

Statistical Exploitation of Measurements



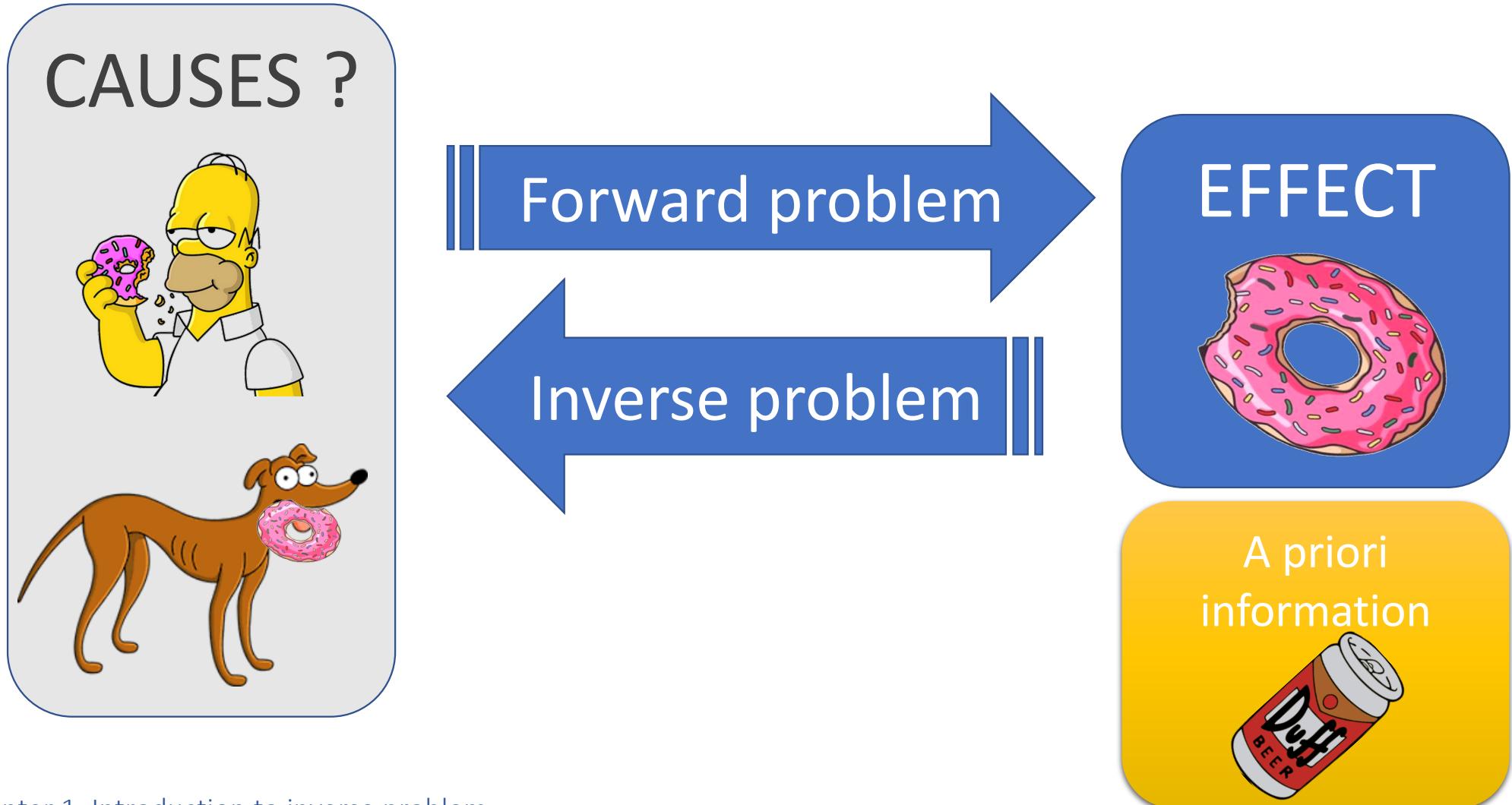
MASTER
FUNDAMENTAL PHYSICS AND APPLICATIONS (UBFC)



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Chapter 1. Introduction to inverse problem

1. Introduction



2. Direct and inverse problem

Let θ be an unknown quantity whose precise value, named θ , will remain unknown because of some uncertainties in the measurement process

How to use at best all the available knowledges to give the most precise information on θ .
These available knowledges consist in:

- The measurements constituting a set of N data named $\mathbf{D} = \{d_1, d_2, d_3, \dots, d_N\}$
- A model of the measurement process
- Any information about θ known before the measurement process, called *a priori* information.

The object



Direct problem : how is formed by a microscope the image of an object?



The image



The object

Inverse problem : what can we infer on the object from the recorded image?

The image

The inverse problem can be formulated as:

Build a probability law on θ , from all the available informations (measurements, model of measurement, a priori information). This probability law is called a posteriori (after the measurements).

3. The Bayes theorem

- An unknown quantity whose precise value is named θ
- Measurements of this unknown quantity constituting a set of N data named $\mathbf{D} = \{d_1, d_2, d_3, \dots, d_N\}$
- *a priori* information $P_{prior}(\theta)$

the Bayes theorem is defined as:

$$P(\theta|\mathbf{D}) = \frac{P(\mathbf{D}|\theta) P_{prior}(\theta)}{P(\mathbf{D})}$$

$P(A|B)$: conditional probability
of A given B, or the probability
of A under the condition B

$P(A)$: prior probability or
probability distribution of A

Example 1 : efficiency of hepatitis test

3% of a population is infected with hepatitis

Sick person : test positive with probability of 95% : $P(+|\text{sick}) = 95\%$

Healthy person: test positive with probability of 10% : $P(+|\text{health}) = 10\%$



A priori information

$$P_{\text{prior}}(\text{sick}) = 3\%$$

Model of measurement

$$P(+|\text{sick}) = 95\%; P(+|\text{health}) = 10\%$$

Inverse problem “How likely is the person tested to be sick?”

The answer is given by the conditional probability :

$$P(\text{sick}|+) = \frac{P(+|\text{sick})P_{\text{prior}}(\text{sick})}{P(+)} = \frac{0.95 \times 0.03}{0.95 \times 0.03 + 0.1 \times 0.97} \approx 0.23 \equiv 23\%$$

$$P(+) = P(+|\text{sick}) \times P_{\text{prior}}(\text{sick}) + P(+|\text{health}) \times [1 - P_{\text{prior}}(\text{sick})]$$

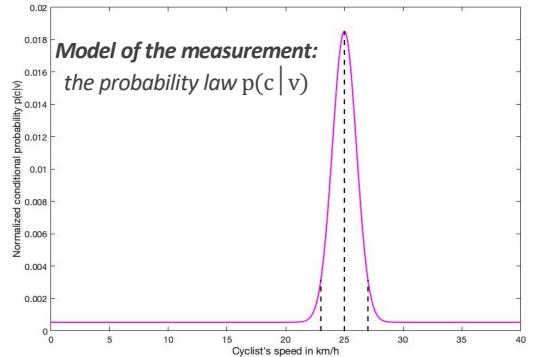
$P_{\text{prior}}(\text{health})$

$$P(\text{sick}|-) = ???$$

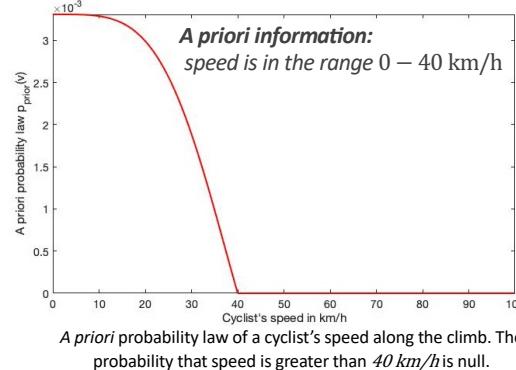


Example 2: Speed of a cyclist on a climb

We want to measure the speed v of a cyclist on a climb (towards the summit!) with a counter with an uncertainty $c = v \pm 2 \text{ km/h}$



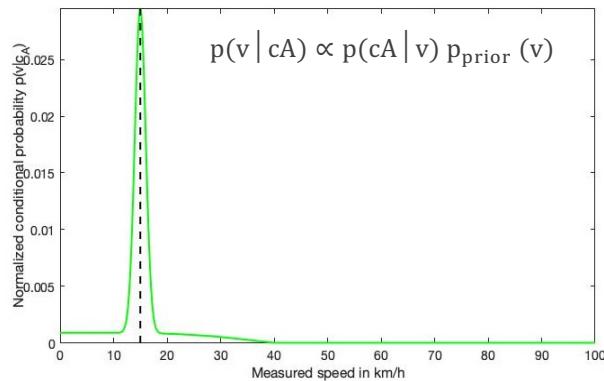
Conditional probability $p(c_0|v)$ when a speed $c_0 = 25 \pm 2 \text{ km/h}$ is measured with the counter. This probability is defined in the range $0 - 40 \text{ km/h}$.



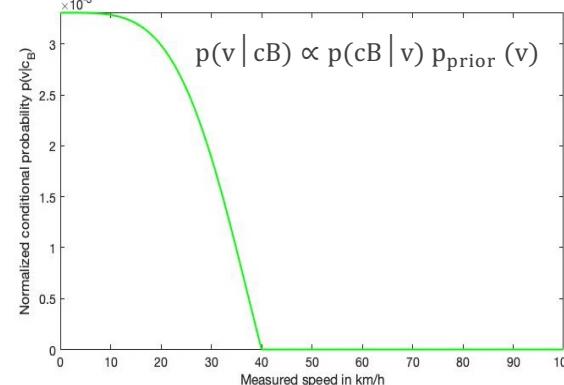
Continuous version of the Bayes theorem:
 $p(v|c) \propto p(c|v) p_{\text{prior}}(v)$

Here $p(c)$ is a constant in the counter range of measurement

A posteriori law when measured speed is $c_A = 15 \text{ km/h}$



A posteriori law when measured speed is $c_B = 80 \text{ km/h}$



To summarize

World	Model	Experimenter
unknown quantity θ	True (but known)	Random variable
measurements	Noised with random variables	Done (known values)
Problem to solve	Direct: the physical model of measurements determines $p(\theta D)$	Inverse: find $p(\theta D)$. The direct problem should be solved before

Actually, it could be useful to give, rather than the full $p(\theta|D)$, two numbers:

- *the mean of the law,*
- *an uncertainty range given by the standard deviation.*

Chapter 2. Estimation

1. Introduction

In the model world, θ is a true but unknown parameter of a probability law

let us perform N measurements d of θ . In the model world d_n is a random variable:

$$d_i = \theta + \varepsilon_i \text{ with } i = 1, \dots, N.$$

The random error ε_i obeys a Gaussian distribution with zero mean

The purpose of estimation is to construct from the measurements and a priori information a new random variable $\hat{\theta}$, called **estimator of θ** such as:

$$\hat{\theta} = T(d_1, \dots, d_N, \text{a priori information})$$

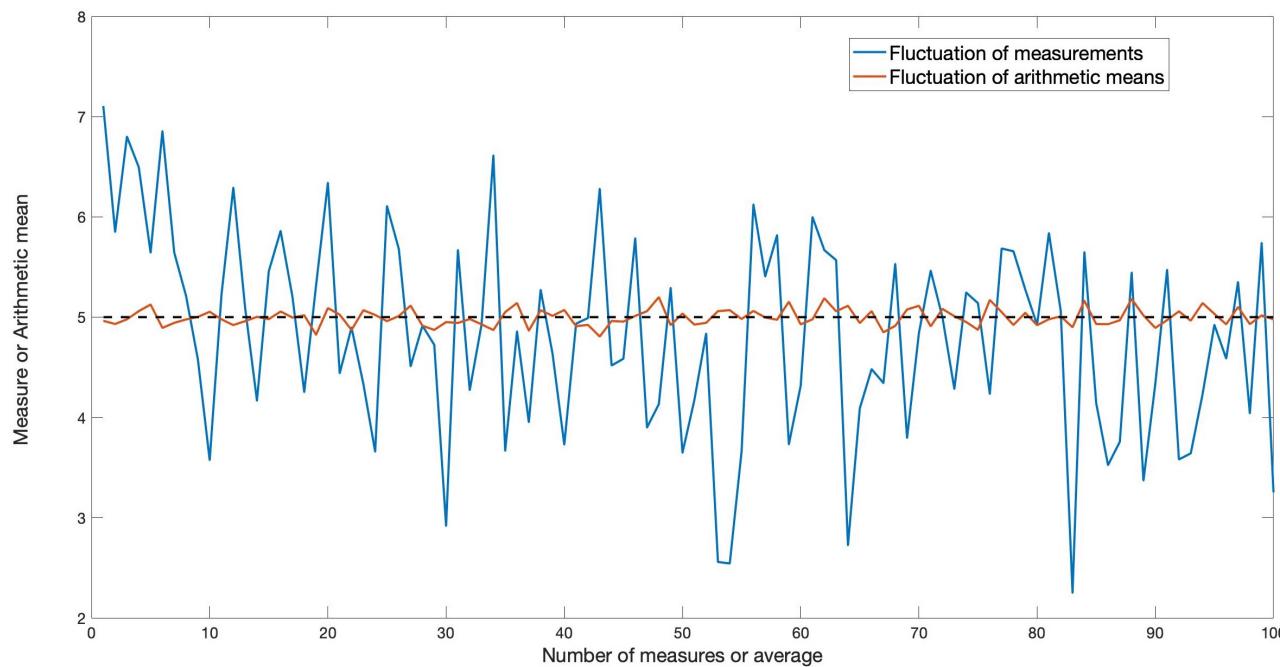
An example of this estimator is the arithmetic average : $\hat{\theta} = \bar{d} = \frac{1}{N} \sum_{i=1}^N d_i$

An estimator is a random variable, just like the measures from which it is derived.

if the measurements are all independent one of each other, the variance of the arithmetic mean is $\frac{\sigma^2}{N}$.

\bar{d} is thus expectation of θ , just like the measurements d_i , but fluctuates less around θ , because of a standard deviation divided by \sqrt{N}

Example : a true parameter $\theta = 5$ is measured N=100 times with a gaussian random error with a standard deviation $\sigma = 1$.



From these data the estimator of θ is:

$$\hat{\theta} = \bar{d} = \frac{1}{N} \sum_{i=1}^N d_i = 4.82$$

with a standard deviation $\sigma = 1.01$ which is close to the standard deviation of the random noise (blue curve).

The 100 measures are repeated 100 times. The red curve shows the fluctuation of the 100-arithmetic means. In that case, the arithmetic mean fluctuates with a smallest standard deviation of 0.09 with is close to:

$$\frac{\sigma}{\sqrt{N}} = \frac{1}{\sqrt{100}} = 0.1.$$

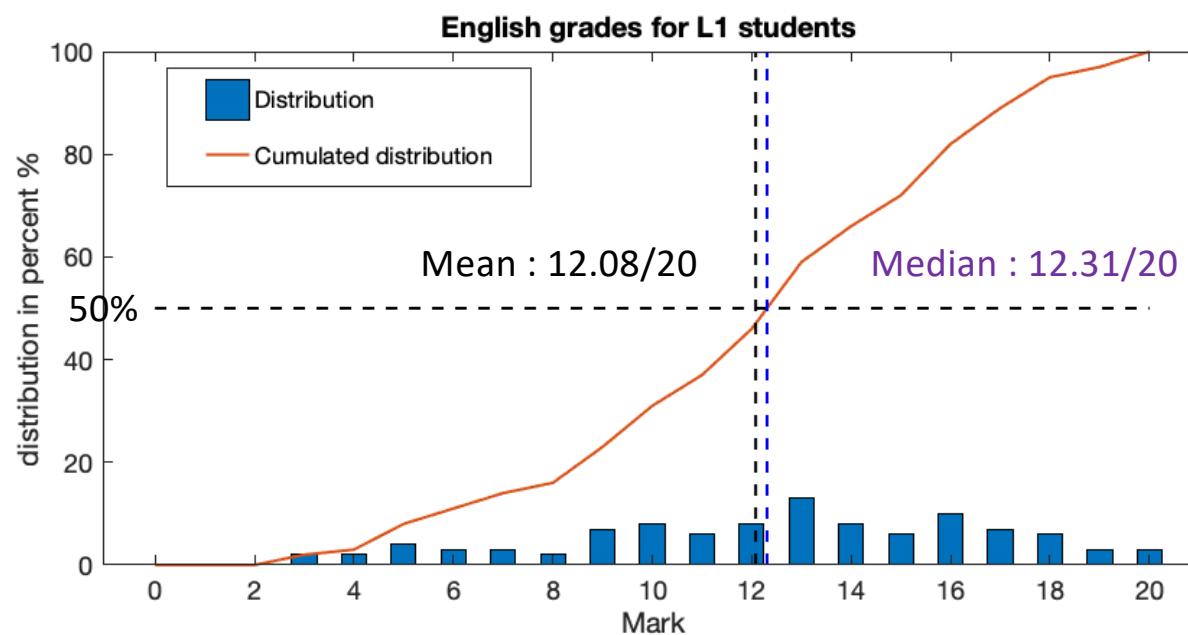
3. Estimators of mean

- Arithmetic mean : $\bar{d} = \frac{1}{N} \sum_{i=1}^N d_i$

if the error is Gaussian and the measurements independent, \bar{d} follows a Gaussian law, of variance $\frac{\sigma^2}{N}$ and mean θ .

- Median : The measurements are ordered from the smallest (d_1) to the largest (d_N). The median is then defined as $d_{(N+1)/2}$ if N is odd, $(d_{N/2} + d_{(N+2)/2})/2$ if N is even.

Median is much less sensitive than mean to outliers



4. Estimators of variance

With known mean:

$$\widehat{\sigma^2} = \frac{1}{N} \sum_{i=1}^N (d_i - \theta)^2$$

With estimated mean:

$$\widehat{\sigma^2} = \frac{1}{N-1} \sum_{i=1}^N (d_i - \bar{d})^2$$

5. Why the measurement errors are often modeled by a Gaussian law?

A consequence of the *central-limit theorem* (CLT) or strong law of large numbers

$X_1, \dots, X_i, \dots, X_N$ being N independent random variables each with the mean m and finite variance σ^2 .
The sum $X_1 + \dots + X_i + \dots + X_N$ has mean Nm and variance $N\sigma^2$.

Consider now the new random variable Z_N such as:

$$Z_N = \frac{X_1 + \dots + X_i + \dots + X_N - Nm}{\sqrt{N\sigma^2}} = \sum_{i=1}^N \frac{X_i - m}{\sqrt{N\sigma^2}} = \sum_{i=1}^N \frac{Y_i}{\sqrt{N}}$$

where $Y_i = \frac{X_i - m}{\sigma}$ is a random variable with zero mean and unit variance.

It can demonstrate that: $\lim_{N \rightarrow \infty} Z_N = N(0,1)$ where $N(0,1)$ is a normal distribution of mean 0 and variance 1.

This theorem applies to a measurement process of good quality, said under control, where all important causes of error have been eliminated. **The residual uncertainty is due to a large number of independent causes, of various origins and of comparable weight.** The measurement error is then expected to be a **Gaussian random variable**, whatever the probability law of each residual error.

Coin toss example

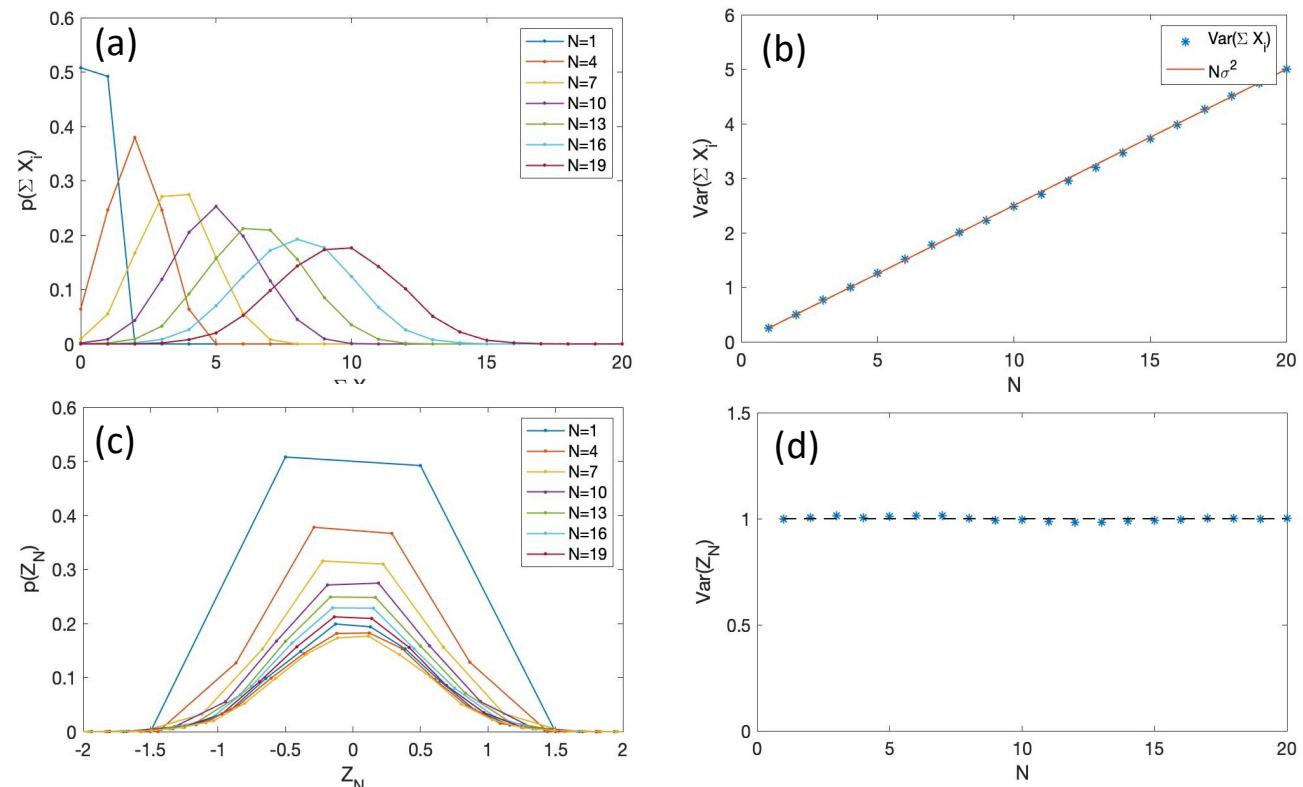
Coin toss is a *Bernoulli* trial with two possible outcomes, "1" (heads) and "0" (tails) with the same probability of 0.5. This random variable has a mean $m = 0.5$ and a variance $\sigma^2 = m(m - 1) = 0.25$. We are interested in the sum of N trials.

Trial 1	Trial 2	Trial 3	Sum
0	0	0	0
0	0	1	1
0	1	0	1
0	1	1	2
1	0	0	1
1	0	1	2
1	1	0	2
1	1	1	3

Possible results with 3 trials and corresponding sums of the trials

Value of the sum	Occurrence	Frequency
0	1	12,5%
1	3	37,5%
2	3	37,5%
3	1	12,5%

Occurrences and frequencies of possible sums of 3 trials



(a) Probability distribution of the sum of N Bernouilli trials. (b) Variance of the sum as a function of the number of summed trials. (c) Probability distribution of the random variable Z_N and (d) its variance as a function of the number of summed trials.

6. Confidence intervals

In the experimenter world, we would like to translate the *a posteriori* law $p(\theta|D)$ in a more intuitive way, by giving an interval where θ lies with a probability of 95%.

In the model world, this is easy:

If the process is under control, \bar{d} follows a Gaussian law, of variance σ^2/N and mean θ , which allows us to write:

$$\theta - \frac{1.96\sigma}{\sqrt{N}} \leq \bar{d} \leq \theta + \frac{1.96\sigma}{\sqrt{N}} \text{ at 95% of confidence.}$$



Two reasons prevent us to simply write
in the experimenter world:

$$\bar{d} - \frac{1.96\sigma}{\sqrt{N}} \leq \theta \leq \bar{d} + \frac{1.96\sigma}{\sqrt{N}}$$

1. This expression assumes $p(\theta|D) = p(\bar{d}|\theta)$, which is true only if $p_{\text{prior}}(\theta) = C^{\text{st}}$

This is a reasonable one for a controlled measurement process, where the measurement error is low and Gaussian. The uncertainty range is then low enough to consider that, within this range, the probability density of θ before measurements is a constant. Of course, if we have an explicit expression of $p_{\text{prior}}(\theta)$, we must renounce this assumption and calculate $p(\theta|\bar{d})$ with $p_{\text{prior}}(\theta)$.

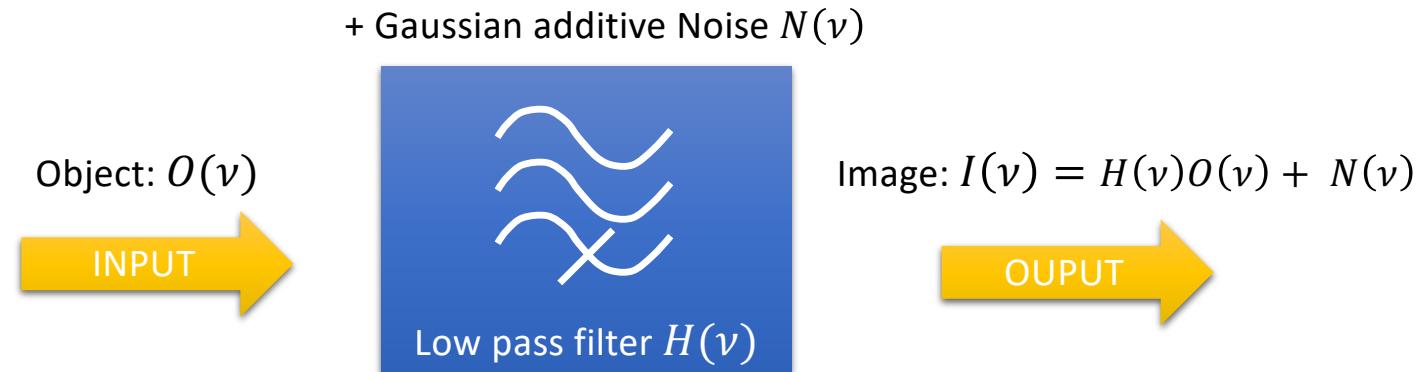
2. σ is not known, but estimated.

if $p_{\text{prior}}(\theta) = C^{\text{st}}, \frac{\bar{d}-\theta}{\sqrt{\hat{\sigma}^2/\sqrt{N}}}$ follows a so-called **Student law** with $N - 1$ degrees of freedom, where θ is the random variable. The range around the arithmetic mean where θ has a 95% chance of being found can then be determined: this range, called the confidence interval, is given by $\bar{d} \pm \alpha \frac{\hat{\sigma}}{\sqrt{N}}$, where α depends on N

N	3	5	10	20	40
α	4.3	2.8	2.3	2.1	2.0

Warning: Using 2 or α has hardly any consequences as soon as you make at least ten measurements. However, it should not be forgotten that the estimated standard deviation of θ from the arithmetic mean is not the estimated standard deviation of the measures $\hat{\sigma}$, but $\hat{\sigma}$! That's the point of repeating the measurements! ...and we will not forget either that this division by \sqrt{N} is intimately linked to the assumption of independence of the measurements. If this assumption is not fully verified, the size of the confidence interval may be underestimated.

7. Wiener filtering: when a biased estimator works better than unbiased one



Inverse problem : "How to retrieve at best $O(\nu)$ from the output?"

$$O(\nu) = I(\nu)/H(\nu)$$

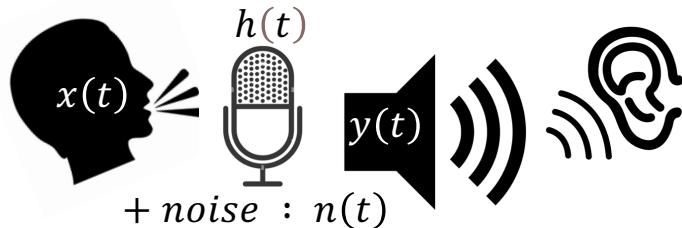
Without noise With noise

Find a function $G(\nu) \leq 1/H(\nu)$, such that:

$$\widehat{O(\nu)} = G(\nu)I(\nu) = G(\nu)H(\nu)O(\nu) + G(\nu)N(\nu)$$

Minimizing the quadratic error $\langle (\widehat{O} - O)^2 \rangle$

Application : sound recorded with a noisy microphone



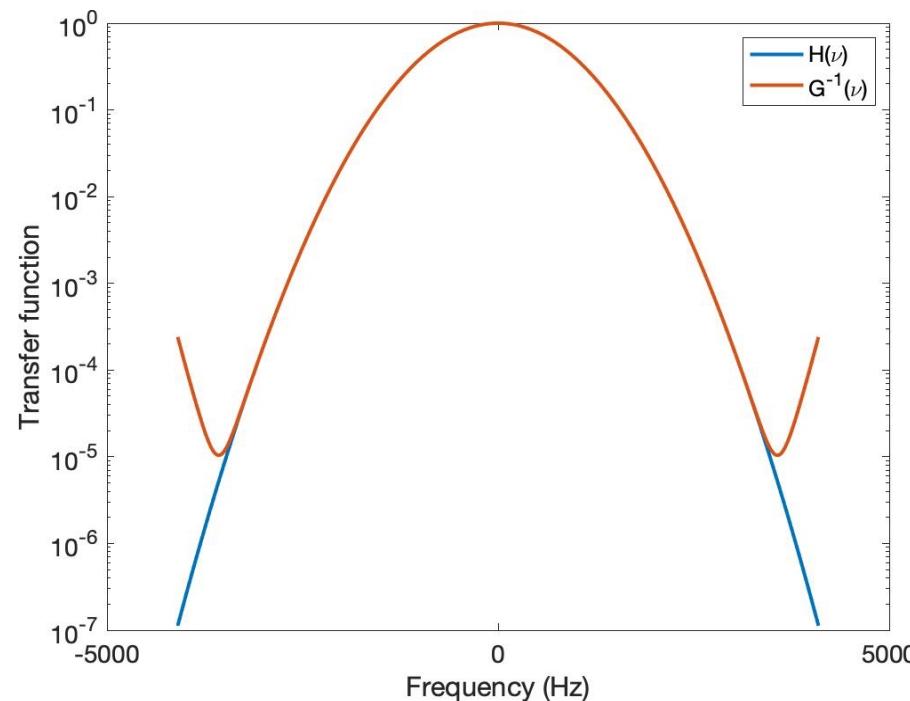
$$y(t) = h(t) * x(t) + n(t)$$

in time domain

$$Y(\nu) = H(\nu)X(\nu) + N(\nu)$$

in frequency domain

Fourier transform

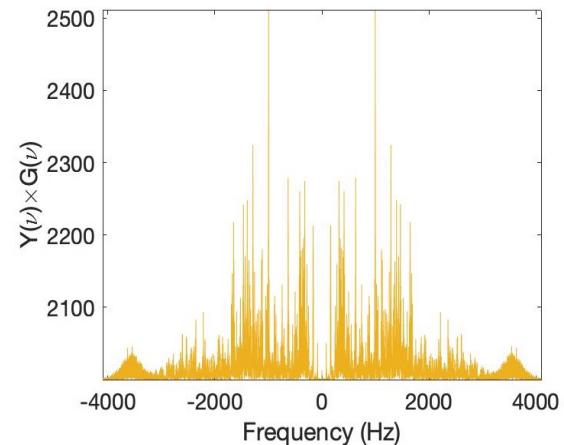
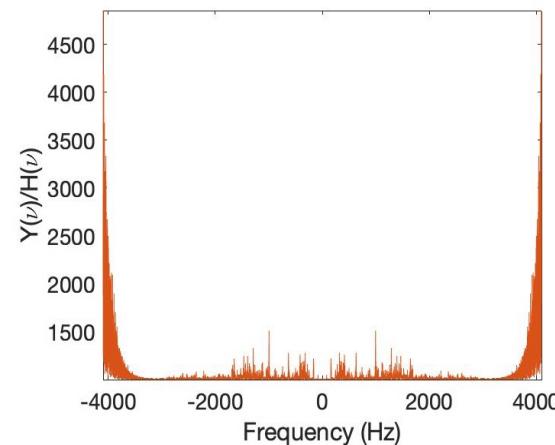
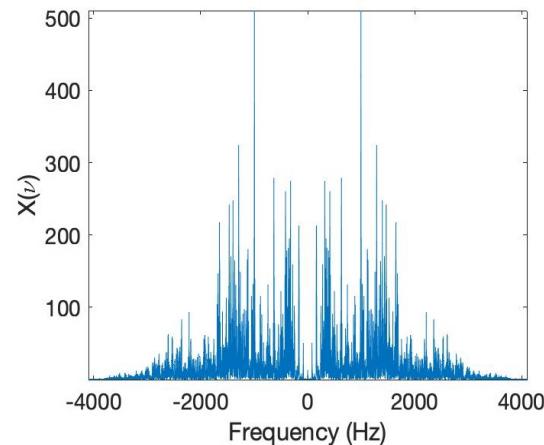
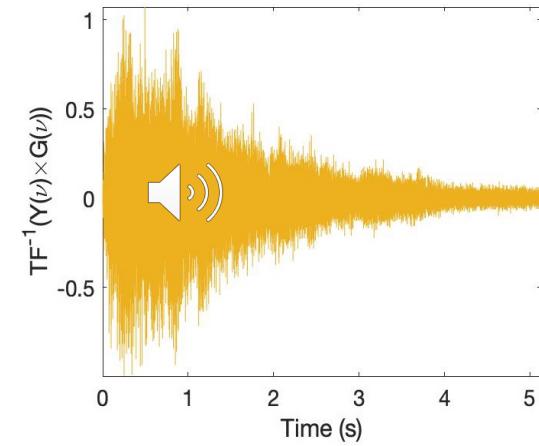
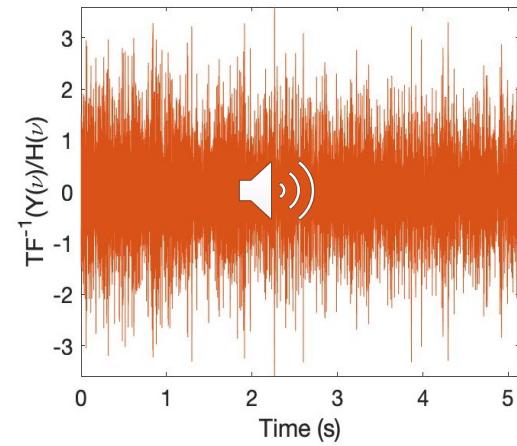
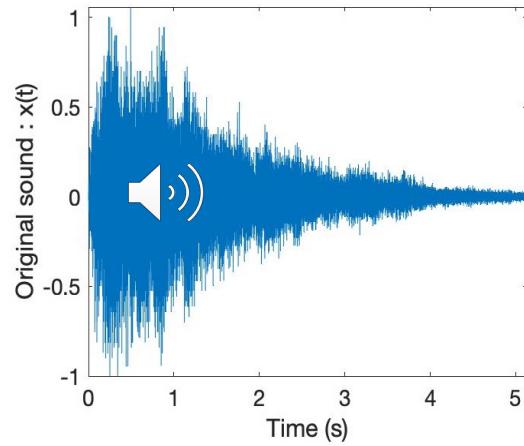


$H(\nu)$: Low pass filter

$G(\nu) = \frac{H\langle X^2 \rangle}{H^2\langle X^2 \rangle + \langle N^2 \rangle}$: Biased estimator

Comparison between the original and the estimated sounds using:

$$\begin{cases} \hat{x}_1(t) = TF^{-1}\left(\frac{Y}{H}\right) \\ \hat{x}_2(t) = TF^{-1}(GY) \end{cases}$$



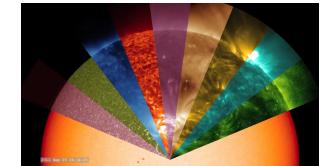
Chapter 3. Karhunen-Loève Transform or Principal Component Analysis

2011 https://upload.wikimedia.org/wikipedia/commons/transcoded/a/ac/NASA_SDO_multispectral_view_of_the_Sun%2C_September_2011.ogv/NASA_SDO_multispectral_view_of_the_Sun%2C_September_2011.ogv.480p.webm

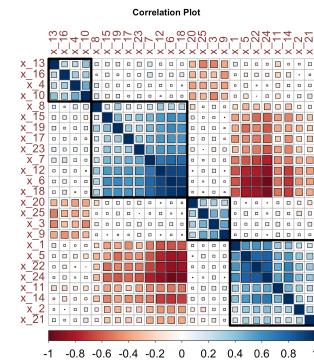
1. Introduction

2 purposes but same mathematical method

- Karhunen-Loève Transform (KLT): compression of information by eliminating redundancy
 - multispectral image compression, encoding bits reduction of images...
- Principal Component Analysis (PCA): studying the redundancy



study of correlated data of large dimension



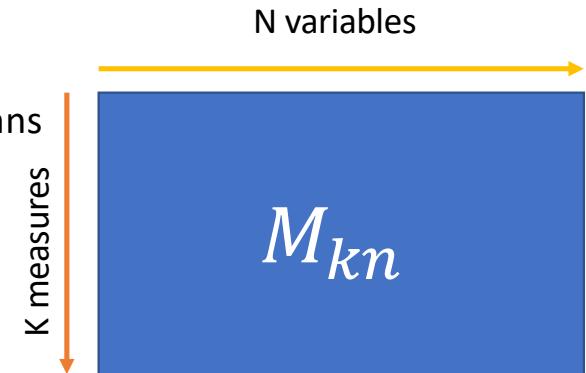
<https://rpubs.com/melike/corrplot>

2. Mathematical description of the Karhunen-Loève Transform

K measures of N joint variables. The data are arranged in a matrix \mathbf{M} of K rows and N columns

A measure of one variable M_{kn} can be represented by a point in a N dimensional space.

Reducing the dimensionality to $L < N$ will be possible if the cloud of points is contained in a L dimensional space



$$\text{Average of the variable } n, \text{ with } 1 \leq n \leq N : \bar{M}_n = \frac{1}{K} \sum_{k=1}^K M_{kn}$$

$$\text{Covariance between the variable } p \text{ and the variable } q: C_{pq} = \frac{1}{K-1} \sum_{k=1}^K (M_{kp} - \bar{M}_p)(M_{kq} - \bar{M}_q)$$

$$\text{With } \mathbf{M}_c = \mathbf{M} - \bar{\mathbf{M}}, \text{ the centered data matrix, } N \times N \text{ covariance matrix } \mathbf{C} \text{ of } \mathbf{M} : \quad \mathbf{C} = cov(\mathbf{M}) = \frac{\mathbf{M}_c^T \mathbf{M}_c}{K-1}$$

The correlation coefficient r_{pq} is obtained by normalizing the covariances using the variances C_{pp} and C_{qq} :

$$r_{pq} = \frac{C_{pq}}{\sqrt{C_{pp}} \sqrt{C_{qq}}} ; \quad -1 \leq r_{pq} \leq 1$$

Let us define a rotation of the coordinates axes in the N -dimensional space: $\mathbf{M}_c = \mathbf{Y}\Phi$, where Φ is a $N \times N$ rotation matrix between orthonormal bases in the N -dimensional space.

Because $\Phi^{-1} = \Phi^T$, it allows us to write the transformed $K \times N$ matrix of data: $\mathbf{Y} = \mathbf{M}_c\Phi^T$

Defining respectively \mathbf{V} and \mathbf{D} as the $N \times N$ eigenvectors matrix and the $N \times N$ diagonal eigenvalues matrix of the covariance matrix \mathbf{C} , we can prove that $\Phi = \mathbf{V}^T$ and $\frac{\mathbf{Y}^T \mathbf{Y}}{K-1} = \mathbf{D}$. It implies that the K.L.T. data \mathbf{Y} are uncorrelated

Now we are looking for the rotation allowing the reconstruction of a $K \times N$ truncated data matrix \mathbf{M}_{trunc} as close as possible of \mathbf{M} with $L < N$ variables such that the quadratic error as a function of L : $\varepsilon_L^2 = \sum_{k=1}^K \sum_{n=1}^N (M_{kn} - M_{kn}^{trunc})^2$ is minimum. This is obtained calculating:

$$\mathbf{M}_{trunc} = \bar{\mathbf{M}} + \mathbf{Z}\Psi$$

where \mathbf{Z} is a $K \times L$ matrix filled with the L last columns of the matrix \mathbf{Y} and Ψ is a $L \times N$ matrix filled with the L last rows of the matrix Φ

In matrix \mathbf{D} the eigenvalues λ_k are ranked in ascending order ($\lambda_1 < \lambda_2 < \dots < \lambda_N$). Consequently, the ratio $\varrho = \frac{\sum_{n=L+1}^N \lambda_n}{\sum_{n=1}^N \lambda_n}$ is the percentage of lost information. In many practical cases, there is a value of L for which this percentage

drops quite abruptly to almost 0, meaning that the original data lie in a L dimensional space. Because of that, to retrieve the original data it is sufficient to conserve L K.L.T. variables, i.e. $K \times L$ numbers, plus the N numbers forming $\bar{\mathbf{M}}$ and the $L \times N$ coefficients forming Ψ .

3. Application of PCA to students' marks

Matrix M of $K \times N$ joint data

Students	Math	Sciences	French	Latin	Music
Jean	6	6	5	5,5	8
Aline	8	8	8	8	9
Annie	6	7	11	9,5	11
Monique	14,5	14,5	15,5	15	8
Didier	14	14	12	12	10
André	11	10	5,5	7	13
Pierre	5,5	7	14	11,5	10
Brigitte	13	12,5	8,5	9,5	12
Evelyne	9	9,5	12,5	12	18

Table marks of $K = 9$ students in $N = 5$ subjects.

Matrix \bar{M}

	Math	Sciences	French	Latin	Music
Average	9,67	9,83	10,22	10,00	11,00

Covariance matrix $C = cov(M_c) = cov(M - \bar{M})$

	Math	Sciences	French	Latin	Music
Math	12,81	11,16	2,99	5,16	0,13
Sciences	11,15	10,06	4,64	5,91	0,06
French	2,99	4,64	13,57	10,34	0,44
Latin	5,16	5,91	10,34	8,63	0,81
Music	0,13	0,06	0,44	0,81	9,75

Correlation coefficients r_{pq}

Subject	Math	Sciences	French	Latin	Music
Math	1,00	0,98	0,23	0,49	0,01
Sciences	0,98	1,00	0,40	0,63	0,01
French	0,23	0,40	1,00	0,96	0,04
Latin	0,49	0,63	0,96	1,00	0,09
Music	0,01	0,01	0,04	0,09	1,00

The 3 last eigenvalues are significative. It means that the 5-dimensional space of the original data can be contracted to a 3-dimensional space defined by the 3 principal components associated to the eigenvalues.

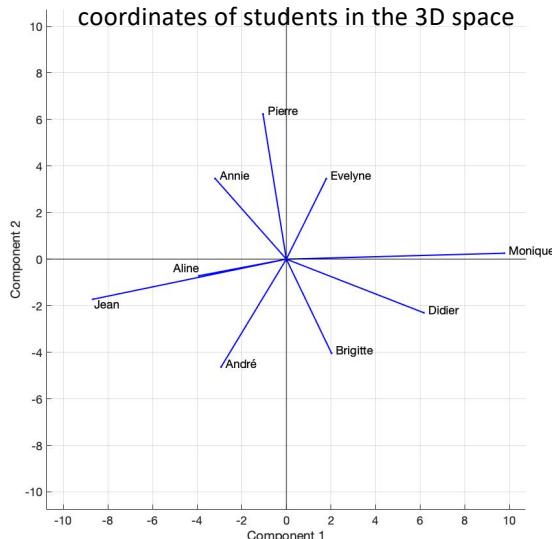
Transformed $K \times N$ matrix of data: $Y = M_c \Phi^T = M_c V$

$N \times N$ rotation matrix: $\Phi = V^T$

$Y: K \times N$ (9×5) matrix

Component	5	4	3	2	1
Jean			2,53	-1,72	-8,67
Aline			1,8	-0,7	-3,91
Annie	Z		0,31	3,46	-3,19
Monique	Z		3,36	0,25	9,77
Didier			0,95	-2,3	6,16
André			-2,66	-4,63	-2,93
Pierre			1,71	6,23	-1,05
Brigitte			-1,41	-4,04	2,02
Evelyne			-6,6	3,46	1,79

Last 3 columns of Y represent the coordinates of students in the 3D space



2D view in the components 1 and 2 of the students' coordinates in the 3D contracted space

Reconstruction

Truncated matrix $\bar{M}_{trunc} = \bar{M} + Z\Psi$

Students	Math	Sciences	French	Latin	Music
Jean	6,02	6,02	5,10	5,36	8,01
Aline	7,95	8,08	8,03	7,94	9,00
Annie	6,04	6,91	10,92	9,64	10,99
Monique	14,40	14,67	15,62	14,80	8,01
Didier	14,11	13,82	11,90	12,19	9,99
André	10,91	10,10	5,47	7,02	13,00
Pierre	5,51	6,96	13,93	11,61	9,99
Brigitte	13,07	12,39	8,45	9,59	11,99
Evelyne	8,99	9,56	12,59	11,86	18,01

Reconstructed table marks of $K = 9$ students with $L = 3$ principal components.

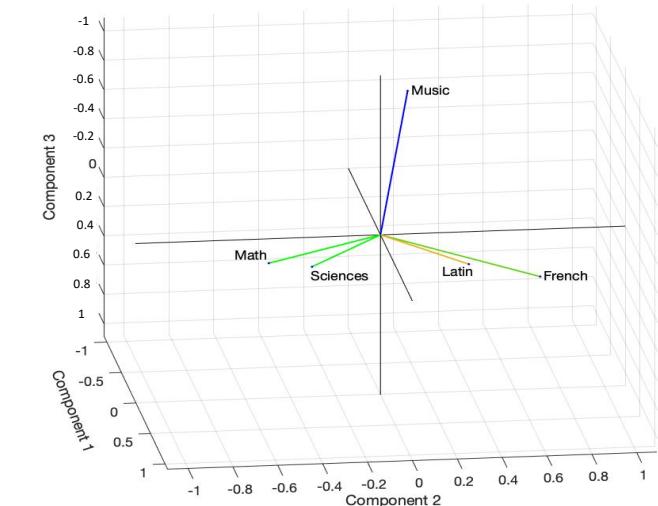
Original matrix M of $K \times N$ joint data. Lost information : $\varrho < 0,1\%$

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Aline	8	8	8	8	9
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Evelyne	9	9,5	12,5	12	18

$\Phi: N \times N$ (5×5) matrix

Component	Math	Sciences	French	Latin	Music
5					
4					
3	-0,05	-0,01	0,11	0,02	-0,99
2	-0,56	-0,37	0,65	0,33	0,12
1	0,51	0,51	0,50	0,47	0,03

Last 3 rows of Φ represent the coordinates of subjects in the 3D space



Representation of the subjects in the 3D space corresponding to the 3 principal components of the data

3. Application of PCA to students' marks

Chapter 4. Hypothesis testing

1. Introduction

DEFINITION : Hypothesis testing means taking a decision with respect to a given hypothesis.

EXAMPLE : Are data **compatible** with $\theta = \theta_0$?

If yes, we **cannot reject** the hypothesis $\theta = \theta_0$.

However, we have **not proved** $\theta = \theta_0$, in any case.

Are the measurements $\bar{d} = 0.5, \frac{\hat{\sigma}}{\sqrt{N}} = 1$ compatible with $\theta = 0$?

This is a question in the experimenter world and the answer is given by the following reasoning in the model world :

- if $\theta = 0$, $P(-2 \leq \bar{d} \leq 2) \sim 95\%$.
- Hence, since $\bar{d} = 0.5$ is comprised in the confidence interval, we cannot reject $\theta = 0$.

TYPES OF TESTS : The most common tests can be divided in three categories:

1. Are data compatible with a value (mean, standard deviation)?
2. Are data compatible with a probability distribution (Gaussian, for example)?
3. Could two samples come from the same population?

Population: ensemble of objects statistically equivalent with respect to a quantitative criterion; only chance gives different values to different objects.

Sample: randomly chosen subset of a population

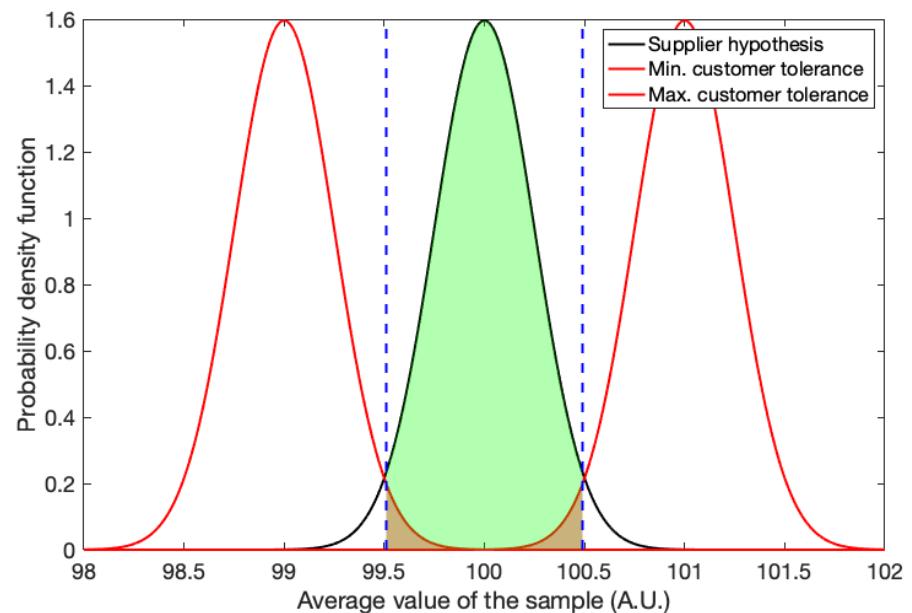
2. Statistical control of quality

2.1 Reception quality control

A customer receives a bundle of N pieces and has defined tolerance limits on the mean (not on the individual pieces!). He wants to be sure, at a given risk of 2,5%, that the mean is actually within the tolerance limits. A lot of pieces fabricated with a mean outside the tolerance limits must be rejected with a probability $P > 97.5\%$.

To be specific, let us consider that θ must be greater than 99 or smaller than 101, (customer or H_1 hypothesis) in some unity. If $\theta \leq 99$ or $\theta \geq 101$, the lot must be rejected with $P > 97.5\%$.

On the other hand, the supplier pretends $\theta = 100$. If this (null) hypothesis is true, the lot must be accepted with $P > 95\%$. $1 - P$ is the supplier's risk.



customer risk

95% Supplier
Hypothesis

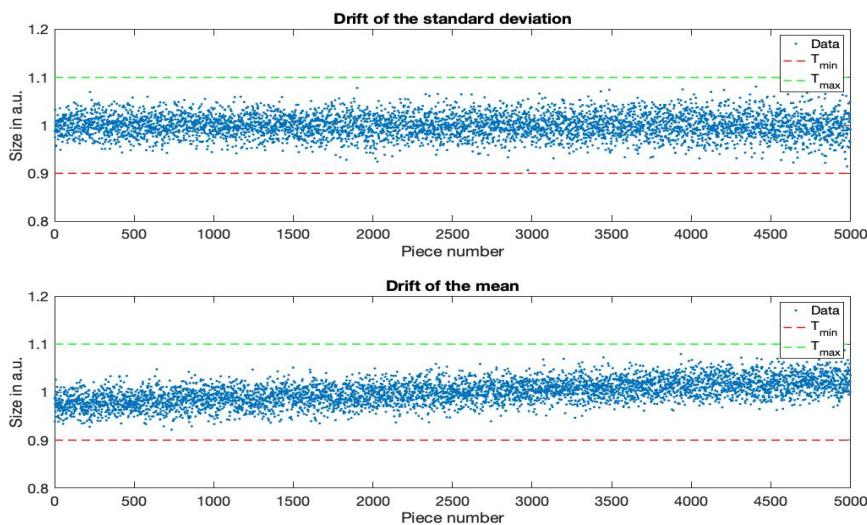
All the probability densities curves are Gaussian with a standard deviation of 0.25.

This only value ensures the right risks for both the supplier and the customer.

In practice, we have to take a lot of N pieces such that $\frac{\hat{\sigma}}{\sqrt{N}} = 0.25$

2.2 Statistical mastering of production

While of great historical importance, the method developed in the preceding paragraph has some important drawbacks. In particular, a drift of the true mean could lead to the rejection of the pieces, with painful consequences for both the supplier and the customer. However, another important requirement is the necessity of avoiding no necessary adjustments: an adjustment has a cost.

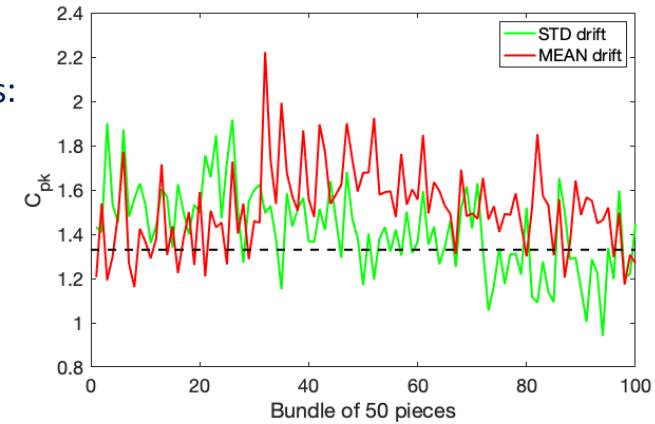


The proposed approach consists in two separate steps:

- Step 1: is the production capable, i.e., can fulfill the customer tolerances on the individual pieces?

Step 1 is fulfilled if the capability verifies:

$$C_{pk} = \text{Inf} \left(\frac{\bar{d} - T_{min}, T_{max} - \bar{d}}{3\sigma} \right) \geq 1.33$$



- Step 2: is the fabrication stable, without drift of either the mean or the standard deviation?

Computation of the arithmetic average and estimated standard deviation on successive samples. The fabrication is stable if the variation of these values can be attributed to randomness

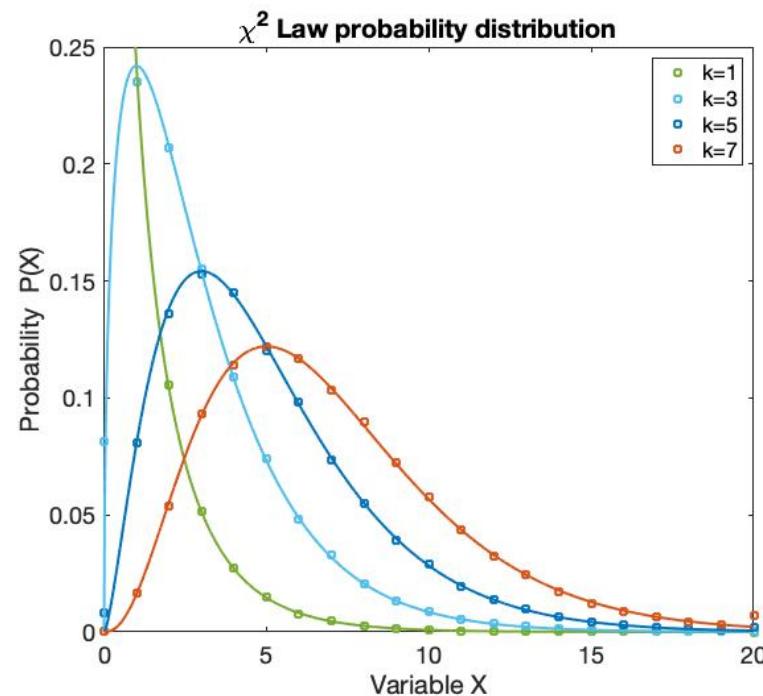
2.2 Fit test: χ^2 test

Definition

χ_k^2 distribution law of k degrees of freedom is the distribution of a sum of the squares of k independent standard normal random variables :

$$p_k(x) = \frac{1}{2^{\frac{k}{2}} \Gamma\left(\frac{k}{2}\right)} x^{\frac{k}{2}-1} e^{-\frac{x}{2}}$$

where Γ is the *gamma* function.



χ^2 test : Is the data behavior compatible with a specific, probability law, here the Gaussian law?



Comparison between the measured frequency to the expected probability.

χ^2 test

N data named $D = \{d_1, d_2, d_3, \dots, d_N\}$

M classes C_j with bounds $[k_j, k_{j+1}]$. A measurement $d_i \in C_j \Leftrightarrow k_j \leq d_i < k_{j+1}$.

n_j elements in the class C_j . The limits of classes are defined such that $n_j > 6$. The total number of data is $N = \sum_{j=1}^M n_j$.

Calculation of the arithmetic average \bar{d} and of the estimated standard deviation $\hat{\sigma}$

If data obey to a Gaussian distribution, we can find the probability of inclusion in the class C_j :

$$P(C_j) = P(k_j \leq d_i < k_{j+1}) = P(k < k_{j+1}) - P(k_j \leq d_i)$$

Given by the *cdf* of a Gaussian of mean \bar{d} and standard deviation $\hat{\sigma}$

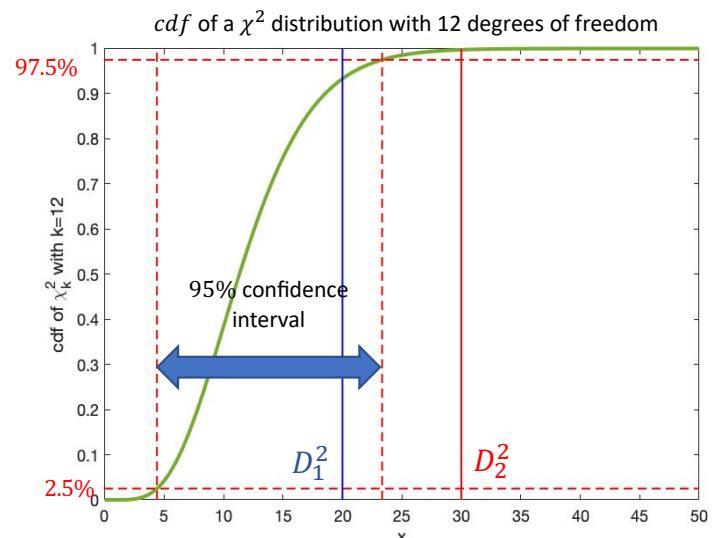
Computation of the distance D^2 between the measured frequencies and the expected probabilities:

$$D^2 = \sum_{j=1}^M \frac{(n_j - NP_j)^2}{NP_j}$$

If the data follow a Gaussian distribution, D^2 follows a χ^2 distribution of $M - 1$ degrees of freedom.

$D_1^2 = 20$ is included in the confidence interval : the Gaussian hypothesis cannot be rejected.

$D_2^2 = 30$ is outside the confidence interval : the Gaussian hypothesis is rejected.



Chapter 5. Inverse problem and least-squares fitting

1. General frame

Assume data (measurements) $D = \{\dots, d_i, \dots\}$ at abscissae $\{\dots, x_i, \dots\}$ modeled by a model M using K parameters $P = (p_1, \dots, p_K)$ such as:

$$d_i = M(x_i; p_1, \dots, p_K)$$

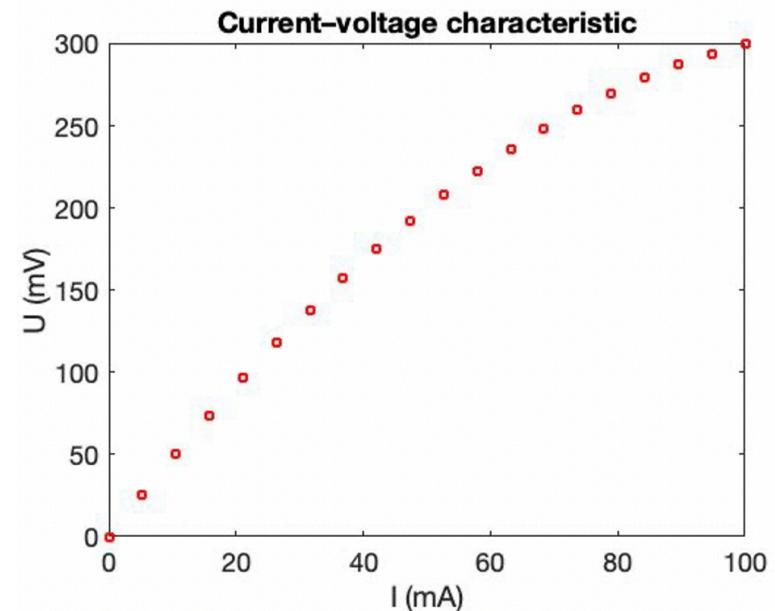
- the direct problem: model the data D (find the model M) for a given value of parameters P .
- the inverse problem: retrieve parameters P from data D , knowing the model M and any other a priori information.

Example: find the resistance R of an electric dipole with a current-voltage characteristic model $U_i = R I_i$ from voltage and current intensity data $\{\dots, U_i, \dots\}$ and $\{\dots, I_i, \dots\}$. Figure shows the plot $U_i = f(I_i)$ of data.

Clearly, the linear model is not correct and the direct problem must be reconsidered

Warning: all tests of linearity will show that the data on the above graph are compatible with a linear assumption, while a look on the graph shows they are not linear.

Make a graph first!



2. Why using least squares?

Using least squares is justified if the errors are Gaussian. If the errors do not obey a Gaussian statistic, least squares fitting can give poor results.

Measurements $D = \{\dots, d_i, \dots\}$ are performed at abscissae $\{\dots, x_i, \dots\}$. Let be a model $M_K(x_i)$ depending on parameters $P = (p_1, \dots, p_K)$. We assume:

$$d_i = M_K(x_i) + n_i$$

where n_i is a centered Gaussian additive noise, independent from a measurement to another, of variance σ_i^2 which can depend on x_i .

in the model world we have an additive noise modelled by the Gaussian probability law:

$$\begin{aligned} p(d_i | M_K(x_i)) &= \frac{1}{\sigma_i^2 \sqrt{2\pi}} e^{-\frac{(d_i - M_K(x_i))^2}{2\sigma_i^2}} \\ \Rightarrow p(D | M_K) &= \prod p(d_i | M_K(x_i)) \propto e^{-\sum \frac{(d_i - M_K(x_i))^2}{2\sigma_i^2}}. \end{aligned}$$

which means that $p(D | M_K)$ is maximum if $\sum \frac{(d_i - M_K(x_i))^2}{2\sigma_i^2}$ is minimum. If $p_{prior}(M_K)$ is constant around the estimated parameters, this is also the maximum of $p(M_K | D)$. This is a reasonable hypothesis for a measurement under control.

3. Linear least squares with two parameters a and b : $y_i = a x_i + b$

We suppose that there is no uncertainty on x and that the uncertainty on the ordinates does not depend on x : $\sigma_i^2 = \sigma^2$. Least squares solution is obtained by minimizing the quadratic error $\varepsilon^2 = \sum (y_i - (ax_i + b))^2$.

The problem is to find a and b coefficients of the linear model such as $\frac{\partial \varepsilon^2}{\partial a} = 0$ and $\frac{\partial \varepsilon^2}{\partial b} = 0$:
$$\begin{cases} a = \frac{\sum_i x_i(\bar{y} - y_i)}{\sum_i x_i(\bar{x} - x_i)} \\ b = \bar{y} - a\bar{x} \end{cases}$$

The uncertainty on the coefficients is given by:
$$\begin{cases} \sigma_a^2 = \frac{\hat{\sigma}^2}{\sum_i (\bar{x} - x_i)^2} = a^2 \left(\frac{\frac{1}{\rho^2} - 1}{N-2} \right) \\ \sigma_b^2 = \hat{\sigma}^2 \left(\frac{1}{N} + \frac{\bar{x}^2}{\sum_i (\bar{x} - x_i)^2} \right) \end{cases}$$
, where $\hat{\sigma}^2 = \frac{1}{N-2} \sum_i (y_i - (ax_i + b))^2$.

4. Linear least squares: matrix formulation

Let be N equations with K parameters, $N > K$: $y_i = \theta_1 f_1(x_i) + \dots + \theta_K f_K(x_i)$

This system can be written in a matrix form as $\mathbf{Y} = \mathbf{J}\boldsymbol{\theta}$, with:

$$\mathbf{Y} = \begin{bmatrix} \vdots \\ y_i \\ \vdots \end{bmatrix} \text{ } N \text{ lines}; \mathbf{J} = \begin{bmatrix} \ddots & \vdots & \ddots \\ \cdots & f_j(x_i) & \cdots \\ \ddots & \vdots & \ddots \end{bmatrix} \text{ } N \times K \text{ matrix}; \boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_K \end{bmatrix} \text{ } K \text{ columns}$$

Least squares method consists in minimizing the quadratic error weighted by the variance of the measures:

$$\varepsilon^2(\boldsymbol{\theta}) = \sum_{i=1}^N \frac{1}{\sigma_i^2} (\sum_{k=1}^K \theta_k f_k(x_i) - y_i)^2 \quad \longrightarrow \text{Finding the solution of the } K \text{ equations } \frac{\partial \varepsilon^2}{\partial \theta_k} = 0$$

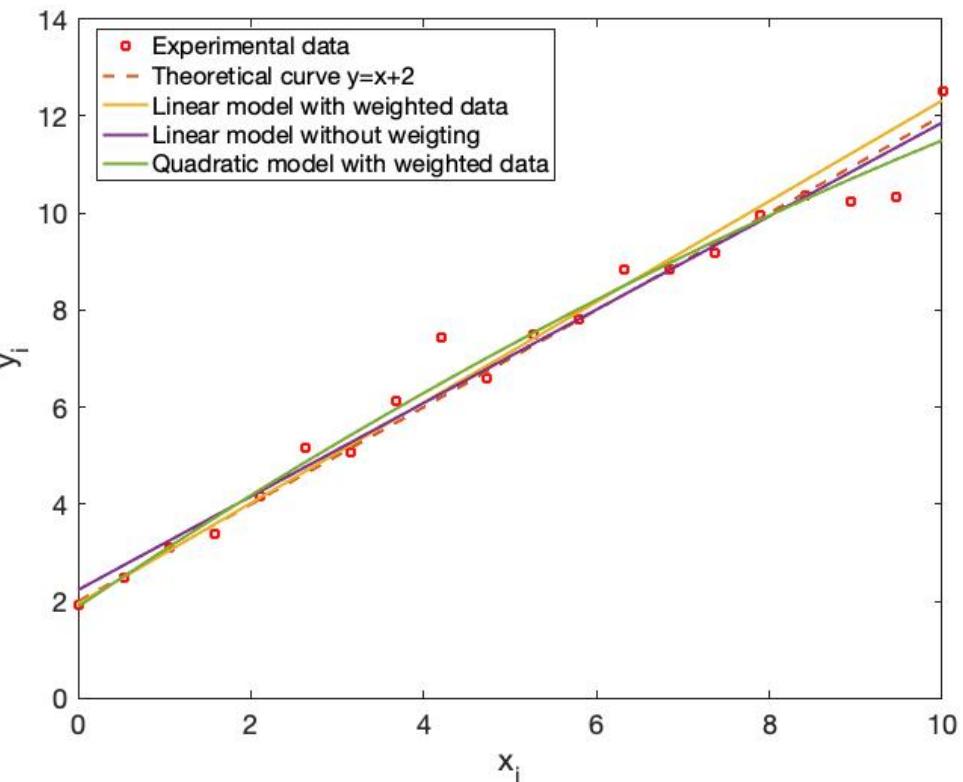
Solution $\boldsymbol{\theta}_{min}$ can be written with in matrix format as: $\boldsymbol{\theta}_{min} = (\mathbf{J}^T \mathbf{W} \mathbf{J})^{-1} \mathbf{J}^T \mathbf{W} \mathbf{Y}$

where $\mathbf{W} = \begin{bmatrix} \frac{1}{\sigma_1^2} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{1}{\sigma_N^2} \end{bmatrix}$ is the diagonal weighting matrix. With no ponderation \mathbf{W} is the identity matrix.

Example of fitted data obeying to the linear function $f(x) = x + 2$

For the least squares method, three cases are considered.

- Linear model where data are weighted by the variance. The model deduced from the linear least squares is:
 $M_1(x) = (1.00 \pm 0.06)x + (2.1 \pm 0.1) ; \varepsilon_1^2(\theta) = 0.02.$
- Linear model but the **data are not weighted** by the variance. In that case the model is:
 $M_2(x) = (1.00 \pm 0.08)x + (2.0 \pm 0.3) ; \varepsilon_2^2(\theta) = 0.06.$
- The last one considers a quadratic model with weighted data. The model is:
 $M_3(x) = (0.00 \pm 0.02)x^2 + (1.0 \pm 0.1)x + (2.0 \pm 0.1) ; \varepsilon_3^2(\theta) = 0.03.$



5. Linearized least squares

Example : retrieve a and τ in a model $y = ae^{-t/\tau}$

Linearized model : $\ln(y) = \ln(a) - t/\tau$ with $\ln(a)$ and $1/\tau$ given by linear regression

In practice, the results are not so good: after linearization, the variance becomes no constant. Even weighting by the inverse of the standard deviation does not give good results.

5. Nonlinear least squares: the Gauss-Newton method

Newton method

Find θ such that $M(x, \theta) = y$ where M is a nonlinear function of θ .

If M is not "too" nonlinear, the solution of $f(\theta) = M(x, \theta) - y = 0$ can be found by using the Newton or dichotomy algorithms

Gauss-Newton method

Combination of the Newton and the least squares (Gauss) method

Let be N nonlinear equations with K parameters, $N > K$: $y_i = M_K(x_i; \theta)$.

The objective is to determine the K parameters of the vector θ by minimizing in an iterative manner the quadratic error

Gauss-Newton method

Let be $\boldsymbol{\theta}_l = \begin{bmatrix} \vdots \\ \theta_k \\ \vdots \end{bmatrix}$ the parameter vector obtained after l^{th} iteration.

The following matrix system will be solved in the least squares sense:

$$\mathbf{M}_K(\mathbf{X}; \boldsymbol{\theta}_l) - \mathbf{Y} = \mathbf{M}'_K(\mathbf{X}; \boldsymbol{\theta}_l)[\boldsymbol{\theta}_l - \boldsymbol{\theta}_{l+1}]$$

with $\mathbf{M}'_K(\mathbf{X}; \boldsymbol{\theta}_l) = \begin{bmatrix} \ddots & \vdots & \ddots \\ \cdots & \frac{\partial M_K(x_i; \boldsymbol{\theta}_l)}{\partial \theta_k} & \cdots \\ \ddots & \vdots & \ddots \end{bmatrix}$ is a $N \times K$ matrix.

parameter vector $\boldsymbol{\theta}_{l+1}$ at $l + 1$ iteration is obtained calculating:

$$\boldsymbol{\theta}_{l+1} = \boldsymbol{\theta}_l - (\mathbf{M}'_K(\mathbf{X}; \boldsymbol{\theta}_l)^T \mathbf{M}'_K(\mathbf{X}; \boldsymbol{\theta}_l))^{-1} \mathbf{M}'_K(\mathbf{X}; \boldsymbol{\theta}_l)^T (\mathbf{M}_K(\mathbf{X}; \boldsymbol{\theta}_l) - \mathbf{Y})$$

Iterative process is stopped when a given tolerance Optimized parameters of the model $\boldsymbol{\theta}_{opt}$ is reached.

Uncertainty on $\boldsymbol{\theta}_{num}$ is given by the $K \times K$ covariance matrix: $\mathbf{C}_{\boldsymbol{\theta}} = (\mathbf{M}'_K(\mathbf{X}; \boldsymbol{\theta}_{opt})^T \mathbf{C}_Y \mathbf{M}'_K(\mathbf{X}; \boldsymbol{\theta}_{opt}))^{-1}$

where \mathbf{C}_Y is the $N \times N$ covariance matrix of data

Gauss-Newton method : Example

$N = 20$ data $Y = \{\dots, y_i, \dots\}$ measured at abscissa equidistant $X = \{\dots, x_i, \dots\}$ with Δx as sampling step.

Hypothesis : data obeys to a Gaussian law: $y = f(x) = Ae^{-\frac{(x-x_0)^2}{2\sigma^2}}$ where the amplitude A , the origin offset x_0 and the standard deviation σ are the parameters to determine : $\theta = \begin{bmatrix} A \\ x_0 \\ \sigma \end{bmatrix}$.

$$\text{Parameter starting values : } \theta_0 = \begin{bmatrix} \max(Y) \\ X(Y == \max(Y)) \\ \text{length}(\frac{Y}{\max(Y)} > 0.5) \times \Delta x / 2 \end{bmatrix}$$

From the model, calculate the matrices $M_K(X; \theta_0)$ and $M'_K(X; \theta_0)$

$$\theta_{th} = \begin{bmatrix} 1 \\ 0.1 \\ 0.2 \end{bmatrix}; \quad \theta_0 = \begin{bmatrix} 0.88 \\ 0.16 \\ 0.26 \end{bmatrix}; \quad \theta_{opt} = \begin{bmatrix} 0.89 \\ 0.09 \\ 0.23 \end{bmatrix}$$

95% confidence interval for optimized parameters:

$$\begin{cases} \hat{A} = 0.9 \pm 0.1 \\ \hat{x}_0 = 0.09 \pm 0.04 \\ \hat{\sigma} = 0.23 \pm 0.04 \end{cases}$$

