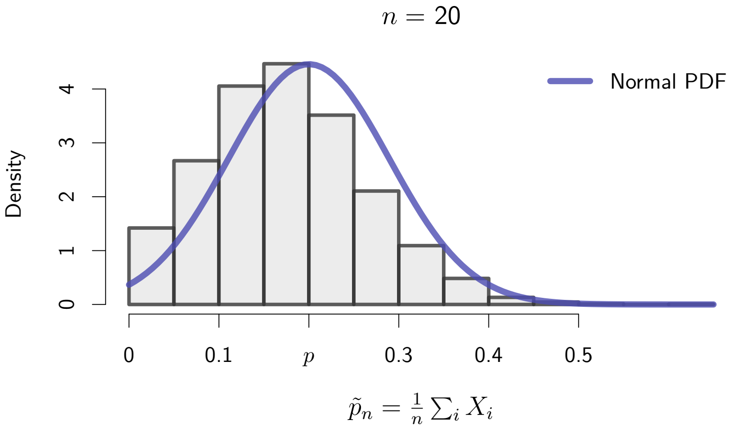


Example of the Bernoulli distribution

Distribution of the mean value — 1e4 samples



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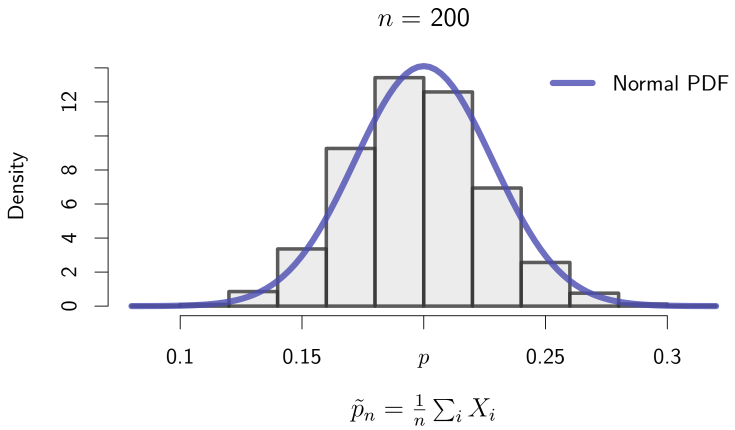

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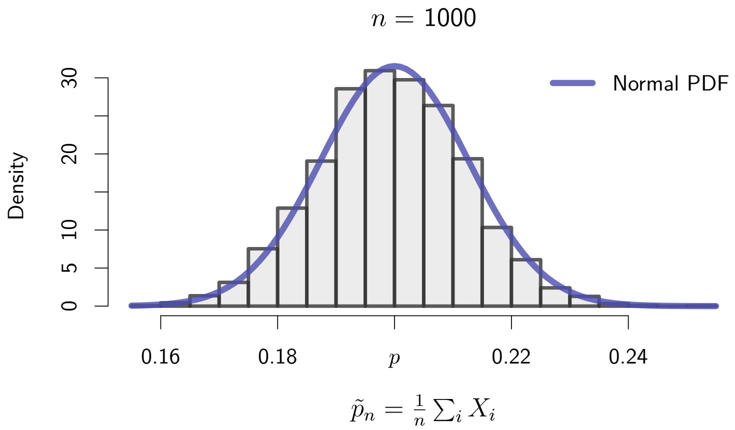

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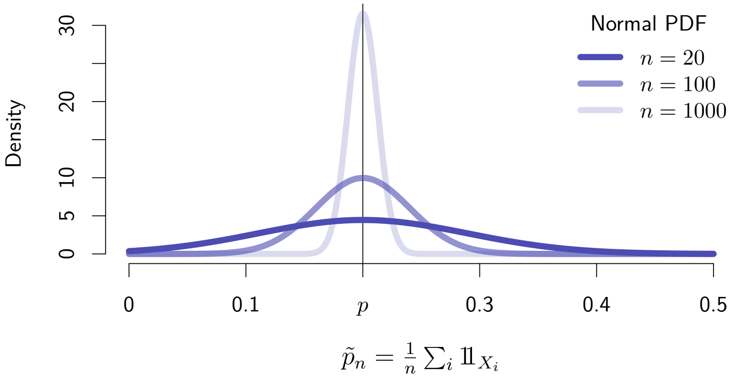

Example of the Cauchy distribution

Cauchy distribution $\mathcal{C}$ has PDF $f(x) = \left(\pi(1+x^2)\right)^{-1}$ with **no expected value**

⚠ Conditions for LLN and CLT are **not satisfied** Mean value does not converge !

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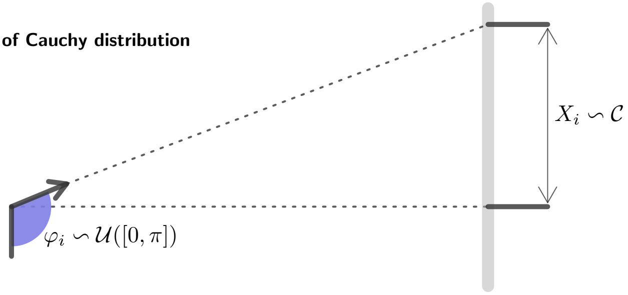

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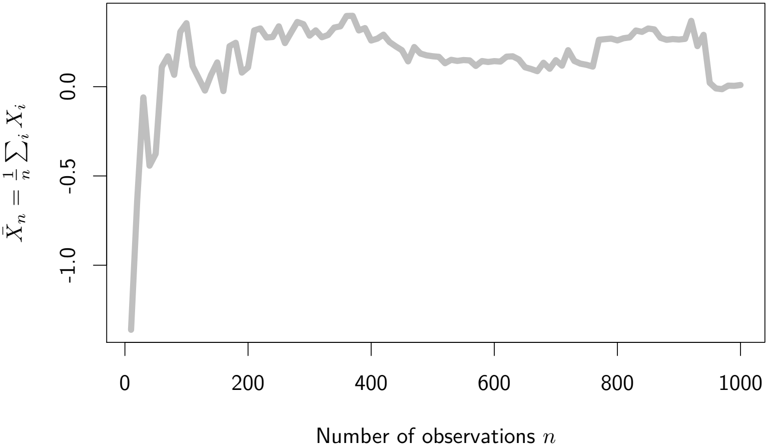

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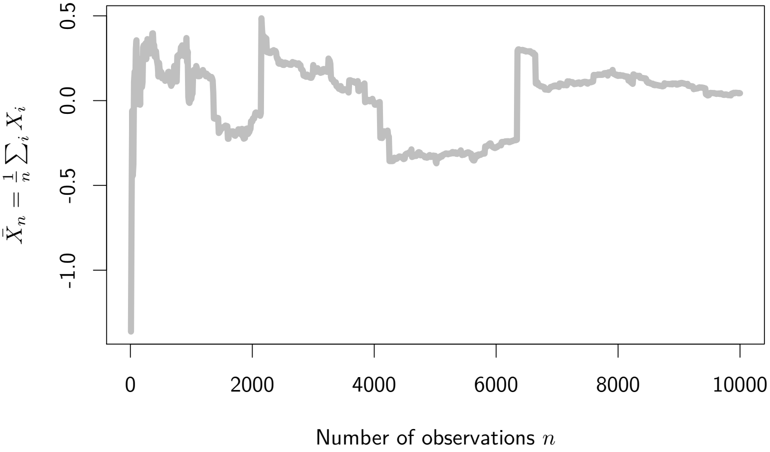

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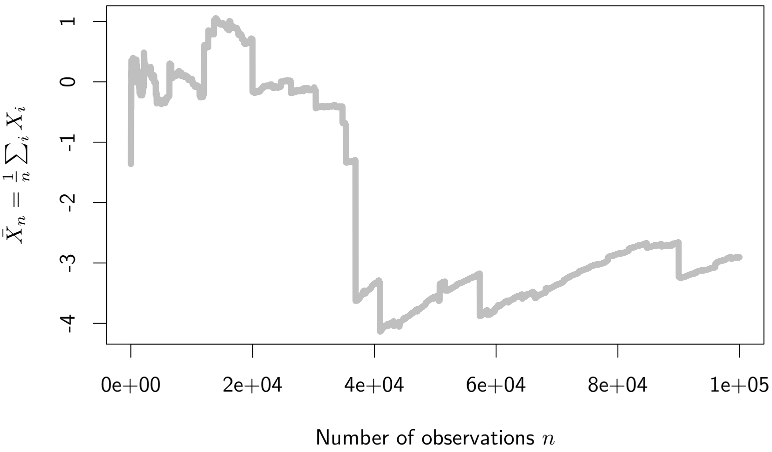

Likelihood function

The likelihood function $L_\theta(x)$ of a set of parameter θ and given data x is

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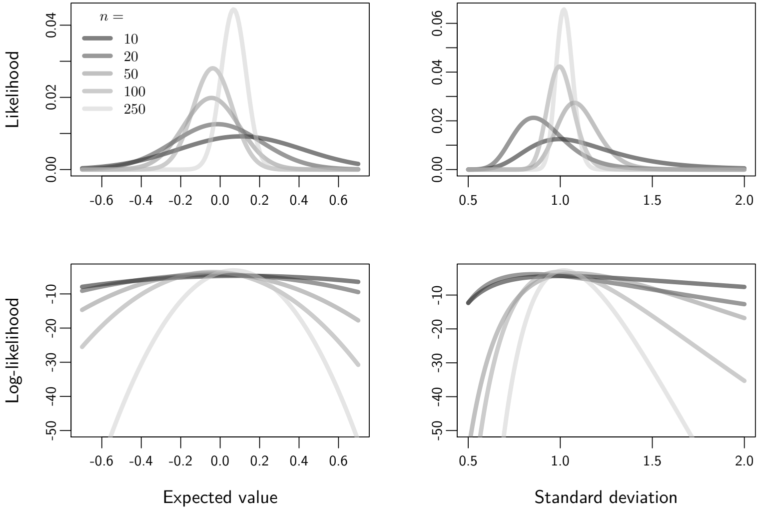
Normal model :

$$\left| \begin{array}{l} L_\theta(x) = \exp\left(-\frac{\sum_i (x_i-\mu)^2}{2\sigma^2}\right)(2\pi\sigma^2)^{-\frac{n}{2}} \\ \mathcal{L}_\theta(x) = -\frac{1}{2\sigma^2}\sum_i (x_i-\mu)^2 - \frac{n}{2}\log\left(2\pi\sigma^2\right) \end{array} \right.$$

Normalised likelihood and log-likelihood for the normal distribution



PDF and random number generation with R

d{*distrib_name*}(*x*)	Density function
p{*distrib_name*}(*q*)	Distribution function
q{*distrib_name*}(*p*)	Quantile function
r{*distrib_name*}(*n*)	Random number generator

More than 20 distributions available with R

Examples

`dnorm(), pnorm(), qnorm(), rnorm()`	Normal distribution
`dunif(), punif(), qunif(), runif()`	Uniform distribution
`dpois(), ppois(), qpois(), rpois()`	Poisson distribution

...

Estimator

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The parameters θ are calibrated using **estimators**

$\rightarrow$ **An estimator** $\tilde{\theta}_n$ is a statistic i.e. a **function of the data**

$$\begin{array}{cccc} \tilde{\theta} & : & \mathbb{R}^n & \mapsto & \mathbb{R}^k \\ & & x & \mapsto & \tilde{\theta}_n(x) \end{array} \quad \text{with} \quad \left| \begin{array}{l} n \text{ the number of observations} \\ k \text{ the number of parameters} \\ x = (x_1, \ldots, x_n) \text{ the observations} \end{array} \right.$$

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- **The distribution of** $\tilde{\theta}_n$ **depends** on the distribution of the data (and so on θ and on n)
- An estimator $\tilde{\theta}_n$ must have specific properties to estimate the parameters θ

Bias of an estimator

$E_\theta \tilde{\theta}_n = \int_{\mathbb{R}^n} \tilde{\theta}_n(x) \prod_i \mathrm{d}P_\theta(x_i)$ is the **expected value** of the estimator $\tilde{\theta}_n$

The bias B of an estimator $\tilde{\theta}_n$ of θ is the quantity

$$B_\theta(\tilde{\theta}_n) = \theta - E_\theta(\tilde{\theta}_n)$$

- An estimator is called **unbiased if**

$$E_\theta(\tilde{\theta}_n) = \theta \qquad \forall \theta \in \mathbb{R}^k$$

- An estimator is **asymptotically unbiased if**

$$E_\theta(\tilde{\theta}_n) \to \theta \quad \text{as} \quad n \to \infty \qquad \forall \theta \in \mathbb{R}^k$$

Bias : Examples

Bias for the mean value

- The mean $\bar{X}$ is a unbiased estimate of the expected value $E_\mu X_i = \mu$

$$E_\mu(\bar{X}) = E_\mu\left(\frac{1}{n}\sum_i X_i\right) = \frac{1}{n}\sum_i E_\mu X_i = \mu \qquad \forall\mu$$

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Bias for the variance

- The empirical variance s_X^2 is asymptotically an unbiased estimate of the variance $var_\sigma(X_i) = \sigma^2$

$$E_\sigma(s_X^2) = E_\sigma\left(\frac{1}{n}\sum_i (X_i - \bar{X})^2\right) = \frac{1}{n}\sum_i E_\sigma(X_i^2) - E_\sigma(\bar{X}^2) = \frac{n-1}{n}\sigma^2 \qquad \forall\sigma$$

$\rightarrow$ $\tilde{s}_X^2 = \frac{n}{n-1}s_X^2 = \frac{1}{n-1}\sum_i(X_i - \bar{X})^2$ is an unbiased estimate of the variance

Error and mean squared error

The error e **of an estimator** $\tilde{\theta}_n$ **of** θ is the quantity

$$e_\theta(\tilde{\theta}_n) = \tilde{\theta}_n - \theta$$

- The error is a **random variable** for which the variability is the one of the estimator
- The error is **centred** if the estimator is **unbiased**

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The mean squared error MSE of an estimator $\tilde{\theta}_n$ **of** θ is the quantity

$$\mathrm{MSE}_\theta(\tilde{\theta}_n) = E_\theta((\tilde{\theta}_n - \theta)^2) = var_\theta(\tilde{\theta}_n) + B_\theta^2(\tilde{\theta}_n)$$

- The mean squared error is a **deterministic quantity** (variance of the error)
- Compromise between **bias and variance** of the estimator

Convergence properties

An estimator $\tilde{\theta}_n$ of θ is called **consistent** if

$$\tilde{\theta}_n \to \theta \quad \text{as} \quad n \to \infty \qquad \forall \theta \in \mathbb{R}^k$$

- Necessary $\mathrm{MSE}_\theta(\tilde{\theta}_n) \to 0$ for a consistent estimator, i.e. at least **asymptotic unbiased** and with **asymptotic variance nil**
- Property generally obtained from the **law of large numbers**

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- Property generally obtained from the **law of large numbers**

The speed of convergence of a consistent estimator $\tilde{\theta}_n$ of θ is $\gamma > 0$ such that

$$n^\gamma(\tilde{\theta}_n - \theta) \to Z \quad \text{as} \quad n \to \infty \qquad \forall \theta \in \mathbb{R}^k$$

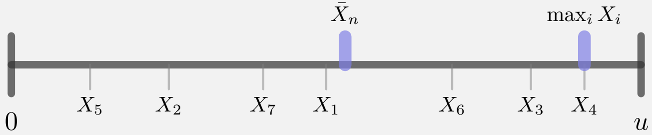
- **Higher the convergence speed, better is the estimator**
- Asymptotic convergence speed of $1/2$ given by the **central limit theorem**

Example of the uniform distribution

$(X_1, \ldots, X_n)$ **uniform random variables** on $[0, u]$ PDF: $f(x) = \frac{1}{u} \mathbb{1}_{[0,u]}(x)$

→ **Two estimators for u**

$$\tilde{u}_1 = 2\bar{X}_n \qquad \text{and} \qquad \tilde{u}_2 = \max_i X_i$$



Example of the uniform distribution

Estimator $\tilde{u}_1 = 2\bar{X}_n = \frac{2}{n}\sum_i X_i$

- **Expected value** : $E(\tilde{u}_1) = \frac{2}{n}\sum_i E(X_i) = u$ since $E(X_i) = u/2$ **Unbiased estimator**
- **Convergence speed** $\gamma = 1/2$ **CLT** : $n^{1/2}(\tilde{u}_1 - u) \to Z$ as $n \to \infty$

Example of the uniform distribution

Estimator $\tilde{u}_1 = 2\bar{X}_n = \frac{2}{n}\sum_i X_i$

- **Expected value**: $E(\tilde{u}_1) = \frac{2}{n}\sum_i E(X_i) = u$ since $E(X_i) = u/2$ **Unbiased estimator**
- **Convergence speed** $\gamma = 1/2$ **CLT**: $n^{1/2}(\tilde{u}_1 - u) \to Z$ as $n \to \infty$

Estimator $\tilde{u}_2 = \max_i X_i$

- $P(\tilde{u}_2 \leq x) = P(\cap_i \{X_i \leq x\}) = (x/u)^n$ therefore a PDF for $\tilde{u}_2$ is $f_2(x) = nx^{n-1}u^{-n}$
  Expected value: $E(\tilde{u}_2) = \int x f_2 \, \mathrm{d}x = \frac{n}{n+1}u$ **Asymptotically unbiased estimator**
- $P\big(n^\gamma(\tilde{u}_2 - u) \geq \varepsilon\big) = 1 - (1 + \varepsilon n^{-\gamma}/u)^n \sim 1 - e^{\varepsilon n^{1-\gamma}/u} \to 0$ as $n \to \infty$ if $\gamma > 1$
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$\tilde{u}_2$ **better than** $\tilde{u}_1$

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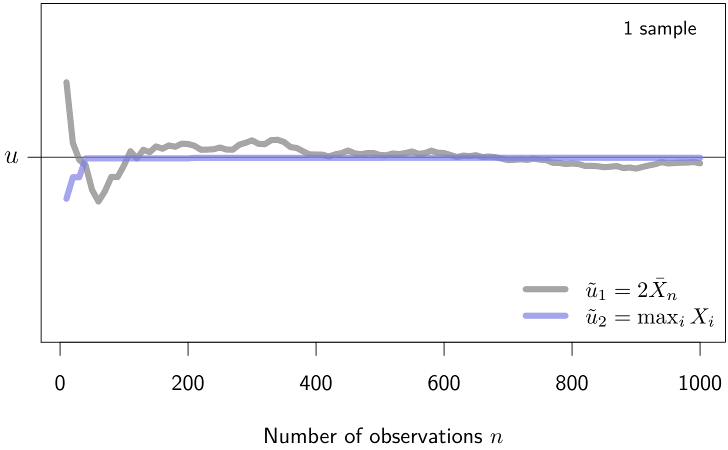

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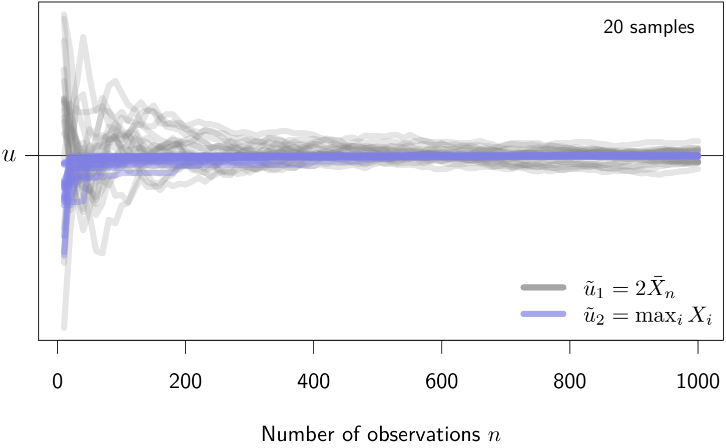
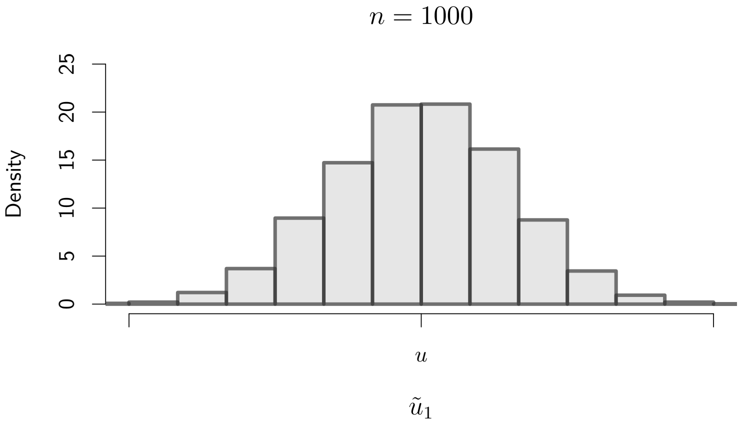


Example of the uniform distribution

Distribution of the estimators — 1e4 samples



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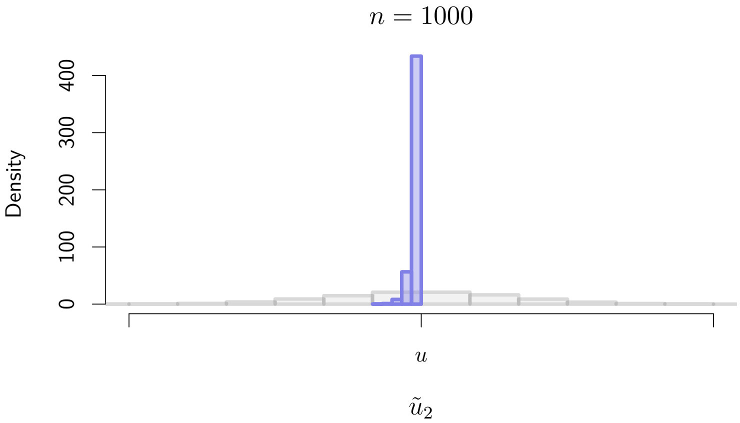

Sufficient statistic, Fisher Information and efficient estimate

A statistic $\tilde{\theta}_n^s(x)$ is **sufficient** (or exhaustive) with respect to an unknown parameter θ if

No other statistic that can be calculated from the same sample provides any additional information as to the value of the parameter (Ronald Fisher)

Fisher–Neyman factorization criterion : $\tilde{\theta}_n$ sufficient for θ iff $\exists\, g, h, \quad L_\theta(x) = h(x)\, g_\theta(\tilde{\theta}_n(x))$

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  → We have in general $I_{\tilde{\theta}(x)}(\theta) \leq I_x(\theta)$ and $I_{\tilde{\theta}^s(x)}(\theta) = I_x(\theta)$ for a sufficient statistic
- **Cramer–Rao bound** : *Under regularity assumptions* $1/I_x(\theta) \leq var_\theta(\tilde{\theta}_n)$, $\forall \tilde{\theta}_n$ unbiased
  → An estimate is called **efficient** iff $var_\theta(\tilde{\theta}_n) = 1/I_x(\theta)$
  → An **efficient** statistic is **necessary sufficient**

Punctual estimation

Introduction

Punctual estimations of parameters are **non-linear optimisation problems** for an

objective function $f_x(\theta)$

| x are the data (given)
| θ are the parameters (to optimize over $\mathbb{R}^k$)

→ Hard problem when f is not regular (discontinuous, multi-modal, noisy, ...)
Convergence to local minima

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Formulation of the objective function f by

- **Least squares** — Non-parametric approach
- **Likelihood** — Maximum likelihood estimate
- **Bayesian approach** — Prior on the parameters

Optimisation with R

MLE and posterior PDF are optimisation problems for functions $f : \mathbb{R}^k \mapsto \mathbb{R}$

Optimisation with R (general case) `optim(par,f)`

with `par` the initial values for the parameters and `f` the function to optimize

> Exist different optimisation methods (Nelder-Mead, quasi-Newton, ...)
> Quasi-Netwon method `''L-BFGS-B''` allows box constraints for the parameter

Least-squares optimisation with R

- Multilinear models `lm(f,X)`
- Non-linear models `nls(f,X,par)`

Maximum likelihood estimation

Maximum Likelihood Estimation (MLE)

$$\tilde{\theta}^{\mathsf{MLE}}(x) = \arg\max_{\theta \in \mathbb{R}^k} L_\theta(x)$$

- **Most probable estimation knowing the data** of parameter θ for the distribution family
- MLE can be determined by **maximizing the log-likelihood**

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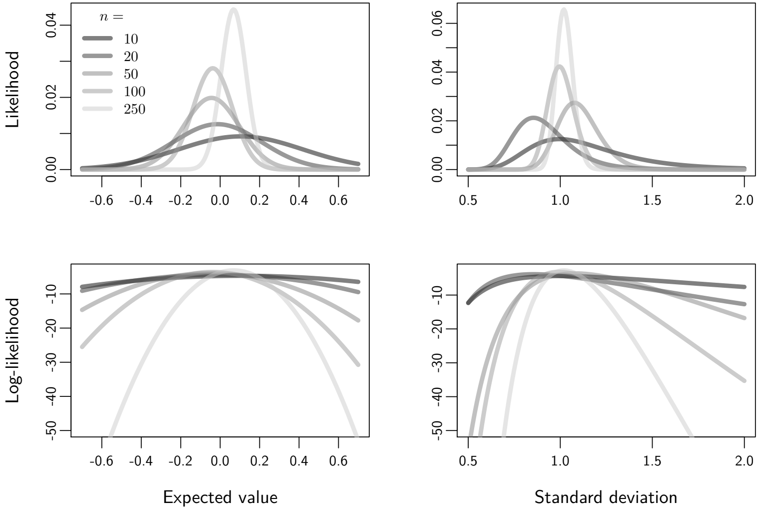
MLE have many **interesting properties** justifying its large use

- MLE not necessary unbiased but is in general **asymptotically unbiased**
- If it exits a **sufficient statistic** then MLE depends on it (but MLE not necessary sufficient)
- If it exits a **efficient statistic** then it is the MLE (regularity assumptions of Cramer-Rao th.)

$\rightarrow$ MLE generally better than least squares or moment methods (cf. uniform distribution)

MLE for the normal distribution



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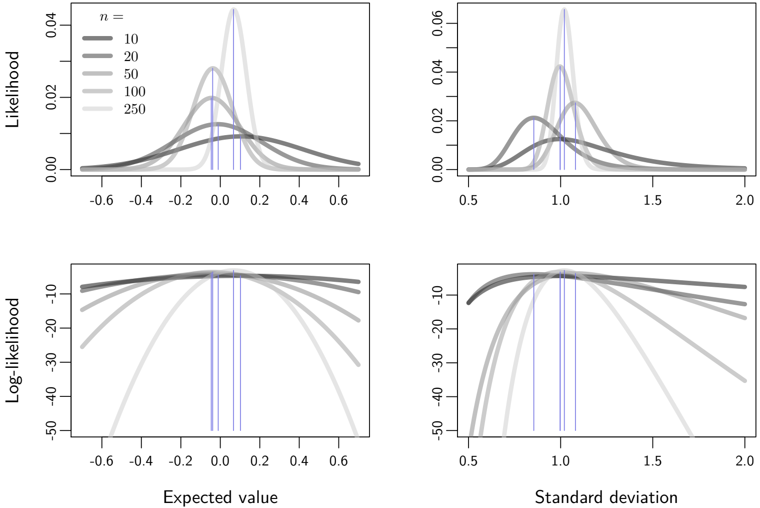

MLE for different distributions

- **Normal distribution**

The likelihood of the Gaussian model is $L_\theta(x) = \frac{1}{(\sqrt{2\pi}\sigma)^n} \exp\big(-\frac{\sum_i (x_i - \mu)^2}{2\sigma^2}\big)$

MLE of μ and σ solution of $\frac{\partial L_\theta}{\partial \mu} = \frac{\partial L_\theta}{\partial \sigma} = 0$ are $\tilde{\mu}_n^{\mathsf{MLE}} = \bar{x}$ and $\tilde{\sigma}_n^{\mathsf{MLE}} = s_x$

$\rightarrow$ **Arithmetic mean and empirical variance are the MLE** for parameters μ and σ^2 of the **normal distribution**

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The likelihood of the uniform model on $[0, u]$ is $L_u(x) = \begin{cases} \frac{1}{u^n} & \text{if } \min_i x_i \geq 0 \text{ and } \max_i x_i \leq u \\ 0 & \text{otherwise} \end{cases}$

MLE of u is $\tilde{u}_n^{\mathsf{MLE}} = \max_i x_i$ (but $\frac{\partial L_u}{\partial u}$ not defined for $u = \max_i x_i$)

$\rightarrow$ **The maximum is the MLE** of u for the **uniform distribution** on $[0, u]$

MLE and the linear regression

Linear model with Gaussian noise

$$y_i = (ax_i + b) + \sigma\mathcal{E}_i, \qquad \text{with } (\mathcal{E}_i) \text{ iid } \mathcal{N}(0,1)$$

$\rightarrow$ **Residuals** $R_i(a,b) = y_i - (ax_i + b)$ **are supposed normally distributed**

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→ **OLS estimates** is **MLE** when the residuals are **Gaussian**
(and the empirical standard deviation is the MLE of noise amplitude σ)

The Bayesian approach

Bayesian approach consists in using **prior distributions for the parameters** and to **analyse posterior distributions conditionally to the data**

- **Data** x are **observable** random variables with **distribution** (likelihood) $P(x \mid \theta)$
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Bayes Theorem assuming $P(x), P(\theta) > 0$

$$P_x(\theta) = P(\theta \,|\, x) = \frac{P(x, \theta)}{P(x)} = \frac{P(\theta) P(x \,|\, \theta)}{P(x)}$$

$$posterior \;\propto\; prior \;*\; likelihood$$

- **Punctual estimations of θ by mode, median or mean of posterior distribution** $P_x(\theta)$
- **Posterior distribution = (normalized) likelihood** when **prior is uniform**
  $\rightarrow$ MLE is the mode of posterior with non-informative prior

Algorithms to calculate MLE and posterior PDF

MLE or posterior PDF are complex problems having in general **no explicit solutions**

$\rightarrow$ Approximation by **iterative algorithms** (starting from initial value $\tilde{\theta}_n^{(0)}$ for the parameters)

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- **Gibbs sampling** — Randomized algorithm – MCMC

  Simulation of $\tilde{\theta}_n^{(i)}$ as random variables with distribution $P\left(\tilde{\theta}_n^{(i-1)}\right)P\left(x \mid \tilde{\theta}_n^{(i-1)}\right)$ (convergence to posterior distribution)

- **Expectation-Maximization (EM)** — Deterministic algorithm

  Iterations of maximisation of the parameters $\tilde{\theta}_n^{(i)}$ of the expected log-likelihood conditionally to the data and values $\tilde{\theta}_n^{(i-1)}$ of the parameters at previous step

- **Variational Bayesian (VB)** — Deterministic algorithm

  Estimation of posterior distribution by minimizing the Kullback-Leibler divergence measure with parameter previous values $\tilde{\theta}_n^{(i-1)}$ over a partition of their domain

Comparing Bayesian, MLE and OLS approaches

OLS and MLE are close when residuals have compact (normal) distributions

Bayesian estimate and MLE are <u>close</u> when :

- **Prior bring few information** (straight distribution) or **data is large** (concentrated likelihood)

Bayesian estimate and MLE are <u>different</u> when :

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MLE or OLS should be substituted by Bayesian estimates when :

- The **dataset is small**
- **Models are complex** (many parameters)
- We have **a priori on the parameter values**
- **Dynamical integration of new data**

Summary

Approach	**Advantage**	**Inconvenient**
OLS	Easy to use	Sensible to extreme values
MLE	Many strong and useful properties	Asymptotic theory (valid if enough data)
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$$\begin{tikzcd}
\textbf{OLS} \arrow[rr, bend left, "\text{Generalisation}"] & \textbf{MLE} \arrow[l, swap, "\text{Normal residuals}"] & \textbf{Bayes} \arrow[l, swap, "\text{Uniform prior}"]
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Precision of estimation

Introduction

Punctual estimates give **no indication on the precision of estimation**

> A fitting can be **insignificant** when it changes from a sample to another (cf. bootstrap)
> Significance of the **differences between different populations** to statute

→ Evaluation of the **precision of estimation** with **confidence intervals**

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→ Evaluation of the **precision of estimation** with **confidence intervals**

CI $= [i_-, i_+]$ is a **confidence interval for θ at the confidence level** $1-\alpha$ if

$$P_\theta(\theta \in \text{CI}) \geq 1-\alpha, \qquad \forall \theta \in \mathbb{R}^k$$

Parameter θ belongs to CI in more than $1-\alpha$ % of the cases

- **Interval of values** with a confidence level instead of **punctual estimation**
- Precision of **estimation of deterministic quantities** : Size of the CI reduces as $n \to \infty$
- Distinct from **prediction intervals** taking into account the noise to predict new observations

Construction of a confidence interval

The **construction of a confidence interval is based on knowledge** on the distribution (variability), or on the asymptotic distribution, of an estimator

> If $q_\theta(u)$ is the quantile of the estimator $\tilde{\theta}_n$, then by construction
> $$P_\theta\left(\tilde{\theta}_n(x) \in [q_\theta(\alpha/2), q_\theta(1-\alpha/2)]\right) \geq 1-\alpha, \qquad \forall\theta \in \mathbb{R}^k, \quad \alpha \in (0,1)$$

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⚠ **Situation generally not accessible** since **estimator distribution is unknown**

- Use of **sufficient conditions** — Tchebychev inequality
- **Asymptotic distribution** — Central limit theorem
- **Posterior distribution** — Bayes approach

Confidence interval with the Tchebychev inequality

Assumption : $x = (X_1, \ldots, X_n)$ is a iid P_θ-sample, $\theta = E(X_i)$, for which exists unbiased estimator $\tilde{\theta}_n$ of θ such that $var_\theta(\tilde{\theta}_n) \leq K_n < \infty$

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The **Tchebychev inequality** gives: $P_\theta\left(|\theta - \tilde{\theta}_n| > \epsilon\right) \leq \frac{K_n}{\epsilon^2}, \quad \forall \epsilon > 0, \quad \theta \in \mathbb{R}$

→ For $\epsilon = \sqrt{K_n/\alpha}$, $\alpha \in (0, 1)$, we get the **symmetric** CI for θ:

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- **Tchebychev inequality very large** : parameter belongs to the CI in more than $1 - \alpha$ % of the cases — **Confidence interval for excess**

Asymptotic confidence intervals

Assumption : $x = (X_1, \ldots, X_n)$ is a iid P_θ-sample, $\theta = E(X_i)$ and $\sigma^2 = var(X_i) < \infty$

Central limit theorem $P_\theta\left(\sqrt{n}\frac{1/n\sum_i X_i - \theta}{\sigma} \in [q_{\mathcal{N}}(\alpha/2), q_{\mathcal{N}}(1-\alpha/2)]\right) \underset{n \to \infty}{\overset{D}{\to}} 1 - \alpha$

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Asymptotic symmetric confidence interval for θ:

$$P_\theta\Big(\theta \in \underbrace{\Big[\frac{1}{n}\sum_i X_i \pm q_{\mathcal{N}}(\alpha/2)\frac{\sigma}{\sqrt{n}}\Big]}_{\text{asymptotic CI level } \alpha}\Big) \to 1-\alpha \qquad \text{as} \quad n \to \infty$$

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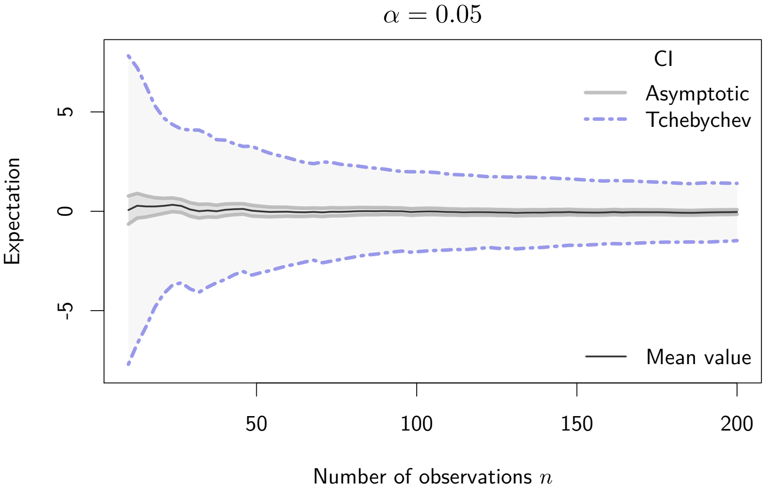
- **CI tends to mean value** if $\sigma^2 = var(X_i) \to 0$ or if $n \to \infty$
- **CI tends to** $\mathbb{R}$ if $\alpha \to 0$
- Asymptotic CI still valid substituting σ by empirical estimator σ_x (exact CI : Student)

CI for the expected value of normal distribution



Bayesian credible interval using posterior PDF

Assumption: $x = (X_1, \ldots, X_n)$ is a iid P_θ-sample and $P(\theta)$ is a prior distribution on the parameters such that $P(\theta) > 0$

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$$P_\theta\big(\theta \in \underbrace{\left[q_x^B(\alpha/2), q_x^B(1-\alpha/2)\right]}_{\text{Bayesian CI}^B \text{ level } \alpha}\big) \geq 1 - \alpha$$

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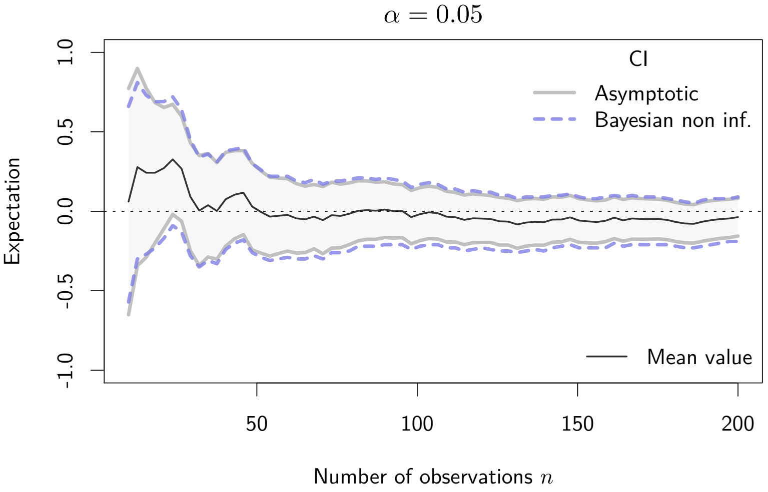
- The **size and symmetry** of CI^B depends on the posterior distribution that depends on **the prior and likelihood**
- Asymptotic CI converges to the uninformed Bayes CI^B with uniform prior

CI for the expected value of normal distribution



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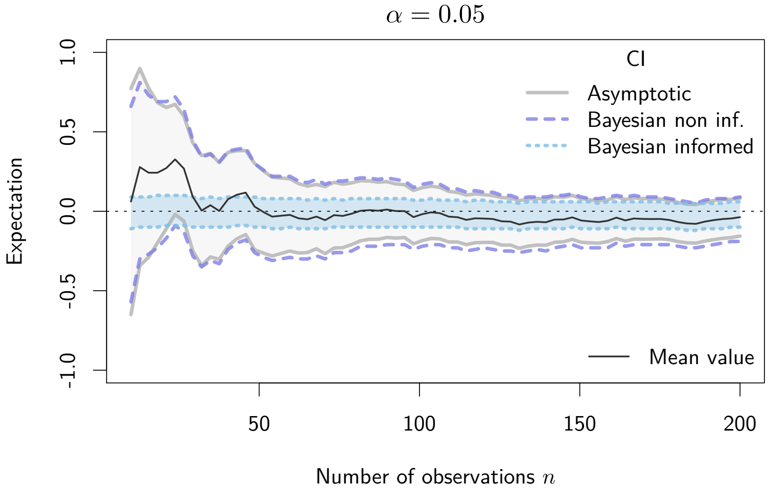

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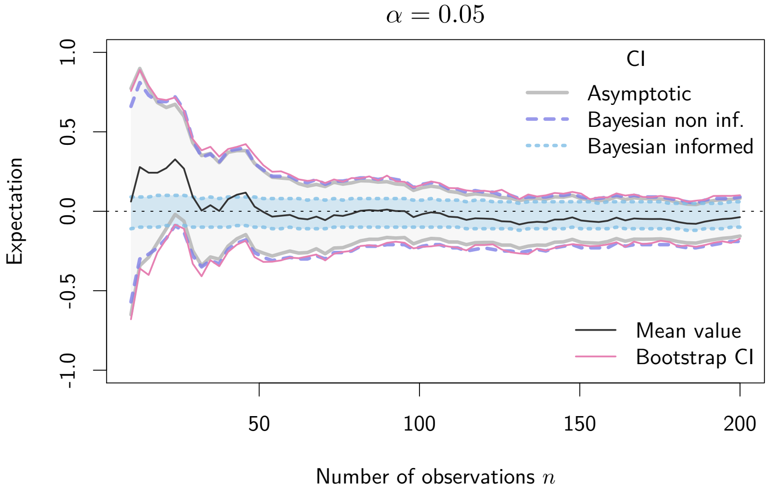

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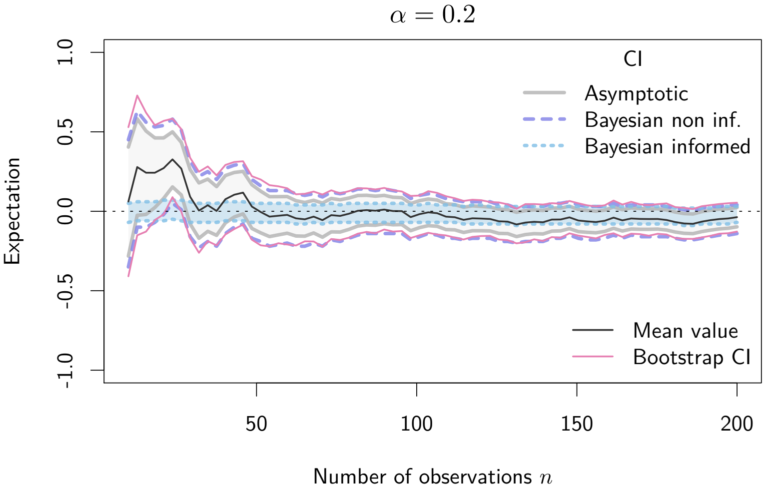

Asymptotic confidence interval for the variance

Calculation of a **asymptotic confidence interval for the variance** parameter σ^2

$$\frac{1}{\sigma}\frac{n-1}{n}\sum_i (x_i - \bar{x}_n)^2 = \frac{(n-1)s}{\sigma} \underset{n \to \infty}{\overset{\mathrm{D}}{\to}} \chi^2(n-1) \qquad \text{(CLT)}$$

with $\chi^2(n-1)$ the Chi-square distribution with $n-1$ degrees of freedom

Then

$$P\Big(\sigma \in \underbrace{\Big[\frac{(n-1)s}{q_{\chi^2}(\alpha/2)}, \frac{(n-1)s}{q_{\chi^2}(1-\alpha/2)}\Big]}_{\text{asymptotic CI level } \alpha}\Big) \underset{n \to \infty}{\to} 1-\alpha$$

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- Do **not required** to know the **expected value**

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- Do **not required** to know the **expected value**
- **Asymmetric CI** since Chi-square distribution is asymmetric

Asymptotic confidence interval for linear regressions

Data $(x, y) = \big((x_1, y_1), \ldots, (x_n, y_n)\big)$ Linear model $y_i = ax_i + b + \varepsilon_i$

OLS estimates : $\tilde{a} = a + \frac{\sum_i x_i \varepsilon_i}{\sum (x_i - \bar{x}_n)^2}$ and $\tilde{b} = b + \bar{x}_n \frac{\frac{1}{n} \sum_i x_i \varepsilon_i}{\sum (x_i - \bar{x}_n)^2}$

The statistics $\dfrac{\tilde{a} - a}{s_{\tilde{a}}}$ and $\dfrac{\tilde{b} - b}{s_{\tilde{b}}}$

with $s_{\tilde{a}} = \sqrt{\frac{1}{n} \sum_i \varepsilon_i^2 / \sum_i (x_i - \bar{x}_n)^2}$ and $s_{\tilde{b}} = \sqrt{\frac{1}{n} \sum_i \varepsilon_i^2 \left(\frac{1}{n} + \frac{\bar{x}_n^2}{\sum_i (x_i - \bar{x}_n)^2} \right)}$

have asymptotically a **Student distribution** t_{n-2} **with** $n - 2$ **degrees of freedom** (CLT)

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have asymptotically a **Student distribution** t_{n-2} **with** $n-2$ **degrees of freedom** (CLT)

→ Therefore

$$\tilde{a} \pm q_{t_{n-2}}(\alpha/2) s_{\tilde{a}} \quad \text{and} \quad \tilde{b} \pm q_{t_{n-2}}(\alpha/2) s_{\tilde{b}}$$

are **asymptotic confidence interval** with confidence level $1-\alpha$ for respectively coefficients a and b of the linear regression

Confidence and prediction bands for linear regressions

Confidence band R : `predict(object,x,'confidence',level)`

Interval of estimation with confidence level $1-\alpha$ for the mean at a given abscissa $x^\star$

$$\tilde{a}\,x^\star + \tilde{b} \pm q_{t_{n-2}}(\alpha/2)\tilde{\sigma}\sqrt{\frac{1}{n} + \frac{(x^\star - \bar{x}_n)^2}{\sum_i (x_i - \bar{x}_n)^2}}$$

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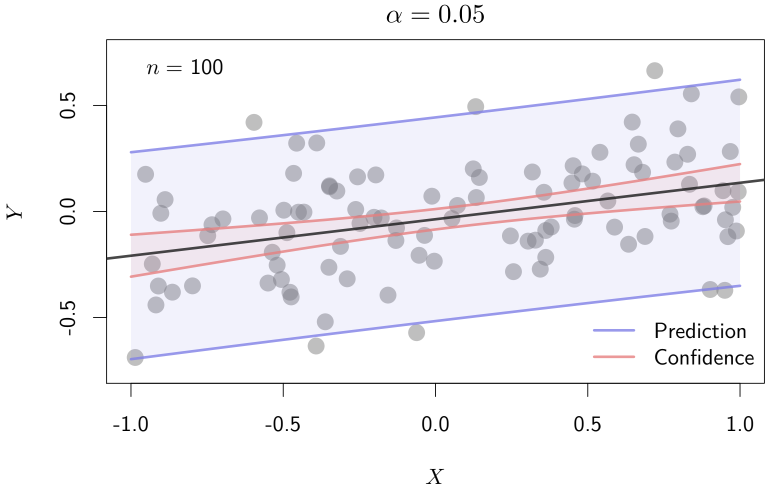
Prediction band R : `predict(object,x,'predict',level)`

Interval of prediction of a new observation at $x^\star$ with confidence level $1-\alpha$

$$\tilde{a}\, x^\star + \tilde{b} \pm q_{t_{n-2}}(\alpha/2)\tilde{\sigma}\sqrt{1 + \frac{1}{n} + \frac{(x^\star - \bar{x}_n)^2}{\sum_i (x_i - \bar{x}_n)^2}}$$

Confidence and prediction bands for a linear regression



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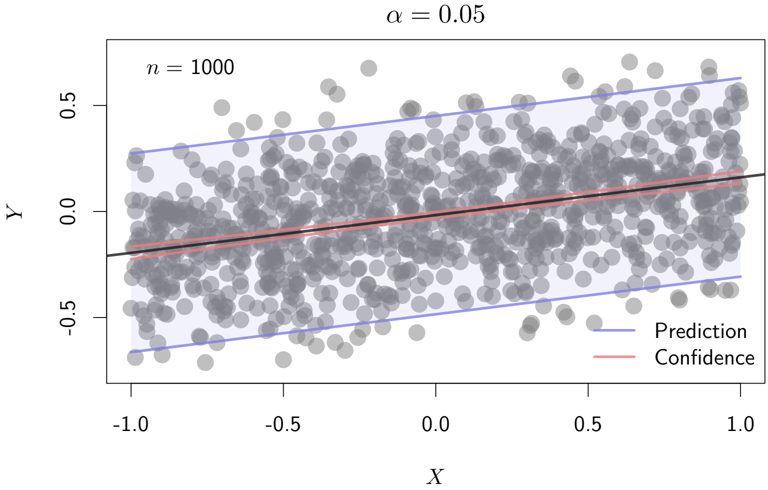

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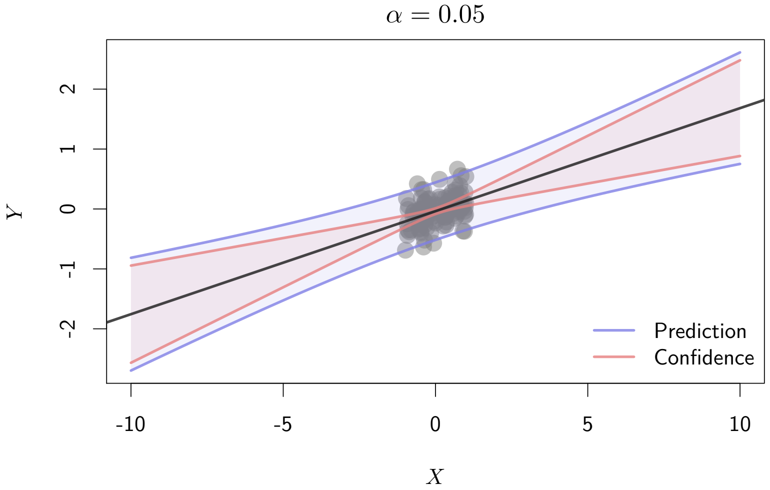


Confidence interval with R

Confident interval `confint(object,level)`

Confident band `predict(object,x,'confidence',level)`

Prediction band `predict(object,x,'predict',level)`

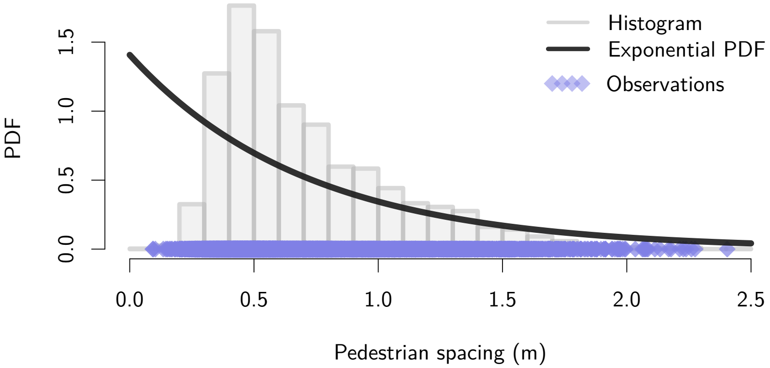
> Generic function for any fitted model object
>
> `level` is the confidence level
>
> Default method assume asymptotic normal distribution for the residuals (asymptotic CI)

Example

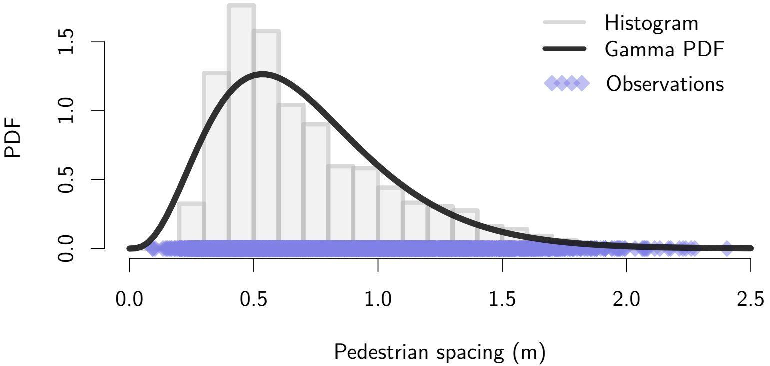
```
object=lm(y~x)
confint(object,0.95)
predict(object,data.frame(1:100),interval='confidence',0.95)
```

Information criteria and test of hypothesis

Fit of the spacing with exponential distribution



Fit of the spacing with gamma distribution



Comparison of models

MLE and posterior PDF allow to find an **optimal fit of the parameters**
CI allows to evaluate the **precision of this fit**

$\rightarrow$ **No indication on the quality of description of the data** using the optimal fit

Cf example : Better fit of pedestrian spacing using gamma distribution than exponential

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Quality of a model evaluated by **information criteria**

Akaike Information Criterion (AIC)

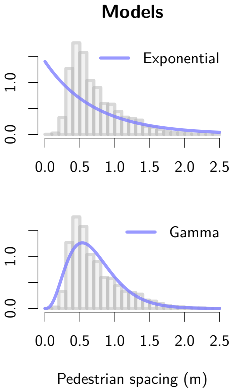
$$\text{AIC} = 2k - 2\ln(L)$$

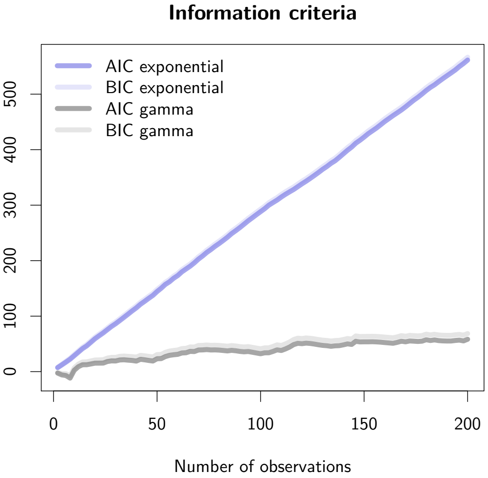
Bayesian Information Criterion (BIC)

$$\text{BIC} = k\ln(2\pi n) - 2\ln(L)$$

- **Compromise between goodness of the fit** through maximum likelihood L and the **complexity of the model** through the parameter number k
- Better model **minimizes criteria**

Information criteria for the fit of the spacing





Likelihood ratio and Bayes factor

The **maximum likelihood ratio** D is

$$\mathsf{D} = \frac{\max_{\theta_1} L_1(\theta_1)}{\max_{\theta_2} L_2(\theta_2)}$$

$\rightarrow$ **Better fit of the model 1** compared to model 2 if $D > 1$ or $\log D > 0$

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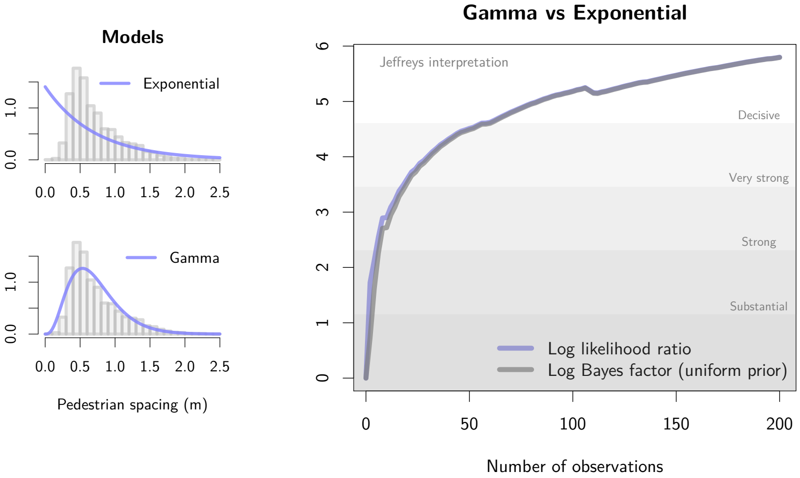
The Bayes factor is the ratio of the **mean likelihood over given prior** f_1 and f_2

$$\mathsf{BF} = \frac{\int L_1(\theta) f_1(\theta)\, \mathrm{d}\theta}{\int L_2(\theta) f_2(\theta)\, \mathrm{d}\theta}$$

$\rightarrow$ **Better fit of the model 1** when $BF > c$ or $\log BF > \log c$ (cf. Jeffreys interpretation)

Likelihood ratio and Bayes factor for the fit of the spacing



Neyman Pearson statistical test

Test of a **null hypothesis** H_0 against an **alternative hypothesis** on a sample of iid data

→ The goal is to **test the validity of** H_0 (and not H_1 — **asymmetric approach**)

→ In general, hypothesis are $H_0 : \{\theta \in \Theta_0\}$ vs $H_1 : \{\theta \notin \Theta_0\}, \quad \Theta_0 \in \mathbb{R}^k$

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Four possible configurations :

Reality / **Test**	H_0 is true	H_0 is false
Reject of H_0	**Error1**	OK
No reject of H_0	OK	**Error2**

- The **probability of occurrence of Error1 is** $\alpha \in (0, 1)$ — Valid for any number of observations
- The **probability of occurrence of Error2** tends to zero as $n \to \infty$ — Power of the test

Construction and usage of a test

A **test is based on a statistic** S for which the distribution
is known under H_0
diverges under H_1

- Construction of a **region of rejection** R_α of H_0

$$P_{H_0}(R_\alpha(S)) = P(\textbf{Error1}) \leq \alpha$$

- **Binary** response of a test for given α

Reject of H_0 **if** $S \in R_\alpha$
No reject otherwise

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The **p-value** is the critical level $\alpha^\star$ such that

$$\left| \begin{array}{ll} \alpha > \alpha^\star : & \text{Reject of } H_0 \\ \alpha < \alpha^\star : & \text{No Reject of } H_0 \end{array} \right.$$

$\alpha^\star$ is the probability to observe the value for S under H_0 — It is not the probability of H_0

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$\alpha^\star$ is the probability to observe the value for S under H_0 — It is not the probability of H_0

Reject of H_0 if $\alpha^\star$ small (e.g. $\alpha^\star < 0.01$) — **No conclusion otherwise**

Example of the machine

$(X_1, \ldots, X_n)$ is a iid sample of Bernoulli distribution with distribution $p = 0.2$

$\rightarrow$ $P(X_i = 1) = p$, $P(X_i = 0) = 1 - p$, $E(X_i) = p$ and $var(X_i) = p(1 - p)$

Test of assumptions $H_0 : \{p = 0.2\}$ VS $H_1 : \{p \neq 0.2\}$

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Test of assumptions $H_0 : \{p = 0.2\}$ VS $H_1 : \{p \neq 0.2\}$

LLN and **TCL** gives

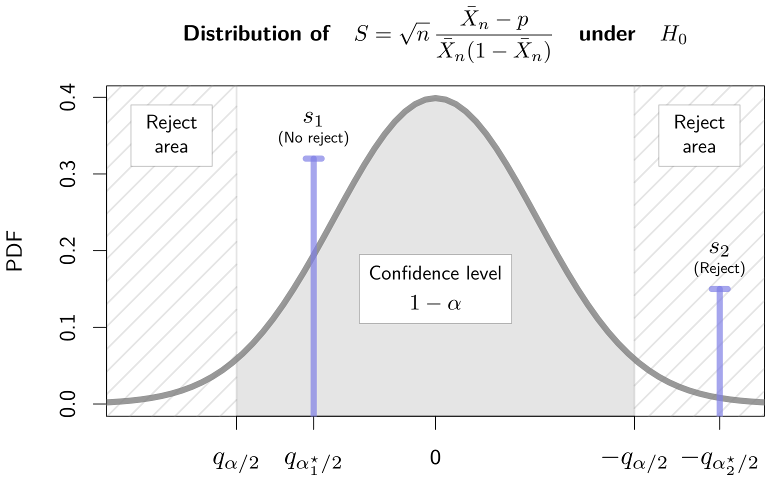
$$S_n = \sqrt{n}\frac{\bar{X}_n - p}{\bar{X}_n(1 - \bar{X}_n)} \quad \rightarrow \quad \begin{cases} \mathcal{N}(0,1) & \text{under } H_0 \\ \pm\infty & \text{under } H_1 \end{cases} \qquad \text{as} \quad n \rightarrow \infty$$

Rejection region $R_\alpha(S_n) = |S_n| > \xi_\alpha$ such that $P_{H_0}(|S_n| > \xi_\alpha) \leq \alpha$

- $\xi_\alpha = -q_{\alpha/2}$ i.e. $R_\alpha(S_n) = |S_n| > -q_{\alpha/2}$ with q quantile of normal distribution
- P-value: $$\alpha^\star = P(|S_n| > s_n) = \begin{cases} 0.5 \ \text{(in average) if } H_0 \text{ is true} \\ 0 \ \text{ as } n \rightarrow \infty \text{ if } H_1 \text{ is true} \end{cases}$$

Example of the machine

$H_0 : \{ p = 0.2 \}$ VS $H_1 : \{ p \neq 0.2 \}$ at level $\alpha = 0.05$



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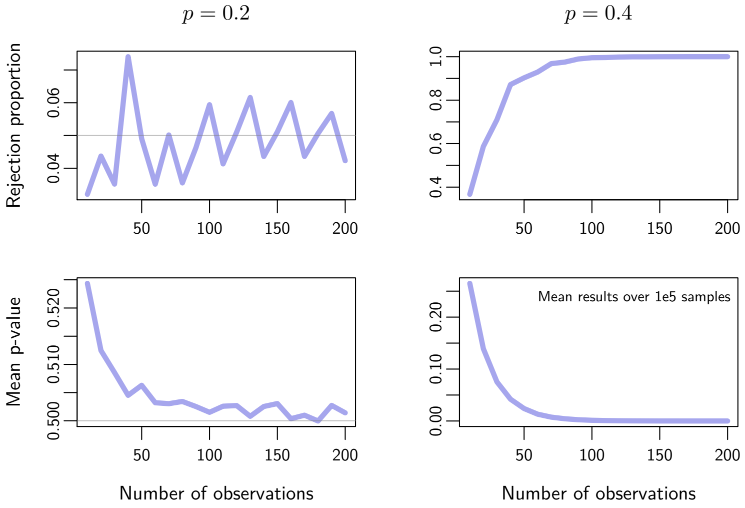

Some tests with R

Test for	Statistic	Distribution	R
Mean value $\{\mu = \mu_0\}$	$\sqrt{n}\,\frac{\bar{x}-\mu_0}{s_x}$	Student	`t.test(x,mu0)`
Variance $\{\sigma = \sigma_0\}$	$(n-1)\,\frac{s_x^2}{\sigma_0^2}$	Chi–squared	—
Mean equality $\{\mu_1 = \mu_2\}$	$\frac{\bar{x}-\bar{y}}{\left(s_x^2/n_1+s_y^2/n_2\right)^{1/2}}$	Student	`t.test(x,y)`
Variance equality $\{\sigma_1 = \sigma_2\}$	s_x^2/s_y^2 (with $s_x < s_y$)	Fisher	`var.test(x,y)`
Adequacy of discrete distribution	$\frac{\sum_i (E_i - O_i)^2}{E_i}$	Chi–squared	`chisq.test(x,p)`
Adequacy of continuous distribution	$\sup_z \lvert D_x(z) - D_y(z) \rvert$	Kolmogorov	`ks.test(x,y)`
Normality	$\frac{\left(\sum_i a_i x^{(i)}\right)^2}{n\,s_x^2}$	Shapiro-Wilk	`shapiro.test(x)`
Independence	$\frac{\sum_i (nE_{i,j} - E_i E_j)^2}{nE_i E_j}$	Chi–squared	`chisq.test(x,y)`

Parametric clustering

Parametric clustering (density- or distribution-based clustering)

Assumption : Observations as **mixture of identical models with different parameter values**

Gaussian mixture model : **Multivariate normal distribution**

- **Observables** : Data x supposed to be iid observations of a multivariate normal distribution f
- **Parameters** : $\theta_k = (\mu_k, \sigma_k)$ of the Gaussian mixture and the proportions of observations per cluster π_k, $k = 1, \ldots, K$

$\rightarrow$ Log-likelihood :

$$\mathcal{L}_\theta(x) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \pi_k f(x_i, \theta_k) \right)$$

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Likelihood maximisation according to parameters (μ_k, σ_k, π_k), $k = 1, \ldots, K$

1. Local optimum for fixed K through iterative algorithms — EM, Gipps sampling, VB, ...
2. Selection of the cluster number K with information criteria — AIC, BIC, likelihood ratio, ...

Gaussian mixture model with R : `Mclust(data)` Package : `mclust`

`Mclust(data,modelNames)` : Gaussian mixture for multivariate dataset fitted via

EM algorithm and **BIC criterion**

Gaussian mixture model with R : `Mclust(data)`

Package : `mclust`

`Mclust(data,modelNames)` : Gaussian mixture for multivariate dataset fitted via

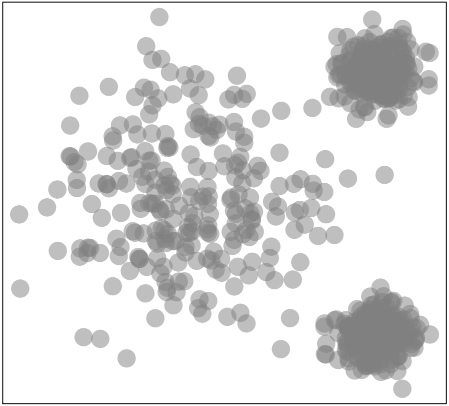
EM algorithm and **BIC criterion**

Several shapes for the cluster can be used — Option : `modelNames`

- `EII` : Spherical, equal volume
- `VII` : Spherical, varying volume

- `EEV` : Ellipsoidal, equal volume & shape
- `VEV` : Ellipsoidal, equal shape
- `EVV` : Ellipsoidal, equal volume
- `VVV` : Ellipsoidal, varying volume & shape

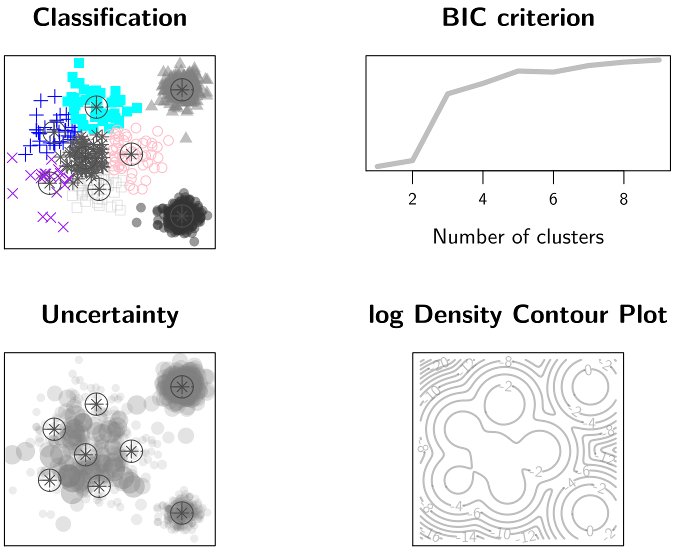
Observations



`Mclust` : Example 1

Spherical clusters

`EII` : Spherical, equal volume

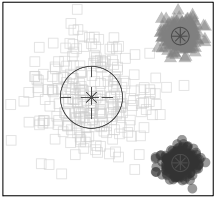


`Mclust` : Example 1

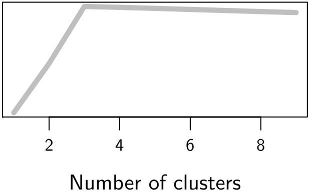
`VII` : Spherical, varying volume

Spherical clusters

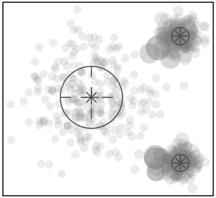
Classification



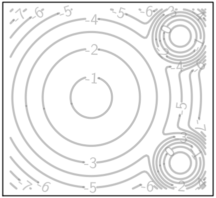
BIC criterion



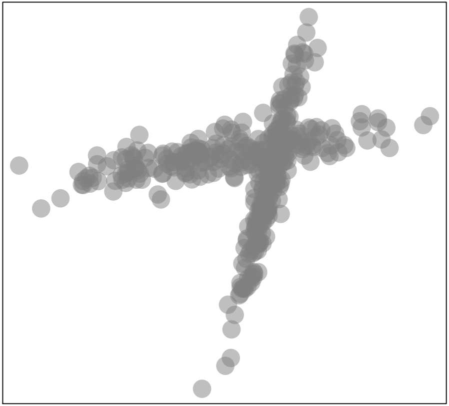
Uncertainty



log Density Contour Plot



Observations

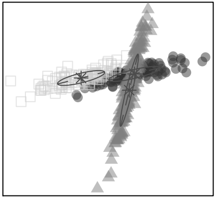


Mclust : Example 2

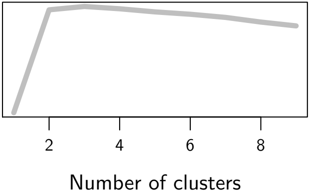
EVV : Ellipsoidal, equal volume

Linear clusters

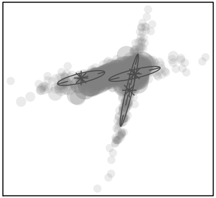
Classification



BIC criterion



Uncertainty



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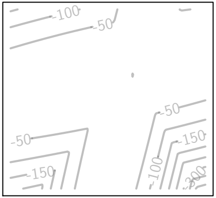
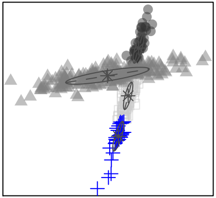


`Mclust` : Example 2

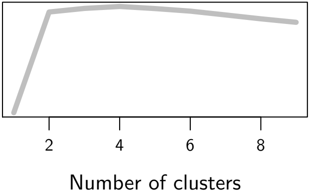
Linear clusters

`VEV` : Ellipsoidal, equal shape

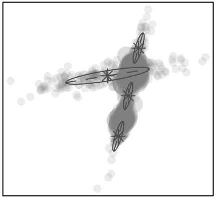
Classification



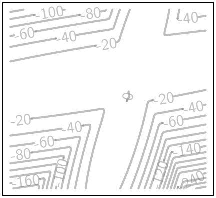
BIC criterion



Uncertainty



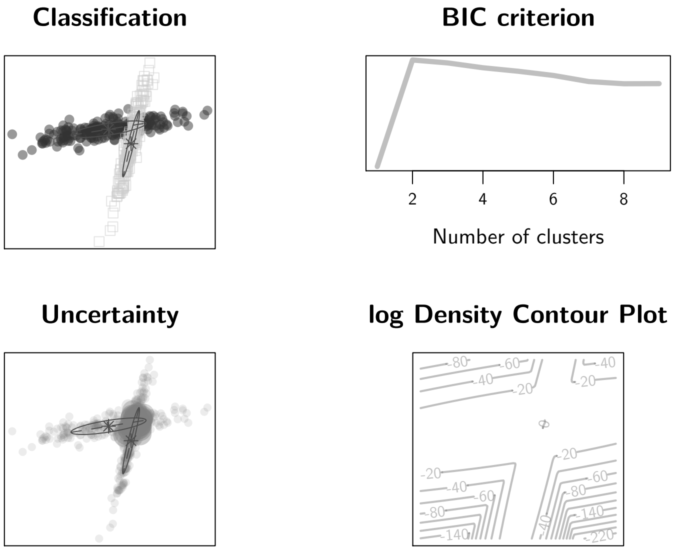
log Density Contour Plot



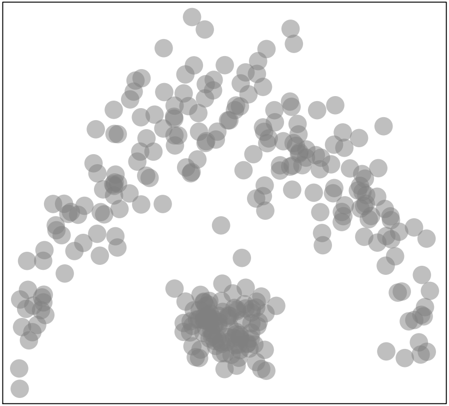
`Mclust` : Example 2

`VVV` : Ellipsoidal, varying volume & shape

See also mixture of linear models here



Observations

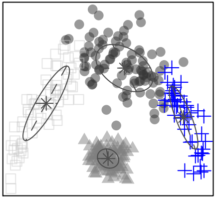


`Mclust` : Example 3

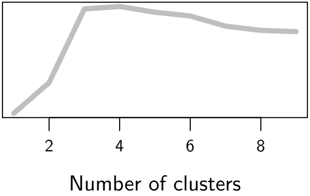
Irregular clusters : Non-parametric clustering

`VVV` : Ellipsoidal, varying volume & shape

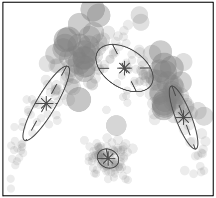
Classification



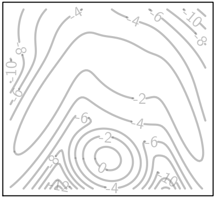
BIC criterion



Uncertainty



log Density Contour Plot



Summary

Descriptive statistic allows to describe data without modelling assumptions

$\rightarrow$ Exploration of the data — Knowledge database discovery, data mining, big data

$\rightarrow$ Elaboration of data-based models — Senseless parameters

Parametric statistic allows to obtain precise assessments on statistical models

$\rightarrow$ Level of information, confidence interval, test of hypothesis or significance

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R and its numerous packages and help forums is a useful software for both descriptive and parametric data analysis

References and links

Books

- T.W. Anderson & J.D. Finn *The statistical analysis of data* Springer 1996
- D. Montgomery & G. Runger *Applied Statistics and Probability for Engineers* Wiley 2010
- P. Congdon *Bayesian statistical modelling* (2nd edition) Wiley 2006

Websites

- The R project for statistical computing `r-project.org`
- Wikipedia : Statistics `wikipedia.org/Statistics`
- Online courses `statistics.com`
- Python & R codes for common machine learning algorithms `analyticsvidhya.com`

Videos

- R vs Python `blog.dominodatalab.com`
- R statistics tutorials `youtube.com`

Integrated development environments for R

- RStudio, Jupyter, Rattle, Red-R, R Commander, JGR, RKWard, Deducer, ...

Abbreviations

PDF	*Probability density function*
ECDF	*Empirical cumulative distribution function*
iff	*If and only if*
th.	*Theorem*
ind.	*Independent*
iid	*Independent and identically distributed*
OLS	*Ordinary least squares*
PCA	*Principal component analysis*
lc	*Linear combination*
D	*Distribution*
P	*Probability*
a.s.	*Almost surely*
LLN	*Law of large numbers*
CLT	*Central limit theorem*
MSE	*Mean squared error*
MLE	*Maximum likelihood estimator*

Overview

Part 1 | Descriptive statistics for univariate and bivariate data

Repartition of the data (histogram, kernel density, empirical cumulative distribution function), order statistic and quantile, statistics for location and variability, boxplot, scatter plot, covariance and correlation, QQplot

Part 2 | Descriptive statistics for multivariate data

Least squares and linear and non-linear regression models, principal component analysis, principal component regression, clustering methods (K-means, hierarchical, density-based), linear discriminant analysis, bootstrap technique

Part 3 | Parametric statistic

Likelihood, estimator definition and main properties (bias, convergence), punctual estimate (maximum likelihood estimation, Bayesian estimation), confidence and credible intervals, information criteria, test of hypothesis, parametric clustering

Appendix LaTeX plots with R and Tikz

Appendix 1 : Plotting with R

R is not only a software for data analysis and mathematical modelling, it is also a software to **get graphics**[3]

→ Basically R allows to produce figures in Metafile, Postscript, PDF, Png, Bmg, TIFF, jpg

→ `tikzDevice` package allows to get LaTeX file (.tex)

Simple plot `plot(x,y)`

- Options `xlab, ylab, main, ...`
- Legends `legend('topright', ...)`
- Specification of the axis label `axis(1, ...)`

Multiplot

- Figures with 2 lines of 3 plots `par(mfrow=c(2,3));plot()...`
- Customized position of the plots `split.screen(rbind(...));screen(1)...`
- Scatterplot of a database `plot(data_base)`

[3] See `demo(graphics)`, package 'ggplot2', CRAN Task View, Google image : R graphics

LaTeX plot with R

Script

```
require(tikzDevice)
tikz('exemple.tex',width=5,height=3,standAlone=T)
curve(sin(x)/x,xlim=c(0,20),xlab='$x$',ylab='$f(x)$',lwd=7,col=rgb(.5,.5,.5))
legend('topright',c('$f(x)=\\frac1x\\sin(x)$'),lwd=7,col=rgb(.5,.5,.5))
dev.off()
```