Lecture 3. Basics for linear estimation, the white box case

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Abstract. We present and illustrate the roadmap for a linear parameter estimation problem, in the case when the structure of the model is known ('white box case'). The Ordinary Least Square case is first considered to introduce all the useful tools (sensitivity coefficients, conditioning, etc). We focus then on optimal ways to implement the best estimation through the study of the sensitivity matrix and other matrices depending on it. The propagation of bias on blocked parameter during the estimation of desired parameters is also studied.

1. Introduction

We present and illustrate the roadmap for a linear parameter estimation problem, in the case when the structure of the model is known ('white box case'). The Ordinary Least Square case is first considered to introduce all the useful tools. We focus then on optimal ways to implement the best estimation through the study of the sensitivity matrix and other matrices depending on it.

2. The roadmap for solving a linear parameter estimation problem: the Ordinary Least Square case

2.1. Generate data

Let us suppose we have realised an experiment that provides m measurements $y_i = y(t_i)$ for i=1, …, m at m discrete values of time t (the 'independent' variable). These measurements are the components of the vector $(m \times 1)$ of experimental measurements $\boldsymbol{y} = [y_1 \ldots y_i \ldots y_m]^t$. Times of measurements are regularly spaced between $t_{\min}$ and $t_{\max}$ and are the components of the time vector $(m \times 1)$ $\boldsymbol{t} = [t_{\min} \ldots t_i \ldots t_{\max}]^t$ with $t_i = t_{min} + (i-1)\,\mathrm{d}t$, i=1, …, m. Let ε_i be the

(unknown) error associated to the measurement y_i (i=1, …, m), then the measurement errors vector $(m \times 1)$ is $\boldsymbol{\varepsilon} = [\varepsilon_1 \ldots \varepsilon_i \ldots \varepsilon_m]^t$. Some assumptions have to be done on these measurement errors. They are detailed in **Table 1**.

Number	Assumption	Explanation
1	Additive errors	$\boldsymbol{y} = \boldsymbol{y}_{perfect} + \boldsymbol{\varepsilon}$
2	Unbiased model	$\boldsymbol{y}_{perfect} = y_{mo}(x^{exact})$
3	Zero mean errors	$\mathrm{E}[\boldsymbol{\varepsilon}] = 0$
4	Constant variance	$\mathrm{var}[\varepsilon] = \sigma_\varepsilon^2$
5	Uncorrelated errors	$cov\,[\varepsilon_i, \varepsilon_j] = 0$ for $i \neq j$
6	Normal probability distribution	
7	Known parameters of the probability density distribution of errors	
8	No error in the S_{ij}	$\boldsymbol{S}$ is not a random matrix
9	No prior information regarding the parameters	

Table 1 : Statistical assumptions regarding the measurement errors

The first assumption on measurement errors is that they are purely additive :

$$\boldsymbol{y} = \boldsymbol{y}_{perfect} + \boldsymbol{\varepsilon} \qquad \textbf{(3. 1)}$$

Here $\boldsymbol{y}_{perfect}$ represents the vector $(m \times 1)$ of (unknown) errorless measurements, which corresponds to the output of a model that is assumed to be perfect[2]. Moreover, measurement errors are assumed to be the realizations of a random variable with any distribution but with a zero mean, that is $\mathrm{E}[\boldsymbol{\varepsilon}] = 0$ (unbiased errors), E[.] being the expected value operator (representing the mean of a large number of realizations of the random variable). On its main diagonal, the covariance matrix $(m \times m)$ $\boldsymbol{\psi} = \mathrm{cov}(\boldsymbol{\varepsilon}) = \mathrm{E}\left[(\boldsymbol{\varepsilon} - \mathrm{E}[\boldsymbol{\varepsilon}])\,(\boldsymbol{\varepsilon} - \mathrm{E}[\boldsymbol{\varepsilon}])^t\right] = \mathrm{E}\left[\boldsymbol{\varepsilon}\,\boldsymbol{\varepsilon}^t\right]$ of measurements errors contains the variance σ_ε^2 of each measurement that is supposed constant for each time t_i, i = 1, …, m. This variance may or may not be known. Finally, measurement errors are assumed uncorrelated (error at time t_i is independent of error at time t_j ($\mathrm{E}[\varepsilon_i\,\varepsilon_j] = 0$ for $i \neq j$) and consequently $\boldsymbol{\psi}$ is a diagonal matrix:

$$\boldsymbol{\psi} = \mathrm{cov}\,(\boldsymbol{\varepsilon}) = \mathrm{diag}\left(\sigma_\varepsilon^2, \cdots, \sigma_\varepsilon^2, \cdots, \sigma_\varepsilon^2\right) = \sigma_\varepsilon^2\,\boldsymbol{I} \qquad \textbf{(3. 2)}$$

These data (3.1) can come from a real experiment or can have been numerically created (for testing the parameter estimation method), using a mathematical model and adding a numerical

[2] The objective of 'direct' modelisation is to give the best approximation of $\boldsymbol{y}_{perfect}$

random noise verifying the preceding assumptions. Now the model and its parameters will be presented.

2.2. Build a model of the measured signal, define the parameters and first contact with the sensitivities

The objective of such a model is to give a mathematical expression, noted $y_{mo}(t, \boldsymbol{x}) = \eta(t, \boldsymbol{x})$ of the perfect measurements $y_{perfect}(t)$ mentioned above. This model is a function of the independent variable (time) and of n parameters composing the parameters vector ($n \times 1$) noted $\boldsymbol{x} = [x_1 \dots x_n]^t$. The model vector ($m \times 1$) is then given by $\boldsymbol{y_{mo}}(\boldsymbol{t}, \boldsymbol{x}) = [y_{mo,1}(t_1, \boldsymbol{x}) \dots y_{mo,i}(t_i, \boldsymbol{x}) \dots y_{mo,m}(t_m, \boldsymbol{x})]^t$, where $\boldsymbol{t} = [t_1 \dots t_i \dots t_m]^t$ is a column vector composed of the m times of measurements t_i. For this example, we choose to analyse the classical two parameters estimation problem consisting in estimating simultaneously the slope and the intercept of a straight line; then the model is given, in a scalar writing, by:

$$y_{mo}(t, \boldsymbol{x}) = x_1\ t + x_2 \qquad \textbf{(3. 3)}$$

The model is linear with respect to its two parameters x_1 and x_2 because:

$$\begin{aligned} &y_{mo}(t, a\boldsymbol{x} + b\boldsymbol{x'}) = (a\,x_1 + b\,x_1')\ t + a\,x_2 + b\,x_2' = a(x_1 t + x_2) + b\,(x_1'\ t + x_2') \\ &y_{mo}(t, a\boldsymbol{x} + b\boldsymbol{x'}) = a\ y_{mo}(t, \boldsymbol{x}) + b\ y_{mo}(t, \boldsymbol{x'}) \end{aligned} \qquad \textbf{(3. 4)}$$

Important remark: the following model:

$$y_{mo}(t, \boldsymbol{x}) = x_1 \sqrt{t} + x_2\, \mathrm{erf}\,(t) \qquad \textbf{(3. 5)}$$

is also linear with respect to its two parameters x_1 and x_2, even if its time behavior is not linear. On the contrary, the following model:

$$y_{mo}(t, \boldsymbol{x}) = x_1 \sqrt{t} + \exp(-x_2\, t) \qquad \textbf{(3. 6)}$$

is linear with respect to x_1 but nonlinear with respect to x_2 and is consequently nonlinear with respect to $\boldsymbol{x}$.

Writing the m model values (3. 3) for the m time values $t_1 \dots t_m$, the m resulting equations can be written in a matrix way as follows:

$$\begin{bmatrix} y_{mo,1} \\ \vdots \\ y_{mo,i} \\ \vdots \\ y_{mo,m} \end{bmatrix} = \begin{bmatrix} t_1 & 1 \\ \vdots & \vdots \\ t_i & 1 \\ \vdots & \vdots \\ t_m & 1 \end{bmatrix} . \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \textbf{(3. 7)}$$

or, in a more compact form:

$$\boldsymbol{y}_{mo} = \boldsymbol{S}\,\boldsymbol{x} \qquad \textbf{(3. 8)}$$

The matrix $\boldsymbol{S}$ ($m \times n$) is called the sensitivity (or Jacobian) matrix. Column k contains the m times values of the sensitivity coefficient of the model with respect to the parameter x_k, given by :

$$S_k(t, \boldsymbol{x}) = \left.\frac{\partial y_{mo}(t, \boldsymbol{x})}{\partial x_k}\right|_{t, x_j \text{ for } j \neq k} \quad , \quad k=1, \ldots, n \qquad \textbf{(3. 9a)}$$

Equation (3. 8) is only valid for a linear model. However, the sensitivity coefficient (3.9a) can be defined for the discrete time values $t = t_i$ (i=1, …, m) to form a sensitivity matrix $\boldsymbol{S}$ defined for any linear or nonlinear model as:

$$\boldsymbol{S}(\boldsymbol{x}) = \left(\nabla_x \boldsymbol{y}^{\,t}_{mo}\right)^t \qquad \textbf{(3.10a)}$$

or, more simply, in a symbolic way

$$\boldsymbol{S}\,(\boldsymbol{x}) = \frac{\mathrm{d}\,\boldsymbol{y}_{mo}\,(\boldsymbol{x})}{\mathrm{d}\,\boldsymbol{x}} \qquad \textbf{(3.10b)}$$

Let us note here that the nabla operator ∇_x, of dimensions n x 1 , can be applied either to a scalar or to a row vector. So,

- $$\nabla_x z = \begin{bmatrix} \dfrac{\partial z}{\partial x_1} \\ \dfrac{\partial z}{\partial x_2} \\ \\ \dfrac{\partial z}{\partial x_n} \end{bmatrix}$$ if z is a scalar **(3.10c)**

- $$\nabla_x \boldsymbol{z} = \begin{bmatrix} \dfrac{\partial z_1}{\partial x_1} & \dfrac{\partial z_2}{\partial x_1} & \cdots & \dfrac{\partial z_m}{\partial x_1} \\ \dfrac{\partial z_1}{\partial x_2} & \dfrac{\partial z_2}{\partial x_2} & \cdots & \dfrac{\partial z_m}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial z_1}{\partial x_n} & \dfrac{\partial z_2}{\partial x_n} & \cdots & \dfrac{\partial z_m}{\partial x_n} \end{bmatrix}$$ if it is a row vector **noted** $\boldsymbol{z}$ of size 1 *x m* **(3.10d)**

Let us note here that, in terms of dimensions, the the left product of the operator ∇_x with another quantity (scalar or matrix), respects the same rule as a normal column vector. For example, the dimensions of $\nabla_x \boldsymbol{z}$ in equation (3.10d) is (n x 1) by (1 x m), that is (n x m).

Important remark: if the model is linear with respect to its parameters (as in the cases (3. 3) and (3. 5)), then the sensitivity coefficients do not depend on the parameters:, and the sensitivity matrix does not depend on $\boldsymbol{x}$.

For model (3. 3), we have $S_1(t) = t$ and $S_2(t) = 1$ then:

$$\boldsymbol{S} = \begin{bmatrix} S_1(t_1) & S_2(t_1) \\ \vdots & \vdots \\ S_1(t_i) & S_2(t_i) \\ \vdots & \vdots \\ S_1(t_m) & S_2(t_m) \end{bmatrix} = \begin{bmatrix} t_1 & 1 \\ \vdots & \vdots \\ t_i & 1 \\ \vdots & \vdots \\ t_m & 1 \end{bmatrix} \qquad \textbf{(3. 10)}$$

A sensitivity coefficient is a measure of the "influence" of a given parameter x_k on the response of the model $\boldsymbol{y}_{mo}(\boldsymbol{t}, \boldsymbol{x})$. If all the sensitivity coefficients are of "high" magnitude and "independent", the simultaneous estimation of the parameters composing $\boldsymbol{x}$ will be possible. The meaning of "high" and "independent" will be developed later.

2.3. Choose the objective function

Assuming that the model has the right form (or "right structure", given by the resolution of the "right" partial differential equations describing the "right" physical phenomena) and is calculated with the right values of parameters $\boldsymbol{x}^{exact}$, then $\boldsymbol{y}_{mo}(\boldsymbol{x}^{exact}) = \boldsymbol{y}_{perfect}$ and Eq. (3. 1) becomes

$$\boldsymbol{y} = \boldsymbol{y}_{mo}(\boldsymbol{x}^{exact}) + \boldsymbol{\varepsilon} \qquad \textbf{(3. 11)}$$

Since the m measurement errors composing $\boldsymbol{\varepsilon}$ are not known, the problem of finding the values of the n components of $\boldsymbol{x}^{exact}$ given m measurements verifying Eq. (3. 11) is underdetermined (m equations with $n + m$ unknowns: n parameters x_k (k=1, …, n) and m noise values ε_i (i = 1, …, m)). The problem consists in using the m measurements for estimating the n unknown parameters, with $m \geq n$. Then the new problem to solve is a minimization problem. For a given value $\boldsymbol{x}$ of the parameter vector, a residual vector $\boldsymbol{r}$ ($m \times 1$) is built in order to calculate the difference between measurement vector $\boldsymbol{y}$ ($m \times 1$) and the corresponding model output $\boldsymbol{y}_{mo}(\boldsymbol{x})$ (m x 1), each component of $\boldsymbol{r}$ being associated with one of the m instants of time where a measurement is available.

$$\boldsymbol{r}(\boldsymbol{x}) = \boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x}) = \left[y_1 - y_{mo,1}(t_1, \boldsymbol{x}) \quad \dots \quad y_i - y_{mo,i}(t_i, \boldsymbol{x}) \quad \dots \quad y_m - y_{mo,m}(t_m, \boldsymbol{x}) \right]^t \qquad \textbf{(3. 12)}$$

This present definition of the residual vector $\boldsymbol{r}(\boldsymbol{x})$ is an extension of the concept of residual vector which is usually defined as $\boldsymbol{r}(\hat{\boldsymbol{x}})$, where $\hat{\boldsymbol{x}}$ corresponds to the minimum of $\boldsymbol{r}(\boldsymbol{x})$, see Eq. (3.17) further on.

Then the norm of this residual vector $\| \boldsymbol{r}(\boldsymbol{x}) \|$ is calculated, it is a scalar value that will be minimized with respect to the different components of parameter $\boldsymbol{x}$ in order to estimate an 'optimal' value for it. One has to choose the way of computing the norm of the residuals $\| \boldsymbol{r}(\boldsymbol{x}) \|$. Without any a priori information about the values of the parameters and given the above assumptions for measurements errors, the chosen norm is the Euclidian norm (or L_2 norm) given by:

$$\| \boldsymbol{r}(\boldsymbol{x}) \| = \left(\sum_{i=1}^{m} r_i^2(\boldsymbol{x}) \right)^{1/2} \qquad \textbf{(3. 13)}$$

In fact, the objective function that will be minimized is the square of that Euclidian norm, it is called the 'Ordinary Least Squares' objective function[3] :

$$J_{OLS}(\boldsymbol{x}) = \| \boldsymbol{r}(\boldsymbol{x}) \|^2 = \| \boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x}) \|^2 \qquad \textbf{(3. 14)}$$

In the particular case of a linear model, $\boldsymbol{y}_{mo}(\boldsymbol{x}) = \boldsymbol{S}\,\boldsymbol{x}$ and this OLS sum becomes:

$$J_{OLS}(\boldsymbol{x}) = \sum_{i=1}^{m} r_i^2(\boldsymbol{x}) = \sum_{i=1}^{m} \left(y_i - y_{mo}(t_i, \boldsymbol{x}) \right)^2 = \sum_{i=1}^{m} \left(y_i - \sum_{j=1}^{n} S_j(t_i)\, x_i \right)^2 \qquad \textbf{(3.16)}$$

With a matrix writing, (3.16) is equivalent to :

$$J_{OLS}(\boldsymbol{x}) = \left[\boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x}) \right]^t \left[\boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x}) \right] \qquad \textbf{(3. 15)}$$

The solution of this minimization will be called $\hat{\boldsymbol{x}}_{OLS}$ here. The hat ($\wedge$) superscript designates an estimator of the corresponding quantity, that is a random variable derived here from the random vector variable $\boldsymbol{\varepsilon}$ (the measurement noise) and the subscript 'OLS' designates the specific minimized norm used here, the *Ordinary Least Squares* sum J_{OLS} defined in Eq. (3.14).

[3] it is here the most *efficient*, *i.e.* that will provide the estimation with the minimal variance if the noise is of zero mean, independent and identically distributed

If the model is linear, this OLS estimator does not require the use of any iterative algorithm and is given in a simple explicit form:

$$\hat{\boldsymbol{x}}_{OLS} = \arg\left(\min\left(J_{OLS}(\boldsymbol{x})\right)\right) \qquad \textbf{(3. 16)}$$

So, the original question was:

> "what are the exact values $\boldsymbol{x}^{exact}$ of parameter vector $\boldsymbol{x}$ for the model $\boldsymbol{y}_{mo}(\boldsymbol{x})$ when *m* corresponding noisy measurements $\boldsymbol{y} = \boldsymbol{y}_{mo}(\boldsymbol{x}^{exact}) + \boldsymbol{\varepsilon}$ are available?"

The answer is:

> "one possible approximation of $\boldsymbol{x}^{exact}$ is the estimator $\hat{\boldsymbol{x}}_{OLS}$, which minimizes the Ordinary Least Squares 'objective' function (sometimes also called 'criterion') $J_{OLS}(\boldsymbol{x})$ defined as the sum of the squares of the differences between the *m* model output and the corresponding measurements".

Or, in simpler words:

> "the natural numerical approximation of the parameters present in $\boldsymbol{x}^{exact}$ is the one that enables the model to be the closest to the whole set of measurements. This Ordinary Least Squares method was first found by Carl Friedrich Gauss in 1795 and later published by Adrien-Marie Legendre (1805)".

The natural question that arises next is: "how far is this $\hat{\boldsymbol{x}}_{OLS}$ estimation from the exact value $\boldsymbol{x}^{exact}$ and what can be done to reduce their difference?" These questions will be discussed now within the linear assumption where an explicit expression for $\hat{\boldsymbol{x}}_{OLS}$ will be given. Readers interested by non-linear estimation can refer to lecture 7 of this series.

2.4. Solve the parameter estimation problem: minimize the objective function

The OLS estimator $\hat{\boldsymbol{x}}_{OLS}$ is defined as the value of parameter vector $\boldsymbol{x}$ that minimizes the scalar function $J_{OLS}(\boldsymbol{x})$. So, it has to verify:

$$\nabla_x J_{OLS}(\hat{\boldsymbol{x}}_{OLS}) = 0 \qquad \textbf{(3.19)}$$

or

$$\nabla_x J_{OLS}(\boldsymbol{x}) = 2\left(\nabla_x\left(\boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x})\right)^t\right)\left(\boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x})\right) \qquad \textbf{(3. 17a)}$$

This equation stems from the following property of the nabla operator ∇_x, applied to a scalar product of vectors, see (Beck and Arnold, 1977, page 221) in the reference list:

$$\nabla_x \left(\boldsymbol{z}^t \boldsymbol{z} \right) = 2 \left(\nabla_x \boldsymbol{z}^t \right) \boldsymbol{z} \quad \text{where } \boldsymbol{z} \text{ is a column-vector of size } m \text{ x } 1 \qquad \textbf{(3.20b)}$$

and, as a consequence, $\boldsymbol{z}^t$ is a line-vector of size 1 x m

As a consequence,

$$\boldsymbol{y}_{mo} = \boldsymbol{S}\, \boldsymbol{x} \quad \text{with} \quad \boldsymbol{S}(\boldsymbol{x}) = \left(\nabla_x \boldsymbol{y}_{mo}^{\,t} \right)^t \qquad \textbf{(3.21)}$$

So, $\nabla_x J_{OLS}(\boldsymbol{x}) = 2 \left(\nabla_x \left(\boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x}) \right)^t \right) \left(\boldsymbol{y} - \boldsymbol{y}_{mo}(\boldsymbol{x}) \right)$ (3. **17a)** becomes:

$$\nabla_x J_{OLS}(\boldsymbol{x}) = -2\, \boldsymbol{S}^t \left[\boldsymbol{y} - \boldsymbol{S}\boldsymbol{x} \right] \qquad \textbf{(3. 18)}$$

Then $\hat{\boldsymbol{x}}_{OLS}$ is solution of:

$$\left[\boldsymbol{S}^t \boldsymbol{S} \right] \hat{\boldsymbol{x}}_{OLS} = \boldsymbol{S}^t \boldsymbol{y} \qquad \textbf{(3. 19)}$$

The n equations composing the linear system (3. 19) are called the 'normal equations'. The solution is straightforward if the ($n \times n$) matrix $\boldsymbol{S}^t\boldsymbol{S}$ is not singular, it is then possible to compute its inverse and obtain:

$$\hat{\boldsymbol{x}}_{OLS} = \left[\boldsymbol{S}^t \boldsymbol{S} \right]^{-1} \boldsymbol{S}^t \boldsymbol{y} \qquad \textbf{(3. 20)}$$

Let us note that it is not necessary to invert matrix $\boldsymbol{S}^t\boldsymbol{S}$, also called information matrix, in order to solve the system of normal equations (3.23): Eq. (3.24) can be used further on to yield a symbolic explicit expression of the OLS solution.

The ($n \times m$) matrix $\left[\boldsymbol{S}^t \boldsymbol{S} \right]^{-1} \boldsymbol{S}^t$ is called the Moore-Penrose matrix, also named as the pseudo-inverse of $\boldsymbol{S}$. Obviously, a necessary condition for $\boldsymbol{S}^t\boldsymbol{S}$ not to be singular is that the sensitivity coefficients are independent, and have a non-zero norm. This condition also requires that the number of measurements m be equal or greater than the number of parameters n to be estimated.

Eq. (3.24) gives an explicit expression for the ordinary least square *estimator* $\hat{\boldsymbol{x}}_{OLS}$ of $\boldsymbol{x}$ for any linear model $\boldsymbol{y}_{mo}(\boldsymbol{x}) = \boldsymbol{S}\, \boldsymbol{x}$ as a function of measurements $\boldsymbol{y}$ defined in Eq. (3.11). Since $\boldsymbol{y}$ is a random vector (because of noise $\boldsymbol{\varepsilon}$), such is also the case for $\hat{\boldsymbol{x}}_{OLS}$. However, equation (3.24) has also another *statistical* meaning: once measurements are available, a realization of

y (that is numerical values for its components) becomes available, and this equation provides the corresponding OLS *estimation* of ***x***.

2.5. Evaluate the confidence in estimations (variance and bias of estimator)

2.5.1. First approach with stochastic simulations (Monte Carlo method)

Before computing the statistical properties of the OLS estimator (expected value and covariance matrix), we present a graphical approach that helps to understand the meaning of such properties. This approach is possible in the case when two parameters are estimated because each estimation $\hat{\boldsymbol{x}}_{OLS} = (\hat{x}_{OLS,1}, \hat{x}_{OLS,2})$ can be plotted as a point in a 2D coordinates frame graduated in (x_1, x_2). The idea is then to simulate K=100 experiments with K different realizations of the random noise vector $\boldsymbol{\varepsilon}$ generated by an independently distributed Gaussian process with the same statistical properties (see Table 1) to produce K samples of measurements vectors **y** according to (3.12). The exact output of the model ($\boldsymbol{y}_{perfect}$) as well as the time of measurements and the standard deviation of the noise used for each simulation is given in *Table 2*. This model structure with this set of associated experimental parameters is called the 'reference case' **Figure 1** shows one of the simulated experiments (circles) and the corresponding recalculated model output corresponding to the OLS estimation $\hat{\boldsymbol{x}}_{OLS} = (\hat{x}_{OLS,1}, \hat{x}_{OLS,2})$ (red line).

x_1^{exact} (K/h)	5
x_2^{exact} (K)	2
Model structure $y_{mo}(t, \boldsymbol{x})$	$x_1\ t + x_2$, Eq. (3. 3)
Number of measurements *m*	20
Start of time range t_{min}	0.5
Time step dt	0.1
Noise standard deviation σ_ε	0.5

Table 2 : conditions of the K=100 simulated 'reference' experiments.

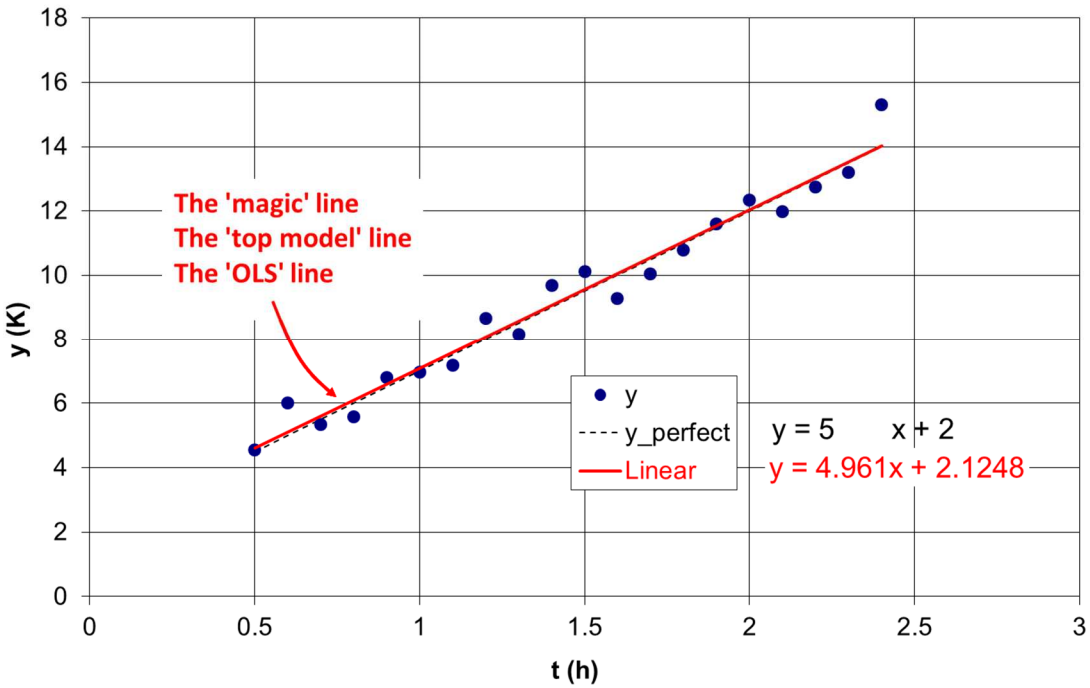

Figure 1 : one of the K=100 experiments of the 'reference case', the corresponding exact model and the corresponding recalculated OLS model output.

The K=100 OLS estimations $\hat{\boldsymbol{x}}_{OLS} = (\hat{x}_{OLS,1}, \hat{x}_{OLS,2})$ are then plotted in a scatter graph graduated in (x_1, x_2) in ***Figure 2***. Because of a different random realization of noise for each of the 100 experiments, each corresponding OLS estimations $\hat{\boldsymbol{x}}_{OLS} = (\hat{x}_{OLS,1}, \hat{x}_{OLS,2})$ is different, showing immediately the consequence of noise measurement on the dispersion of estimations. In that figure the position (square) of the exact value $\boldsymbol{x}^{exact} = (x_1^{exact} = 5, x_2^{exact} = 2)$ and the position (star) of the mean value of the K estimations $\hat{\boldsymbol{x}}_{mean} = (\text{mean}(\hat{x}_{1,OLS}) = 4.994, \text{mean}(\hat{x}_{2,OLS}) = 2.019)$ (the center of the scatter) are very close.

Another interesting way of looking at the estimation results is to plot them in a scatter graph with normalized coordinates indicating the distance of each estimation from the center of the scatter in %, see ***Figure 3***:

$$e_{OLS,1,i} = 100\left(\hat{x}_{OLS,1,i} - \hat{x}_{mean,1}\right) / \hat{x}_{mean,1} \qquad \textbf{(3. 21)}$$

$$e_{OLS,2,i} = 100\left(\hat{x}_{OLS,2,i} - \hat{x}_{mean,2}\right) / \hat{x}_{mean,2} \qquad \textbf{(3. 22)}$$

If we consider that $\hat{\boldsymbol{x}}_{mean} \approx \boldsymbol{x}_{exact}$ the quantities (3. 21) and (3. 22) that are the relative estimation errors in % of x_1^{exact} and of x_2^{exact}. That plot enables to quantify in % the dispersion of the estimations of each parameter around its mean value. This dispersion is what one often wants to minimize.

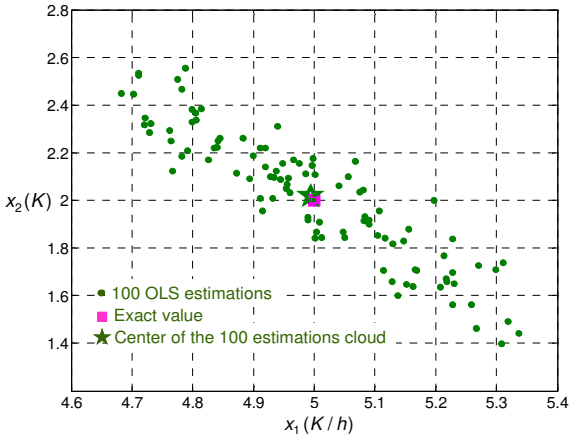

Figure 2 : dispersion of the 100 estimations around their central value (star) that is very close to the exact value (square)

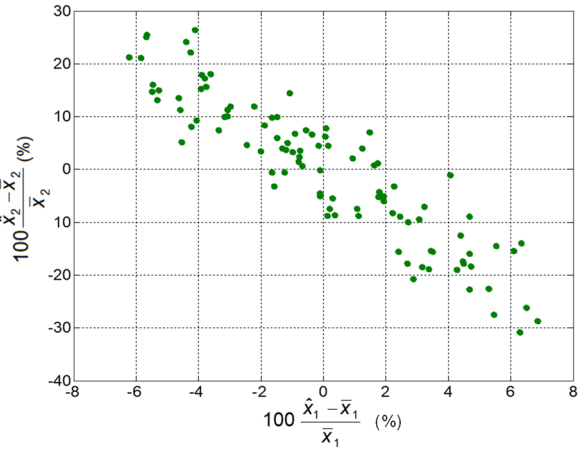

Figure 3* : *relative estimation errors in % centred and scaled using the mean value of the scatter

At this point, after having quantified the central value $\hat{\boldsymbol{x}}_{mean}$ of the K=100 $\hat{\boldsymbol{x}}_{OLS}$ estimations and after having evaluated the dispersion of the majority of estimations around this central value (that indicates the confidence we associate to it), we can sum up the result of the estimation problem in the following way:

" x_1^{exact} is equal to $\hat{x}_{mean,1} = 2.0 \pm 20\%$ and
x_2^{exact} is equal to $\hat{x}_{mean,2} = 4.9 \pm 40\%$"

But in reality, we never realize 100 experiments with 100 estimations $\hat{\boldsymbol{x}}_{OLS} = (\hat{x}_{OLS,1}, \hat{x}_{OLS,2})$ in order to calculate the mean value $\hat{\boldsymbol{x}}_{mean} = (\text{mean}(\hat{x}_1), \text{mean}(\hat{x}_2))$. We generally do one single experiment and obtain only one of the 100 points of ***Figure 2*** and ***Figure 3***. We must keep in mind that this point can be one of the points 'far' from the exact value! Whatever the realized experiment among these 100, what we want to do is to associate a 'confidence region' to the particular estimation $\hat{\boldsymbol{x}}_{OLS} = (\hat{x}_{OLS,1}, \hat{x}_{OLS,2})$ (or 'confidence intervals' for each parameter) that has about the same dimension than the scatter we have just obtained with these 100 simulated experiments. That is the objective of the following section.

2.5.2. Calculation of statistical properties of the OLS estimator

Here we become more general and we consider the case when not all the n parameters are estimated but only r, the (n-r) remaining parameters are supposed to be known and they are fixed during the estimation of the r unknown parameters. Usually a parameter is set to a supposed known values for two major reasons: i) the model is not sensitive enough to that parameters or ii) the sensitivity of the model to that parameter 'looks like' the sensitivity to

another parameter (see Section 3.1.1). Unknown parameters are noted with subscript *r* and known parameters are noted with subscript *c*. We must consider that the fixed parameters have not been fixed to their exact value, and at the end of estimation of the *r* parameters, we have to evaluate the bias made on the estimations because of the error in the (*n* - *r*) parameters that are supposed to be known.

We can split (3. 8) into:

$$\boldsymbol{y}_{mo} = \boldsymbol{S}_r \boldsymbol{x}_r + \boldsymbol{S}_c \boldsymbol{x}_c \qquad \textbf{(3. 23)}$$

The matrix $\boldsymbol{S}_r$ ($n \times r$) is the sensitivity matrix to estimated parameters. It is a part of the "complete" sensitivity matrix $\boldsymbol{S}$, relative to all the parameters (unknown $\boldsymbol{x}_r$ ($r \times 1$) and known $\boldsymbol{x}_c$ ((n-r) × 1)):

$$\boldsymbol{S} = [\boldsymbol{S}_r \vdots \boldsymbol{S}_c] = \left[\begin{bmatrix} S_1(t_1) & \dots & S_r(t_1) \\ \vdots & \dots & \vdots \\ S_1(t_m) & \dots & S_r(t_m) \end{bmatrix} \vdots \begin{bmatrix} S_{r+1}(t_1) & \dots & S_{n-r}(t_1) \\ \vdots & \dots & \vdots \\ S_{r+1}(t_m) & \dots & S_{n-r}(t_m) \end{bmatrix}\right] \qquad \textbf{(3. 24)}$$

The matrix $\boldsymbol{S}_c$ (n × r) is the sensitivity matrix to estimated parameters. It is a part of the "complete" sensitivity matrix $\boldsymbol{S}$, relative to all the parameters (estimated $\boldsymbol{x}_r$ ($r \times 1$) and fixed $\boldsymbol{x}_c$ ((n-r) × 1)):

The OLS solution (3. 20) becomes:

$$\hat{\boldsymbol{x}}_{OLS} = \left[\boldsymbol{S}_r^t \boldsymbol{S}_r\right]^{-1} \boldsymbol{S}_r^t (\boldsymbol{y} - \boldsymbol{S}_c \boldsymbol{x}_c) \qquad \textbf{(3. 25)}$$

Let $\hat{\boldsymbol{x}}_{r,OLS}(\tilde{\boldsymbol{x}}_c)$ be the estimated parameters for a value of fixed parameters $\tilde{\boldsymbol{x}}_c$ different from their exact value $\boldsymbol{x}_c^{exact}$. Let $\boldsymbol{e}_r$ be the vector ($r \times 1$) of the estimation error (the difference between estimated $\hat{\boldsymbol{x}}_r$ and exact $\boldsymbol{x}_r^{exact}$ values of $\boldsymbol{x}_r$) and let $\boldsymbol{e}_c$ be the deterministic error (the bias) for the fixed values of the parameters that are supposed to be known:

$$\boldsymbol{e}_r = \hat{\boldsymbol{x}}_{r,OLS}(\tilde{\boldsymbol{x}}_c) - \boldsymbol{x}_r^{exact} \qquad \textbf{(3. 26)}$$

$$\boldsymbol{e}_c = \tilde{\boldsymbol{x}}_c - \boldsymbol{x}_c^{exact} \qquad \textbf{(3. 27)}$$

One can write, with $\boldsymbol{A}_r = \left[\boldsymbol{S}_r^t \boldsymbol{S}_r\right]^{-1} \boldsymbol{S}_r^t$ the Moore-Penrose matrix:

$$\hat{\boldsymbol{x}}_{r,OLS}(\tilde{\boldsymbol{x}}_c) = \boldsymbol{A}_r (\boldsymbol{y} - \boldsymbol{S}_c \tilde{\boldsymbol{x}}_c) \qquad \textbf{(3. 28)}$$

Eq. (3. 11) can be developed:

$$\boldsymbol{y} = \boldsymbol{y}_{mo}(\boldsymbol{x}^{exact}) + \boldsymbol{\varepsilon} = \boldsymbol{S}_r \boldsymbol{x}_r^{exact} + \boldsymbol{S}_c \boldsymbol{x}_c^{exact} + \boldsymbol{\varepsilon} \quad \textbf{(3. 29)}$$

Combining Eq. (3. 29) and (3. 28), the estimation error (3. 26) may then be approximated by:

$$\boldsymbol{e}_r = \hat{\boldsymbol{x}}_{r,OLS}(\tilde{\boldsymbol{x}}_c) - \boldsymbol{x}_r^{exact} = \boldsymbol{A}_r \boldsymbol{\varepsilon} - \boldsymbol{A}_r \boldsymbol{S}_c \boldsymbol{e}_c = \boldsymbol{e}_{r1} + \boldsymbol{e}_{r2} \quad \textbf{(3.34)}$$

The first term $\boldsymbol{e}_{r1} = \boldsymbol{A}_r \boldsymbol{\varepsilon}$ is the random contribution to the total error; it represents the error due to measurement errors $\boldsymbol{\varepsilon}$ whose covariance matrix $\boldsymbol{\Psi}$ is given by Eq. (3. 2). The second term $\boldsymbol{e}_{r2} = -\boldsymbol{A}_r \boldsymbol{S}_c \boldsymbol{e}_c$ is the non-random (deterministic) contribution to the total error vector due to the deterministic error on the fixed parameters $\boldsymbol{e}_c$. The expected value of $\boldsymbol{e}_{r1}$ is:

$$\mathrm{E}[\boldsymbol{e}_{r1}] = \boldsymbol{A}_r \, \mathrm{E}[\boldsymbol{\varepsilon}] = 0 \quad \textbf{(3. 30)}$$

meaning that no systematic bias is introduced by the random measurement errors.

Remark: this explains that the mean $\hat{\boldsymbol{x}}_{mean}$ of the 100 scattered estimations in ***Figure 2*** is very close to the exact value $\boldsymbol{x}^{exact}$.

The covariance matrix of $\boldsymbol{e}_{r1}$ is given by:

$$\boldsymbol{C}_1 = \mathrm{cov}(\boldsymbol{e}_{r1}) = \mathrm{E}[\boldsymbol{e}_{r1} \boldsymbol{e}_{r1}^t] = \boldsymbol{A}_r \, \mathrm{E}[\boldsymbol{\varepsilon}\, \boldsymbol{\varepsilon}^t] \, \boldsymbol{A}_r^t = \boldsymbol{A}_r \, \boldsymbol{\psi} \, \boldsymbol{A}_r^t = \sigma_\varepsilon^2 \left[\boldsymbol{S}_r^t \, \boldsymbol{S}_r \right]^{-1} \quad \textbf{(3.31)}$$

The matrix $\boldsymbol{P}_r = \left[\boldsymbol{S}_r^t \boldsymbol{S}_r \right]^{-1}$ may thus be seen as the matrix of "amplification" of measurement errors. The expected value of $\boldsymbol{e}_{r2}$ is:

$$\mathrm{E}\left[\boldsymbol{e}_{r2} \right] = - \, \boldsymbol{A}_r \, \boldsymbol{S}_c \, \boldsymbol{e}_c = - \left[\boldsymbol{S}_r^t \, \boldsymbol{S}_r \right]^{-1} \boldsymbol{S}_r^t \, \boldsymbol{S}_c \, \boldsymbol{e}_c \neq 0 \quad \textbf{(3.37)}$$

This expected value is different from zero, which means that estimation $\hat{\boldsymbol{x}}_{r,OLS}$ is biased, if the error $\boldsymbol{e_c}$ of the parameters supposed to be known is different from zero itself. This means that in the preceding stochastic simulation if only one part of $\boldsymbol{x}_r$ had been estimated (with a non-zero error on the remaining part $\boldsymbol{x}_c$) the scatter of 100 estimations would not have been centred on $\boldsymbol{x}_r^{exact}$. This bias is computed using the corresponding sensitivity coefficients matrix $\boldsymbol{S}_c$. The covariance matrix ((n-*r*)×(*n*-*r*)) of $\boldsymbol{e}_{r2}$ error is $\boldsymbol{C}_2 = \mathrm{cov}(\boldsymbol{e}_{r2}) = 0$ because $\boldsymbol{e}_c$ is not a random error. Finally, the total bias associated to the estimation $\hat{\boldsymbol{x}}_{r,OLS}(\tilde{\boldsymbol{x}}_c)$ is due to the biased value of $\tilde{\boldsymbol{x}}_c$ and its value is given by:

$$\mathrm{E}\left[\boldsymbol{e}_r \right] = \mathrm{E}\left[\boldsymbol{e}_{r2} \right] = - \left[\boldsymbol{S}_r^t \, \boldsymbol{S}_r \right]^{-1} \boldsymbol{S}_r^t \, \boldsymbol{S}_c \, \boldsymbol{e}_c \quad \textbf{(3.38)}$$

The matrix $\left[\boldsymbol{S}_r^t \boldsymbol{S}_r\right]^{-1} \boldsymbol{S}_r^t \boldsymbol{S}_c = \boldsymbol{P}_r \boldsymbol{S}_r^t \boldsymbol{S}_c$ ($r \times (n\text{-}r)$) may thus be seen as the "amplification" of bias on the fixed parameters . For a fixed value of , the covariance matrix of estimation error is:

$$\boldsymbol{C}_r = \mathrm{cov}(\boldsymbol{e}_r) = \mathrm{E}\left[(\boldsymbol{e}_r - \mathrm{E}\left[\boldsymbol{e}_r\right])\,(\boldsymbol{e}_r - \mathrm{E}\left[\boldsymbol{e}_r\right])^t\right] = \mathrm{cov}(\boldsymbol{e}_{r1}) \qquad \textbf{(3. 32)}$$

The coefficients of the covariance matrix of the estimation error are defined by:

$$\boldsymbol{C}_r = \begin{bmatrix} \sigma_1^2 & \mathrm{cov}(e_{r1}, e_{r2}) & \dots & \mathrm{cov}(e_{r1}, e_{rr}) \\ & \sigma_2^2 & & \mathrm{cov}(e_{r2}, e_{rr}) \\ & & \ddots & \vdots \\ sym & & & \sigma_r^2 \end{bmatrix} \qquad \textbf{(3. 33)}$$

Its main diagonal elements is composed of the individual variances of the error associated to each component of the estimated vector $\hat{\boldsymbol{x}}_{r,OLS}$ and its other coefficients are the covariance of crossed errors. Eq. (3.31) shows that knowledge of the variance of measurement errors σ_ε^2 is needed in order to compute the covariance matrix. If σ_ε^2 is not measured before the experiment, an estimation of it may be obtained at the end of estimation thanks to the final value of the objective function $J_{OLS}(\hat{\boldsymbol{x}}_{r,OLS}(\tilde{\boldsymbol{x}}_c)) = \sum_{i=1}^{m} r_i^2\,(\hat{\boldsymbol{x}}_{OLS}(\tilde{\boldsymbol{x}}_c))$. In fact, this estimation is based on the fact that, at the end of the estimation, the only difference that subsists between measurements and model (if its structure and its parameters are correct) must be the measurement errors. In fact, exact parameters are not exactly obtained, and the remaining differences between measurements and model are the residuals given by (3. 12). If the estimated parameters are not too far from the exact parameters, the residuals should have some statistical properties close to those of measurement errors. That is why a non-biased estimation of σ_ε^2 for the estimation of *r* parameters from the use of *m* measurements is thus given by:

$$\hat{\sigma}_\varepsilon^2 = \frac{J_{OLS}(\hat{\boldsymbol{x}}_{r,OLS}(\tilde{\boldsymbol{x}}_c))}{m - r} \qquad \textbf{(3. 34)}$$

This estimation is only valid for an independent and identically distributed (i.i.d.) noise $\boldsymbol{\varepsilon}$ and if there is no bias in the parameters supposed to be known, that is $\tilde{\boldsymbol{x}}_c = \boldsymbol{x}_c^{exact}$. Let us note that in the case of 'exact matching', where the number of measurements m is equal to the number *r* of parameters that are looked for, both numerator and denominator of equation (3.41) are equal to zero and, consequently, no information about the noise level can be brought by the calculation of the residuals.

2.5.3. The correlation matrix

The estimation error associated to $\hat{\boldsymbol{x}}_{r,OLS}(i)$ cannot be arbitrarily low independently of the corresponding error in $\hat{\boldsymbol{x}}_{r,OLS}(j)$ in the case where cov (e_{ri}, e_{rj}) : $\hat{x}_{ri}$ and $\hat{x}_{rj}$ are said correlated through the link that exists between their errors. The correlation level between estimations $\hat{x}_{ri}$ and $\hat{x}_{rj}$ is thus measured by the quantity:

$$\rho_{ij} = \frac{\mathrm{cov}(e_{ri}, e_{rj})}{\sigma_i \sigma_j} = \frac{C_{r,ij}}{\sqrt{C_{r,ii} C_{r,jj}}} = \frac{P_{r,ij}}{\sqrt{P_{r,ii} P_{r,jj}}} \quad \text{for } i, j = 1, \ldots, r \qquad \textbf{(3. 35)}$$

that lies between -1 and 1.

One considers that two estimation errors are highly correlated when $|\rho_{ij}| \geq 0.9$ (Beck et al., 1977). This quantity is independent of the magnitude of measurement errors and corresponds only to the degree of collinearity of the sensitivity coefficients. In the example of ***Figure 3***, $\rho_{12} = -0.99$ indicates that the error in the estimation of the slope (x_1) is highly linked to the error in the estimation of the intercept x_2: they will have the same sign (both estimations will be either under- or over-valued with a very high level of probability). However, this correlation coefficient does not bring any information about the level of these errors: this is brought by the calculation of their variances, the diagonal coefficients in Eq. (3.36). The high negative coefficient of correlation between the two parameters in our example explains why the scatter of the 100 estimations is contained inside a 'narrow' and 'inclined' ellipse whose main axis has a negative slope in ***Figure 3***.

2.5.4. The confidence region and interval for OLS with Gaussian assumptions

If the noise is Gaussian and i.i.d. the confidence region in the plane $(\hat{x}_1, \hat{x}_2)$ plane in ***Figure 2***, for a given confidence level α is an ellipse (for *n*=2 parameters, see ***Figure 4***). Its equation in $\boldsymbol{\delta x}$ coordinates centered on $\hat{\boldsymbol{x}}_{OLS}$ is:

$$\begin{aligned} &\boldsymbol{\delta x}^t \, \boldsymbol{S}^t \boldsymbol{S} \, \boldsymbol{\delta x} = \Delta^2 \\ &\Delta^2 = \chi^2_{1-\alpha}(2) \, \sigma_\varepsilon^2 \end{aligned} \qquad \textbf{(3. 36)}$$

$\chi^2_{1-\alpha}(2)$ is computed by the function *chi2inv(1-alpha,2)* in MATLAB® (or GNU-Octave) or *LOI.KHIDEUX.INVERSE(1-alpha;2)* in Excel® if we search for the confidence region at a 95% level (α=0.05) for the estimation of 2 parameters.

Typical values for classical confidence intervals are indicated in the Table 3

1-α	ν=1	ν=2	ν=3	ν=4
68.30%	**1.00**	**2.30**	**3.53**	**4.72**
95.45%	**4.00**	**6.17**	**8.02**	**9.72**
99.73%	**9.00**	**11.83**	**14.16**	**16.25**

Table 3 : **Chi-Square law for given confidence levels (1 - α) and ν degrees of freedom that will be used to compute the size of the ellipsoidal confidence regions. Square root of values in first column gives the classical rules '1σ, 2σ and 3σ'**

σ_ε^2 is the variance of noisy measurements. It is worth noting that the lengths of half axes ρ_1 and ρ_2 in the principal directions of the ellipse are given by:

$$\rho_1 = \Delta / \sqrt{\lambda_1}$$
$$\rho_2 = \Delta / \sqrt{\lambda_2} \qquad \textbf{(3. 37)}$$

λ_1 and λ_2 are the eigenvalues of $\boldsymbol{S}^t\boldsymbol{S}$. The product of these two eigenvalues is equal to the determinant of $\boldsymbol{S}^t\boldsymbol{S}$. Finally, the area of the confidence region inside the ellipse is given by:

$$A = \pi.\rho_1.\rho_2 = \frac{\pi\chi^2_{1-\alpha}(2)\sigma^2_\varepsilon}{\sqrt{\det(\boldsymbol{S}^t\boldsymbol{S})}} = \frac{\pi\chi^2_{1-\alpha}(2)\sigma^2_\varepsilon}{\sqrt{\lambda_1\lambda_2}} \qquad \textbf{(3. 38)}$$

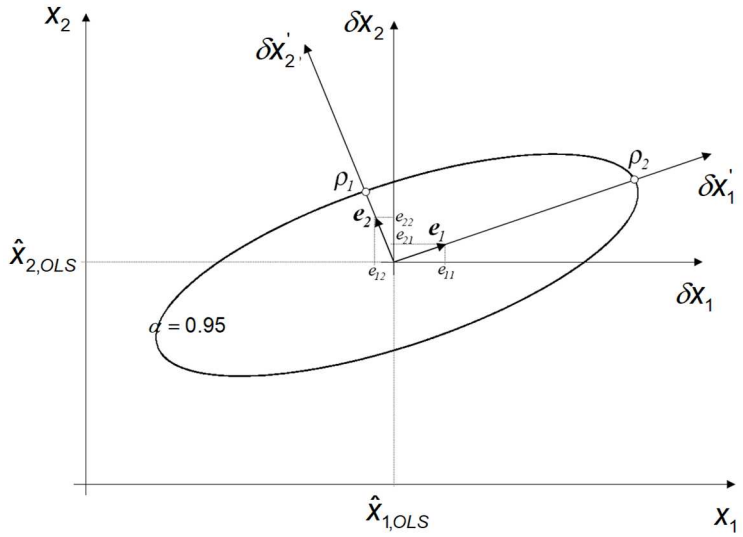

Figure 4 : elliptical confidence region associated to the estimation of two parameters (with Gaussian i.i.d. measurement noise), at a confidence level 1-α=0.95.

So, the product of eigenvalues of $\boldsymbol{S}^t\boldsymbol{S}$ gives information on the area of the confidence region, while the individual eigenvalues give information on the lengths of each principal direction of the ellipse : a 'long' ellipse in a direction corresponds to a low eigenvalue. The experiment that will maximize $\det\left(\boldsymbol{S}^t\boldsymbol{S}\right) = \lambda_1\,\lambda_2$ in order to minimize the confidence region is called a 'D-optimal' experiment.

In the case of estimation of $r = n$ parameters, the n variances associated to each component of the estimated vector $\hat{\boldsymbol{x}}_{OLS}$ constitute the main diagonal of matrix $\boldsymbol{C}$ (Eq. 3.39). The square root of the ith diagonal component of $\boldsymbol{C}$ is then the standard deviation associated to the estimation $\hat{x}_{i,OLS}$ and can be expressed in %. Then, the half width of confidence interval $CI_i^{1-\alpha}$, at a level of confidence of $100(1-\alpha)\%$, associated to the estimation $\hat{x}_{i,OLS}$ is now given by:

$$CI_i^{1-\alpha} = t_{1-\alpha/2}(m-n)\times\sqrt{C_{ii}}\ ,\ \text{for}\ \ i = 1,\ldots,n \qquad \textbf{(3. 39)}$$

The quantity $t_{1-\alpha/2}(m-n)$ is the t-statistic for m - n degrees of freedom at the confidence level of $100(1-\alpha)\%$ (function *tinv(1-alpha/2,m-n)* in MALTAB® or *LOI.STUDENT.INVERSE.N(1 – alpha/2;m - n)* in Excel®). For example, for m = 20 measurements, if n = 2 parameters are estimated, and if the 95% confidence is wanted, then $\alpha = 0.05$ and $t_{0.975}(20-2) = 2.1$. For a high number of measurements (>200), the t-statistic tends to the Gaussian statistic and we have $t_{0.975} \to 1.96$. Finally, the result of the estimation process of the unknown exact parameter x_i^{exact} can be presented in the following way:

' x_i^{exact} has a 95% chance of being in the interval $\left[\hat{x}_{i,OLS} - CI_i^{0.95} \qquad \hat{x}_{i,OLS} + CI_i^{0.95}\right]$',
or: ' $x_i^{exact} = \hat{x}_{i,OLS} \pm CI_i^{0.95}$ with 95% chance'

2.5.5. <u>The residuals analysis</u>

When estimation is achieved, the graphical analysis of residuals given by Eq. (3.13) $\boldsymbol{r}(\hat{\boldsymbol{x}})$ enables to detect some inconsistency of the result. Difference between measurements and model response with optimal parameters must 'look like' measurement noise , or in other words : 'the right model with the right parameters must explain the measurements except its random part'. For a Gaussian noise with standard assumptions, the statistical properties of residuals must be close to the measurement error properties (zero mean and variance $(m-n)\ \sigma_\varepsilon^2$). If the residuals are signed, the problem may be due to an error in the statistical assumptions regarding the measurements or in the structure or parameters of the direct model.

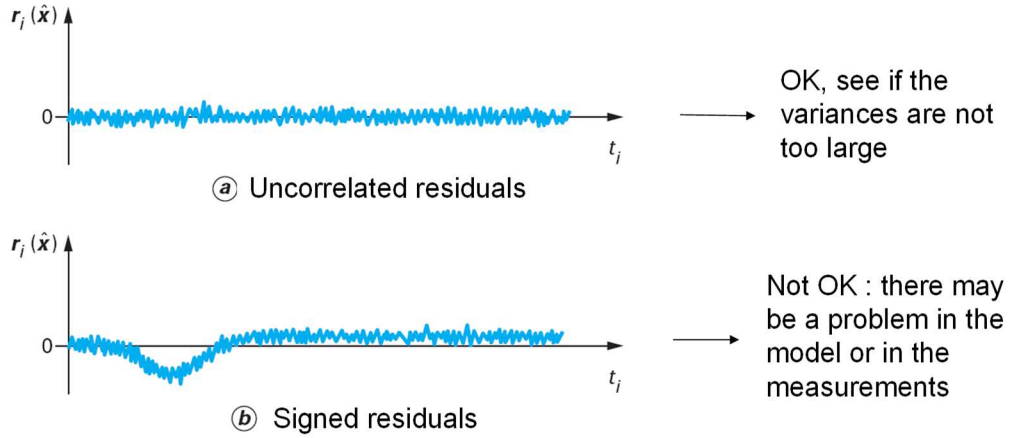

Figure 5 : graphical analysis of residuals at the end of the estimation

3. Indicators for a successful estimation

It has been shown above that matrix $\boldsymbol{S}^t\boldsymbol{S}$, also called the *information matrix*, is fundamental in the process of parameter estimation:

- it has to be invertible (that is non-singular: $\det(\boldsymbol{S}^t\boldsymbol{S}) \neq 0$) in order for **the OLS estimation** to be possible, according to Eq. **(3. 20),**
- it also has to be inverted to **compute the covariance matrix** according to Eq. **(3.31)** associated to the OLS estimation. The diagonal terms of this matrix are equal (within the σ_ε^2 factor and in case of an i.i.d. noise) to the variances of each estimation, and the off-diagonal terms enable to compute the correlation matrix. The inverse of $\boldsymbol{S}^t\boldsymbol{S}$ play the role of "noise amplification",
- the eigenvalues of $\boldsymbol{S}^t\boldsymbol{S}$, in the case of a Gaussian i.i.d. noise, enable the **calculation of the lengths of the half principal axes of the elliptical confidence region,**
- the determinant of $\boldsymbol{S}^t\boldsymbol{S}$ enables the **calculation of the area of the elliptical confidence region.**

The difficulty is clear : $\boldsymbol{S}^t\boldsymbol{S}$ has to be non-singular to be inverted and $\boldsymbol{S}^t\boldsymbol{S}$ has to be not 'quasi-singular' in order to limit the noise amplification. This notion of non-singular character of the information matrix $\boldsymbol{S}^t\boldsymbol{S}$ makes sense only if all the parameters x_j have the same physical units. Otherwise, one should study matrix $\boldsymbol{S}^{*t}\boldsymbol{S}^*$ where $\boldsymbol{S}^*$ is the reduced (sometimes called 'scaled') sensitivity matrix, see section Sections 3.1 and 3.3**.**

We then have to find some indicators to evaluate the singularity and the quasi-singularity of $\boldsymbol{S}^t\boldsymbol{S}$. The first indication can be simply graphical. Indeed, the singularity would happen if a sensitivity coefficient $S_i(t)$ was purely proportional to another $S_i(t)$; in that case the rank of $\boldsymbol{S}^t\boldsymbol{S}$ is lower than n, and its determinant is zero. More difficult is to find a linear combination of more than two sensitivity coefficients for which the consequences would be the same. The quasi-singularity would happen if the sensitivity coefficients are linked for all values of the

independent variable (time here). This case happens most of the time, the rank of $\boldsymbol{S}^t\boldsymbol{S}$ is not zero but its determinant is low and its condition number built with the ratio of extreme eigenvalues:

$$cond(\boldsymbol{S}^t\boldsymbol{S}) = \frac{\lambda_{\max}(\boldsymbol{S}^t\boldsymbol{S})}{\lambda_{\min}(\boldsymbol{S}^t\boldsymbol{S})} \qquad \textbf{(3. 40)}$$

takes high values.

Another explanation stems from linear algebra arguments: one can consider that each sensitivity coefficient $\boldsymbol{S}_j$, that forms a ($m \times 1$) matrix, a so-called 'column-vector', is the components of a real vector $\vec{\boldsymbol{S}}_j$ in a *m*-dimensional space: the possible quasi-singularity of matrix $\boldsymbol{S}$ is caused by the fact that the vectors of the corresponding system of real vectors are 'nearly' dependent, which means that a non-zero set of *n* coefficients exists that makes the corresponding linear combination of these real vectors 'nearly' equal to zero (the interested reader can refer to lecture L7 of this series). Of course, the term 'nearly' needs to be quantified, that is that either all the sensitivity coefficients must have the same physical units or this analysis must be made using reduced sensitivity coefficients otherwise (see section 3.1 further down). Let us note that

'Visual' and 'quantitative' criteria will now be illustrated. We introduce first the reduced sensitivity matrix $\boldsymbol{S}^*$, that enables to compare the sensitivity coefficients between themselves and to compute a covariance matrix associated to *relative* estimations (and then to compute directly relative standard deviation associated to each parameter).

3.1. The reduced, or scaled, sensitivity matrix $\boldsymbol{S}^*$

It is given by:

$$\boldsymbol{S}^* = \boldsymbol{S}\ \mathrm{diag}(\boldsymbol{x}) \qquad \textbf{(3. 41)}$$

$$\text{with } \mathrm{diag}(\boldsymbol{x}) = \begin{pmatrix} x_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & x_n \end{pmatrix} \qquad \textbf{(3. 42)}$$

It is built with the reduce, or scaled, sensitivity coefficients that are defined as:

$$S_k^*(t,\boldsymbol{x}) = x_k S_k(t,\boldsymbol{x}) = x_k \left.\frac{\partial y_{mo}(t,\boldsymbol{x})}{\partial x_k}\right|_{t,x_j \text{ for } j\neq k} = \frac{\partial y_{mo}(t,\boldsymbol{x})}{\dfrac{\partial x_k}{x_k}}\Big|_{t,x_j \text{ for } j\neq k} \qquad \textbf{(3. 50)}$$

Eq. (3.50) shows that the reduced sensitivity S_k^* represents the *absolute* variation of model $\partial y_{mo}(t,\boldsymbol{x})$ due to a *relative* variation of parameter $\partial x_k / x_k$. They can be also considered as the sensitivity coefficients with respect to the natural logarithm of each parameter. These reduced sensitivity coefficients have then the same unit as both model output y_{mo} and

standard deviation σ_ε of the measurement noise. If their magnitude is lower than the magnitude of the measurement noise σ_ε, it means that the influence of the considered parameter on the model response will not be measurable with a correct accuracy. Consequently, the estimation of this parameter through the use of experimental measurements, if it is possible, will be highly inaccurate. Rapid information may then be given by comparing the magnitude of each reduced sensitivity coefficient to the magnitude of the measurement noise, with respect to the independent variable (here time).

In the preceding example, we have then (with $n = 2$ parameters):

$$\boldsymbol{S}^* = \begin{bmatrix} S_1^*(t_1) & S_2^*(t_1) \dots S_n^*(t_1) \\ \vdots & \vdots \quad \vdots \\ S_1^*(t_i) & S_2^*(t_i) \dots S_n^*(t_i) \\ \vdots & \vdots \quad \vdots \\ S_1^*(t_m) & S_2^*(t_m) \dots S_n^*(t_m) \end{bmatrix} = \begin{bmatrix} S_1^*(t_1) & S_2^*(t_1) \\ \vdots & \vdots \\ S_1^*(t_i) & S_2^*(t_i) \\ \vdots & \vdots \\ S_1^*(t_m) & S_2^*(t_m) \end{bmatrix} = \begin{bmatrix} x_1 t_1 & x_2 \\ \vdots & \vdots \\ x_1 t_i & x_2 \\ \vdots & \vdots \\ x_1 t_m & x_2 \end{bmatrix} \qquad \textbf{(3. 51)}$$

Let us notice that all the coefficients defining $\boldsymbol{x}$ have to be chosen in order to calculate (and compare) the reduced sensitivity coefficients: contrary to the sensitivity coefficients of a linear model, they do depend on the value of the parameter vector x. That is why a 'nominal' value for this vector is used for this calculation, that is a value that is a priori expected to be close to its exact value in a parameter estimation problem.

3.1.1. Graphical analysis of reduced sensitivity coefficients

As said before, when nominal values of the parameters have been chosen, it could be very instructive to plot all the reduced sensitivity coefficients composing each column of $\boldsymbol{S}^*$ in the same graph in order to 'visually' detect some future ill-conditioning of matrices $\boldsymbol{S}^{*t}\boldsymbol{S}^*$ and $\boldsymbol{S}^t\boldsymbol{S}$ due to several factors:

- One or more columns of $\boldsymbol{S}^*$ have low values (in absolute value) with respect to both the other ones and to the noise level σ_ε, indicating poor sensitivities of the model to some parameters.

- Two or more column are linearly dependent, indicating correlations between some parameters that will prevent their simultaneous identification. The simplest dependence to check is the proportionality between two coefficients (see ***Figure 6*** and ***Figure 7*** for favorable and unfavorable situations). Let us note that this linear dependence has to concern the whole time interval [t_{min}, t_{max}] in order to imply an ill-conditioning of the inversion.

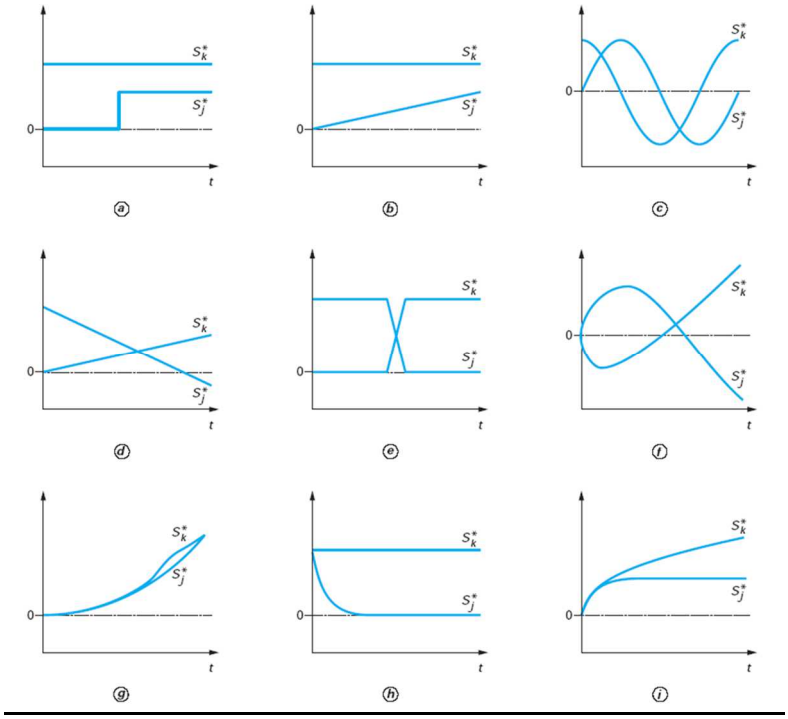

Figure 6 : some situations where reduced sensitivity coefficients S^*_k and S^*_j are linearly independent

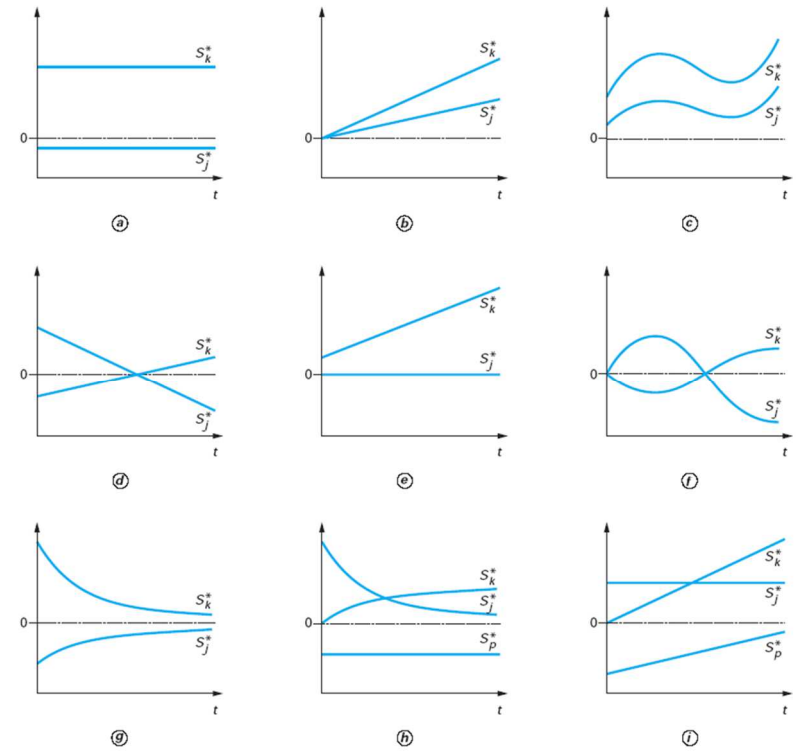

Figure 7 : some situations where reduced sensitivity coefficients S^*_k and S^*_j (and sometimes S^*_p) are linearly dependent, implying an ill-conditioning of the information matrix $S^{*t}S^*$ making it difficult, or impossible, to inverse it.

3.1.2. The relative covariance matrix, and relative confidence intervals

The *relative* variance-covariance matrix (size $n \times n$ for estimation of n parameters) is built the same way as the absolute variance-covariance matrix (see Eq. (3.36) and (3.39)) but the amplification matrix (inverse of the information matrix) is now built with the reduced sensitivity matrix $\boldsymbol{S^*}$ instead of $\boldsymbol{S}$:

$$\boldsymbol{C}^* = \sigma_\varepsilon^2 \left[\boldsymbol{S}^{*t} \boldsymbol{S}^* \right]^{-1} = \sigma_\varepsilon^2 \begin{bmatrix} \left(\frac{\sigma_1}{\hat{x}_{1,OLS}}\right)^2 & \frac{\mathrm{cov}(e_1,e_2)}{\hat{x}_{1,OLS}\hat{x}_{2,OLS}} & \cdots & \frac{\mathrm{cov}(e_1,e_n)}{\hat{x}_{1,OLS}\hat{x}_{n,OLS}} \\ & \left(\frac{\sigma_2}{\hat{x}_{2,OLS}}\right)^2 & & \frac{\mathrm{cov}(e_2,e_n)}{\hat{x}_{2,OLS}\hat{x}_{n,OLS}} \\ & & \ddots & \vdots \\ sym & & & \left(\frac{\sigma_n}{\hat{x}_{n,OLS}}\right)^2 \end{bmatrix} \quad \textbf{(3. 43)}$$

Then, the $\boldsymbol{C^*}$ matrix contains on its main diagonal the n *relative* variances associated to each component of the estimated vector $\hat{\boldsymbol{x}}_{OLS}$. The square root of the i[th] diagonal component of $\boldsymbol{C}^*$ is then the *relative* standard deviation (dimensionless) associated to the estimation $\hat{x}_{i,OLS}$ and can be expressed in %.

$$\sqrt{C_{ii}^*}(\%) = \frac{\sigma_i}{\hat{x}_{i,OLS}}, \text{ for } \quad i = 1,\ldots,n \quad \textbf{(3. 52)}$$

Last, the half width of relative confidence interval $CI_i^{1-\alpha}(\%)$, at a level of confidence of $100(1-\alpha)\%$, associated to the estimation $\hat{x}_{i,OLS}$ (and that was evaluated with 100 stochastic simulations in Section 3.5.1.) is now given by:

$$CI_i^{1-\alpha}(\%) = t_{1-\alpha/2}(m-n) \times \sqrt{C_{ii}^*}, \text{ for } \; i = 1,\ldots,n \quad \textbf{(3. 53)}$$

Finally, the result of the estimation process of the unknown exact parameter x_i^{exact} can be presented as the following, with the *relative* confidence interval:

' x_i^{exact} has 95% chance of being in the interval $\left[\hat{x}_{i,OLS} - CI_i^{0.95}(\%) \quad \hat{x}_{i,OLS} + CI_i^{0.95}(\%)\right]$',
or : ' $x_i^{exact} = \hat{x}_{i,OLS} \pm CI_i^{0.95}(\%)$ with 95% chance'

The elliptical *relative* confidence region corresponding to the scattering of estimations of ***Figure 3*** can also be computed with the *relative* information matrix $\boldsymbol{S}^{*t}\boldsymbol{S}^*$, the resulting equation expressed in the reduced coordinates $\boldsymbol{\delta x}^*$ is:

$$\begin{aligned} &\boldsymbol{\delta x}^{*t}.\boldsymbol{S}^{*t}\boldsymbol{S}^*.\boldsymbol{\delta x}^* = \Delta^2 \\ &\boldsymbol{\delta x}^* = \boldsymbol{\delta x}.diag(\hat{\boldsymbol{x}}_{OLS})^{-1} \end{aligned} \quad \textbf{(3. 44)}$$

'Absolute' and 'relative' ellipses are plotted respectively in ***Figure 9*** and ***Figure 9*** to show that they correctly predict the extent of the 100 estimations cloud.

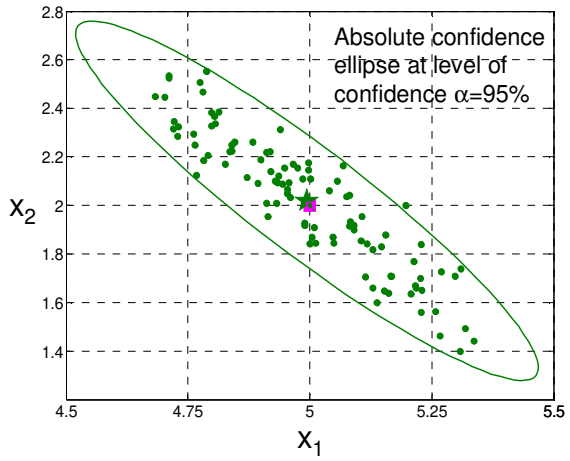

Figure 8 : 100 estimations cloud and 95% absolute confidence elliptical region around the cloud mean

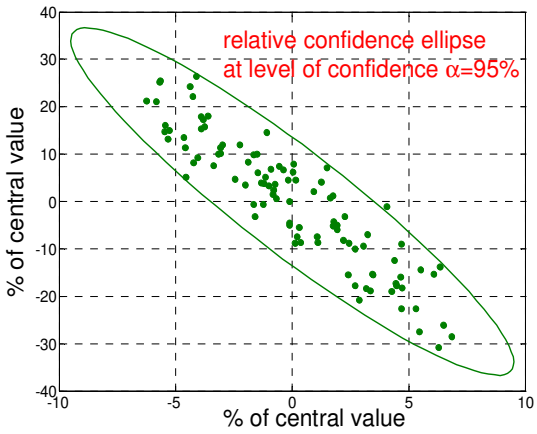

Figure 9 : 100 estimations cloud and 95% relative confidence elliptical region

3.2. Illustration, with a simple example, of different situations that modify the quality of estimation

In this section, the influence of some experimental parameters on the quality of estimation are illustrated for the example described in Table 2. This quality is visualized by the extent of the confidence region and some of the quantitative indicators presented above are also observed.

3.2.1. Influence of noise standard deviation σ_ε

The extension of the confidence region with respect to the standard deviation of noise measurement σ_ε, without changing its orientation, is shown in ***Figure 10***. This is conform to Eq. (3.45) giving the ellipse area proportional to the square of σ_ε.

3.2.2. Influence of number of measurements m (in the same time range)

The extension of the 95 % confidence region with respect to the number of measurements *m*, without changing its orientation, is shown in ***Figure 11***. This is conform to Eq. (3.45) giving the ellipse area inversely proportional to the square root of $\det(\boldsymbol{S}^t\boldsymbol{S})$, then area is inversely proportional to *m*. Then halving the noise level is better than doubling the number of measurements. This is quite obvious if one uses Eq. (3.36) and (3.39) to calculate the standard deviations and the correlation coefficient of the two OLS estimates $\hat{x}_1$ and $\hat{x}_2$:

$$\sigma_1 = \frac{\sigma}{s_t\sqrt{m}} \quad ; \quad \sigma_2 = \frac{\sigma}{\sqrt{m}}\left(1+\frac{\bar{t}^2}{s_t^2}\right)^{1/2} ; \qquad \rho_{12} = -\frac{1}{(1+s_t^2/\bar{t}^2)^{1/2}} \tag{3.55a}$$

where:

$$\bar{t} = \frac{1}{m}\sum_{i=1}^{m} t_i \qquad s_t^2 = \frac{1}{m}\sum_{i=1}^{m} (t_i - \bar{t})^2 \tag{3.55b}$$

One clearly sees that the standard deviation of each parameter is proportional to the standard deviation of the noise and inversely proportional to the square root of the number of measurements, if the average and the standard deviation (3.55b) of the times of measurement are not changed when their number is changed.

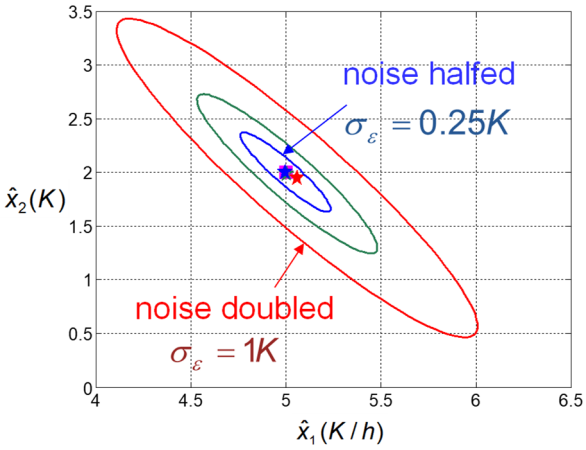

Figure 10 : Confidence ellipse extent as a function of noise level : in green (reference case) $\sigma_\varepsilon = 0.5K$ ***.***

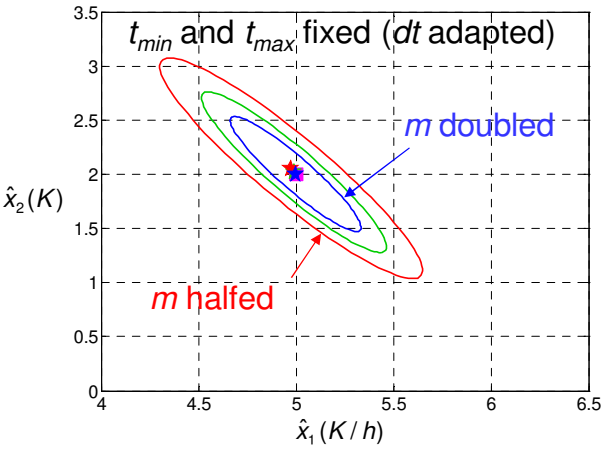

Figure 11 : Confidence ellipse extent as a function of the number of measurements m : in green (reference case) m=20.

3.2.3. Influence of time range (for m=20 measurements)

The last tested experimental factor to be varied is the time range, with a constant number of measurements (m=20), see ***Figure 12***. The results are presented in *Figure 13* and in ***Table 4***.

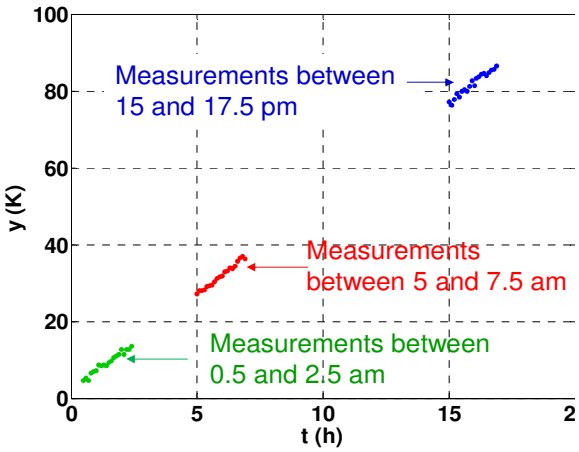

Figure 12: three time ranges are tested, giving three clouds of estimations on Figure 13.

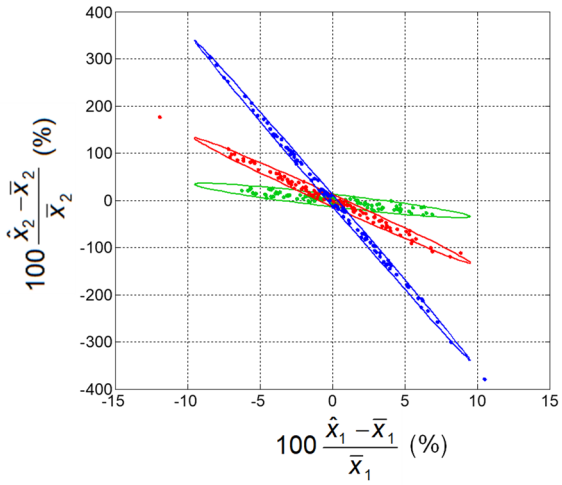

Figure 13: three clouds of estimations (corresponding to the three time ranges for the experiments) and relative 95% confidence ellipse.

Figure 13 shows that when experiments are done at 'high' time values, the confidence ellipse is growing, especially along the x_2 axis: the estimation of x_2 (intercept of the model $x_1 t + x_2$) is more and more inaccurate when the measurements are realized at high time values (far from $t = 0$). This is confirmed by the reduced sensitivity plots on ***Figure 14*** and ***Figure 15*** (see comments in legends).

Time range (h)	0.5 h -2.5 h	5 h -7.5 h	15 h -17.5 h
Central value $\bar{X}_1$ (K/h)	4.994 K/h	4.738 K/h	4.985 K/h
Absolute interval (K/h)	±0.3 K/h	±0.35 K/h	±0.35 K/h
Relative interval (%)	± 6 %	± 7 %	± 7 %
Central value $\bar{X}_2$ (K)	2.019	3.52	2.223
Absolute interval (K)	±0.5 K	±1 K/h	±5.3 K/h
Relative interval (%)	± 10 %	± 28 %	± 106 %

Table 4 : results of estimations for three different time ranges, with m=20 measurements.

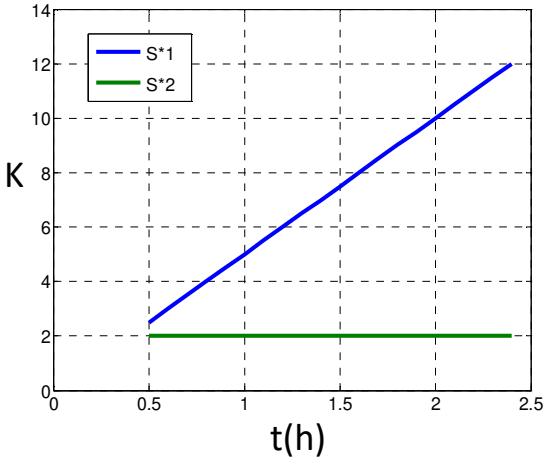

Figure 14 : first time range (between 0.5h and 2.5h). Reduced sensitivities are of same order of magnitude, sensitivity to x_1 is better than to x_2 and is increasing with time.

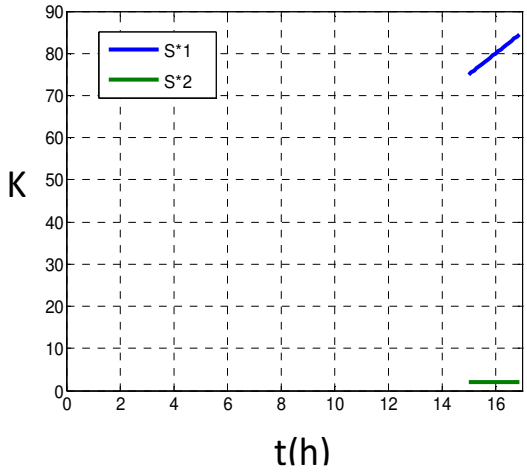

Figure 15 : third time range (between 15h and 17.5h). Reduced sensitivity to x_1 is far better than sensitivity to x_2 that appears now very close to zero comparing to S^*_1.

Last, ***Table 5*** shows multiple indicators confirming that increasing the beginning of the time range for the estimation of x_1 and x_2 is degrading the conditioning and then the quality of estimation.

Time range (h)	0.5 h -2.5 h	5 h -7.5 h	15 h -17.5 h
λ_{min} of $S^{*t}S^*$ ↑	1.03e1	6.5e-1 ↓	6.2e-2 ↓
λ_{max} of $S^{*t}S^*$ ↓	1.29e3	1.8e4 ↑	1.3e5 ↑
det($S^{*t}S^*$) ↑	1.34e4	1.18e4 ↓	8.0e3 ↓
Ellipse area ↓	3.52e-4	3.99e-4 ↑	5.9e-4 ↑
cond($S^{*t}S^*$) = λ_{max} / λ_{min} ↓	1.24e2	2.78e4 ↑↑	2.1e6 ↑↑
ρ_{12} ↓	-0.93	-0.995 ↑	-0.993 ↔

Table 5 : indicators values for the three experiments. In the first column, the arrows indicate if the indicator should be high (arrow up) or low (arrow down) to improve the conditioning.

3.3. Singular Value Decomposition of a matrix and condition number

3.3.1 Singular Value Decomposition (SVD) of a rectangular matrix

Any rectangular matrix (called $\boldsymbol{K}$ here) with real coefficients and dimension (m, n) with $m \geq n$, can be written under the form:

$$\boldsymbol{K} = \boldsymbol{U}\,\boldsymbol{W}\,\boldsymbol{V}^t, \text{ that is } \begin{bmatrix} & \\ & \boldsymbol{K} \\ & \end{bmatrix} = \begin{bmatrix} & \\ & \boldsymbol{U} \\ & \end{bmatrix} \begin{bmatrix} w_1 & & \boldsymbol{0} \\ & \ddots & \\ \boldsymbol{0} & & w_n \end{bmatrix} \begin{bmatrix} & \\ & \boldsymbol{V}^t \\ & \end{bmatrix} \quad (3.56)$$

Eq. (3.56) is sometimes called "lean" singular decomposition or "economical" SVD and involves:

- $\boldsymbol{U}$, an orthogonal matrix of dimensions (m, n) : its column vectors (the *left* singular vectors of $\boldsymbol{K}$) have a unit norm and are orthogonal by pairs : $\boldsymbol{U}^t\boldsymbol{U} = \boldsymbol{I}_n$, where $\boldsymbol{I}_n$ is the identity matrix of dimension n. Its columns are composed of the first n eigenvectors $\boldsymbol{U}_k$, ordered according to decreasing values of the eigenvalues of matrix $\boldsymbol{K}\,\boldsymbol{K}^t$. Let us note that, in the general case, $\boldsymbol{U}\boldsymbol{U}^t \neq \boldsymbol{I}_m$,

- $\boldsymbol{V}$, a square orthogonal matrix of dimensions (n, n), : $\boldsymbol{V}\,\boldsymbol{V}^t = \boldsymbol{V}^t\boldsymbol{V} = \boldsymbol{I}_n$. Its column vectors (the *right* singular vectors of $\boldsymbol{K}$), are the n eigenvectors $\boldsymbol{V}_k$, ordered according to decreasing eigenvalues, of matrix $\boldsymbol{K}^t\boldsymbol{K}$,

- $\boldsymbol{W}$, a square diagonal matrix of dimensions (n x n), that contains the n so-called *singular* values of matrix $\boldsymbol{K}$, ordered according to decreasing values : $w_1 \geq w_2 \geq \cdots \geq w_n$. The singular values of matrix $\boldsymbol{K}$ are defined as the square roots of the eigenvalues of matrix $\boldsymbol{K}^t\boldsymbol{K}$. If matrix $\boldsymbol{K}$ is square and positive-definite, eigenvalues and singular values of $\boldsymbol{K}$ are the same.

Another SVD form called "Full Singular Value Decomposition" is available for matrix $\boldsymbol{K}$. In this equivalent definition, both matrices $\boldsymbol{U}$ and $\boldsymbol{W}$ are changed: the matrix replacing $\boldsymbol{U}$ is now square (size m x m) and the matrix replacing $\boldsymbol{W}$ is now diagonal but non square (size m x n). In the case $m \geq n$, this can be written:

$$\boldsymbol{K} = \boldsymbol{U}_0\,\boldsymbol{W}_0\,\boldsymbol{V}^t \quad \text{with} \quad \boldsymbol{U}_0 = \begin{bmatrix} \boldsymbol{U} & \boldsymbol{U}_{comp} \end{bmatrix};\ \boldsymbol{W}_0 = \begin{bmatrix} \boldsymbol{W} \\ \boldsymbol{0}_{(m-n)\ \mathrm{x}\ n} \end{bmatrix} \quad \text{and} \quad \dim(\boldsymbol{U}_{comp}) = m\ x\ (m - n) \quad (3.57a)$$

or:

$$\begin{bmatrix} \\ \boldsymbol{K} \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \boldsymbol{U} \qquad \boldsymbol{U}_{comp} \\ \\ \end{bmatrix} \begin{bmatrix} w_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & w_n \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} \\ \boldsymbol{V}^t \\ \\ \end{bmatrix} \qquad (3.57b)$$

Matrix $\boldsymbol{U}_{comp}$ is composed of the (m - n) left singular column vectors not present in $\boldsymbol{U}$. So, the concanated matrix $\boldsymbol{U}_0$ verifies now:

$$\boldsymbol{U}_0^t \boldsymbol{U}_0 = \boldsymbol{U}_0 \boldsymbol{U}_0^t = \boldsymbol{U}\boldsymbol{U}^t + \boldsymbol{U}_{comp}\boldsymbol{U}_{comp}^t = \boldsymbol{I}_m \qquad (3.58)$$

This singular value decomposition (3.55b) can be implemented for any matrix $\boldsymbol{K}$, with real value coefficients, for $m \geq n$.

3.3.2 Interest of the Singular Value Decomposition in linear parameter estimation

We have seen above that if all the n parameters in a parameter vector $\boldsymbol{x}$ are sought for a linear model $\boldsymbol{y}_{mo}(\boldsymbol{x}) = \boldsymbol{S}\,\boldsymbol{x}$, where m noised measurements $\boldsymbol{y} = \boldsymbol{S}\,\boldsymbol{x} + \boldsymbol{\varepsilon}$ are available, and if noised $\boldsymbol{\varepsilon}$ is i.i.d., that is $\mathrm{cov}(\boldsymbol{\varepsilon}) = \sigma_\varepsilon^2\, \boldsymbol{I}_m$, its OLS estimator can be written:

$$\hat{\boldsymbol{x}}_{OLS} = \left(\boldsymbol{S}^t \boldsymbol{S}\right)^{-1} \boldsymbol{S}^t y \quad \text{with} \quad \mathrm{E}(\boldsymbol{\varepsilon}) = \mathbf{0} \quad \text{and} \quad \mathrm{cov}(\hat{\boldsymbol{x}}_{OLS}) = \sigma_\varepsilon^2 \left(\boldsymbol{S}^t \boldsymbol{S}\right)^{-1} \qquad (3.59)$$

The potential difficulty in its estimation may stem from the possible ill-conditioning of the square information matrix $\boldsymbol{S}^t \boldsymbol{S}$ whose inversion makes the standard deviations of its different parameters $\hat{x}_j$ become very large with respect to their exact value, see Eq. (3.51). So, a normalized criterion can be built in order to assess the quality of the estimation of the n parameters.

This can be made through normalization of all the parameters x_j present in parameter vector $\boldsymbol{x}$ by a a nominal value $x_{nom,\,j}$ (which, in parameter estimation results from a prior knowledge of the order of magnitude of the corresponding parameter) to get a reduced parameter vector $\boldsymbol{x}^{red}$ without any physical unit:

$$\boldsymbol{x}^{red} = \boldsymbol{R}_{nom}^{-1}\, \boldsymbol{x} = \begin{bmatrix} x_1 / x_1^{nom} \\ x_2 / x_2^{nom} \\ \vdots \\ x_n / x_n^{nom} \end{bmatrix} \quad \text{with} \quad \boldsymbol{R}_{nom} = \mathrm{diag}(\boldsymbol{x}^{red}) = \begin{bmatrix} x_1^{nom} & 0 & \cdots & 0 \\ 0 & x_2^{nom} & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & x_n^{nom} \end{bmatrix} \qquad (3.60)$$

So the output of the linear model can be expressed in terms of the reduced sensitivity matrix $\boldsymbol{S}^*$ already presented in Section 3.1 and of the reduced (or scaled) parameter vector $\boldsymbol{x}^{red}$:

$$\boldsymbol{y}_{mo} = \boldsymbol{S}\ \boldsymbol{x} = \boldsymbol{S}\ \boldsymbol{R}_{nom}\ \boldsymbol{R}_{nom}^{-1}\ \boldsymbol{x} = \boldsymbol{S}^*\ \boldsymbol{x}^{red} \qquad \text{since} \quad \boldsymbol{S}^* = \boldsymbol{S}\ \boldsymbol{R}_{nom} \tag{3.61}$$

OLS estimation of this reduced parameter vector becomes, using Eq. (3.23):

$$\begin{aligned} \hat{\boldsymbol{x}}^{red} &= \boldsymbol{R}_{nom}^{-1}\ \hat{\boldsymbol{x}}_{OLS} = \boldsymbol{R}_{nom}^{-1}\ (\boldsymbol{S}^t\ \boldsymbol{S})^{-1}\ \boldsymbol{S}^t\ \boldsymbol{y} = \boldsymbol{R}_{nom}^{-1}\ (\boldsymbol{R}_{nom}^{-1}\ \boldsymbol{S}^{*t}\ \boldsymbol{S}^*\ \boldsymbol{R}_{nom}^{-1})^{-1}\ \boldsymbol{R}_{nom}^{-1}\ \boldsymbol{S}^{*t}\ \boldsymbol{y} \\ &= \boldsymbol{R}_{nom}^{-1}\ \boldsymbol{R}_{nom}\ (\boldsymbol{S}^{*t}\ \boldsymbol{S}^*)^{-1}\ \boldsymbol{R}_{nom}\ \boldsymbol{R}_{nom}^{-1}\ \boldsymbol{S}^{*t}\ \boldsymbol{y} = (\boldsymbol{S}^{*t}\ \boldsymbol{S}^*)^{-1}\ \boldsymbol{S}^{*t}\ \boldsymbol{y} \end{aligned} \tag{3.62}$$

And its covariance can be easily derived:

$$\text{cov}\,(\hat{\boldsymbol{x}}^{red}) = \sigma_\varepsilon^2\ \left(\boldsymbol{S}^{*t}\ \boldsymbol{S}^*\right)^{-1} \tag{3.63}$$

It is the same equation as Eq. (3.51). Since all the components of the reduced sensitivity matrix have the same unit as signal $\boldsymbol{y}$, and because $\boldsymbol{x}^{red}$ is dimensionless, it is possible to consider $\boldsymbol{S}^*$ as a linear application from a vector space of dimension n into a vector space of dimension m. That was not possible for the original parameter column-vector $\boldsymbol{x}$, which did not belong to a true mathematical vector space, because its coefficients had not the same units.

So, it is now possible to write the lean SVD of $\boldsymbol{S}^*$, which uses the notion of Euclidian norm of different true vectors, see Eq. (3.56):

$$\boldsymbol{S}^* = \boldsymbol{U}\ \boldsymbol{W}\ \boldsymbol{V}^t \tag{3.64}$$

One can also calculate the amplification coefficient of the relative error k_r, see Eq. (1.7) in Lecture 1 of the same series:

$$k_r\ (\boldsymbol{\varepsilon}) = \frac{\left\| \boldsymbol{e}_{x\,red} \right\| \,/\, \left\| \boldsymbol{x}_{exact}^{red} \right\|}{\left\| \boldsymbol{\varepsilon} \right\| \,/\, \left\| \boldsymbol{y}_{mo}\left(\boldsymbol{x}_{exact}^{red}\right) \right\|} \quad \text{with} \quad \boldsymbol{e}_{x\,red} = \hat{\boldsymbol{x}}^{red} - \boldsymbol{x}_{exact}^{red} \tag{3.65}$$

Using the properties of matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ described above, as well as Eq. (3.62), one can show:

$$\left.\begin{aligned} \left\| \boldsymbol{e}_{x\,red} \right\| &= \left\| \boldsymbol{V}\ \boldsymbol{W}^{-1}\ \boldsymbol{U}^t\ \boldsymbol{\varepsilon} \right\| \le \left\| \boldsymbol{V}\ \boldsymbol{W}^{-1}\ \boldsymbol{U}^t \right\|\ \left\| \boldsymbol{\varepsilon} \right\| \\ \left\| \boldsymbol{y}_{mo}\left(\boldsymbol{x}_{exact}^{red}\right) \right\| &= \left\| \boldsymbol{S}^*\ \boldsymbol{x}^{red} \right\| \le \left\| \boldsymbol{U}\ \boldsymbol{W}\ \boldsymbol{V}^t \right\|\ \left\| \boldsymbol{x}^{red} \right\| \end{aligned}\right\} \Rightarrow k_r\ (\boldsymbol{\varepsilon}) \le \left\| \boldsymbol{V}\ \boldsymbol{W}^{-1}\ \boldsymbol{U}^t \right\|\ \left\| \left\| \boldsymbol{U}\ \boldsymbol{W}\ \boldsymbol{V}^t \right\| \right\| \tag{3.66}$$

One can recognize in the right-hand term of the last inequality (3.66) the product of norms of two matrices. The second matrix is simply the SVD form of the reduced sensitivity matrix $\boldsymbol{S}^*$ while the first one is just the pseudo inverse of $\boldsymbol{S}^*$, which is noted $\boldsymbol{S}^{*+}$ here.

Let us remind that the norm of any matrix $\boldsymbol{K}$ (which has not to be square) is defined by:

$$\left\| \boldsymbol{K} \right\|^2 = \underset{\left\| \boldsymbol{z} \right\|=1}{\text{Max}} \left(\boldsymbol{z}^t \boldsymbol{K}^t \boldsymbol{K} \boldsymbol{z} \right) = w_1^2(\boldsymbol{K}) \tag{3.67}$$

where $w_1(\boldsymbol{K})$ is the largest singular value of $\boldsymbol{K}$. This singular value is simply the square root of the largest (positive) value of the reduced information matrix $\lambda_1(\boldsymbol{S}^{*t}\boldsymbol{S}^*)$, see Eq. (3.46). One can show that:

$$\left\| \boldsymbol{S}^* \right\| = w_1(\boldsymbol{S}^*) \text{ and } \quad \left\| \boldsymbol{S}^{*+} \right\| = w_1(\boldsymbol{S}^{*+}) = \frac{1}{w_n(\boldsymbol{S}^*)} \tag{3.68}$$

So, it can be shown, using Eq. (3.65), (3.66) and (3.68) that the maximum value of the amplification coefficient of the relative error k_r, that is the criterion that assesses the ill-posed character of the OLS parameter estimation problem is equal to the condition number, noted cond (.) here, of the reduced sensitivity matrix:

$$k_r\ (\boldsymbol{\varepsilon}) \leq \text{cond}(\boldsymbol{S}^*) = \frac{w_1(\boldsymbol{S}^*)}{w_n(\boldsymbol{S}^*)} \tag{3.69}$$

So, this condition number, defined here with the Euclidian L_2 norm, is the pertinent criterion that can be used to measure the degree of ill-posedness of a linear parameter estimation problem, whatever the value of the noise level (for an i.i.d. noise). Since it requires the construction of the reduced sensitivity matrix, it depends on the nominal values of the parameters and can change strongly, depending on this choice, even if the problem is linear.

4. Illustration on a three parameters case

Here are the characteristics of the new model and the experimental parameters:

x_{1nom} [x_1]	10
x_{2nom} [x_2]	2
x_{3nom} [x_3]	3
Model structure $y_{mo}(t, \boldsymbol{x})$	$x_1 \sqrt{t} + x_2 erfc(t) + x_3 / \sqrt{t}$
Number of measurements m	100
Start of time range t_{min}	0.02
Time step dt	0.02
Noise standard deviation σ_ε	0.5

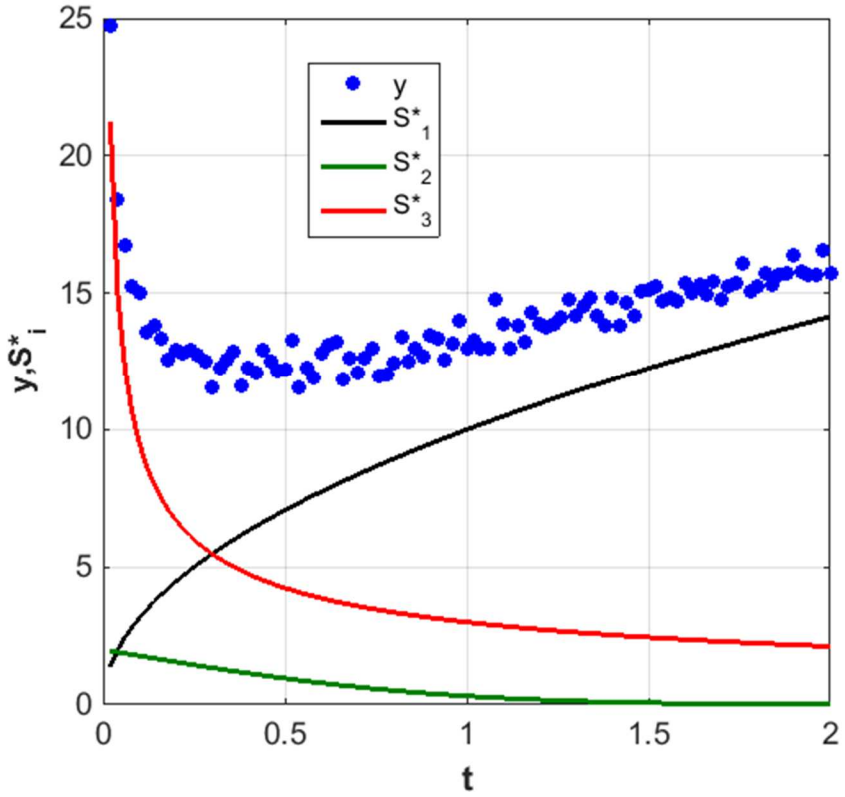

Figure 16 : **Three parameters example, measurements and reduced sensitivities (at nominal values of parameters).**

Figure 17 and ***Figure 18*** shows the 100 Monte Carlo estimations of the three parameters, perfectly centred on the exact values. The condition number of $\boldsymbol{S}^{*t}\,\boldsymbol{S}^{*}$ here is 1325.

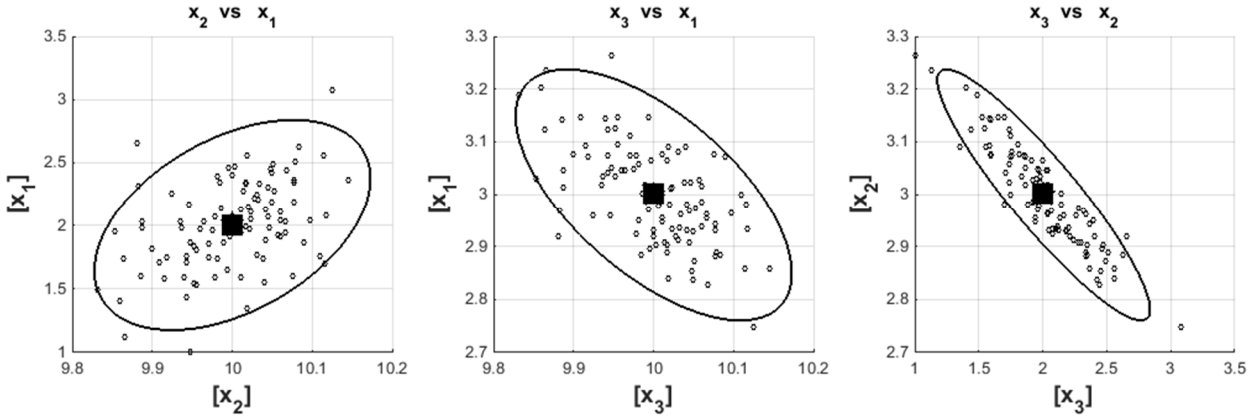

Figure 17 : Unbiaised estimation of the three parameters: the clouds are centered on the exact value (the black square). Axes are scaled with the parameters units

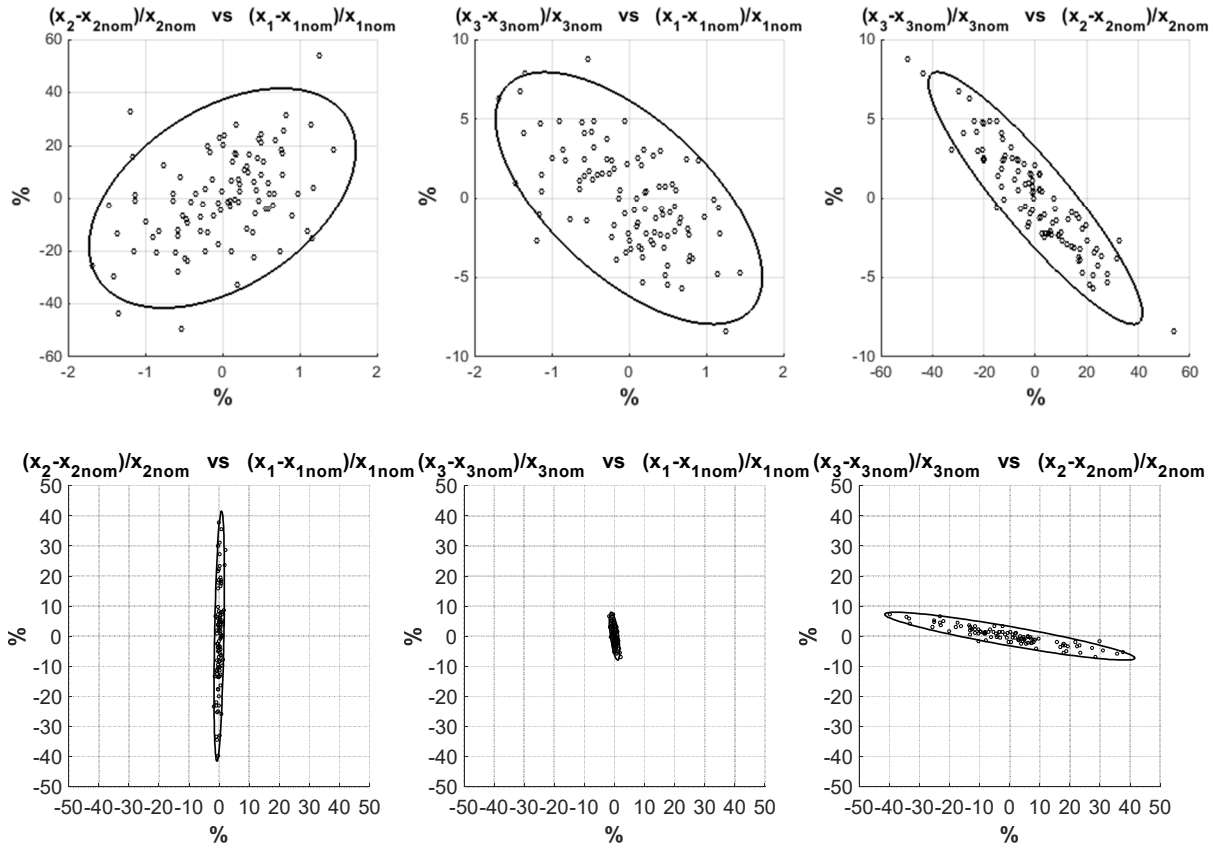

Figure 18 : Unbiaised estimation of the three parameters. Ellipses are the relative confidence region (at level 95%) of each parameter, in axes graduated in % of the nominal values. In the second line, axes are equally graduated between -50% and 50% to visually compare the relative variance associated to each estimated parameter (dispersion of points projected on each axe) and the correlation between errors (inclination of ellipses).

If x_1 is fixed to a wrong value (11 instead of 10, bias equal to +10%), then estimation of x_2 and x_3 is biased, see ***Figure 19*** (blue right plot). In that case, error due to fixed parameter (bias) is even higher than error due to noise measurement (variance). The condition number is better (227) for the simultaneous estimation of only 2 parameters (x_2 and x_3) but care has to be taken on the fixed value of x_1: this illustrates the 'bias-variance trade-off'.

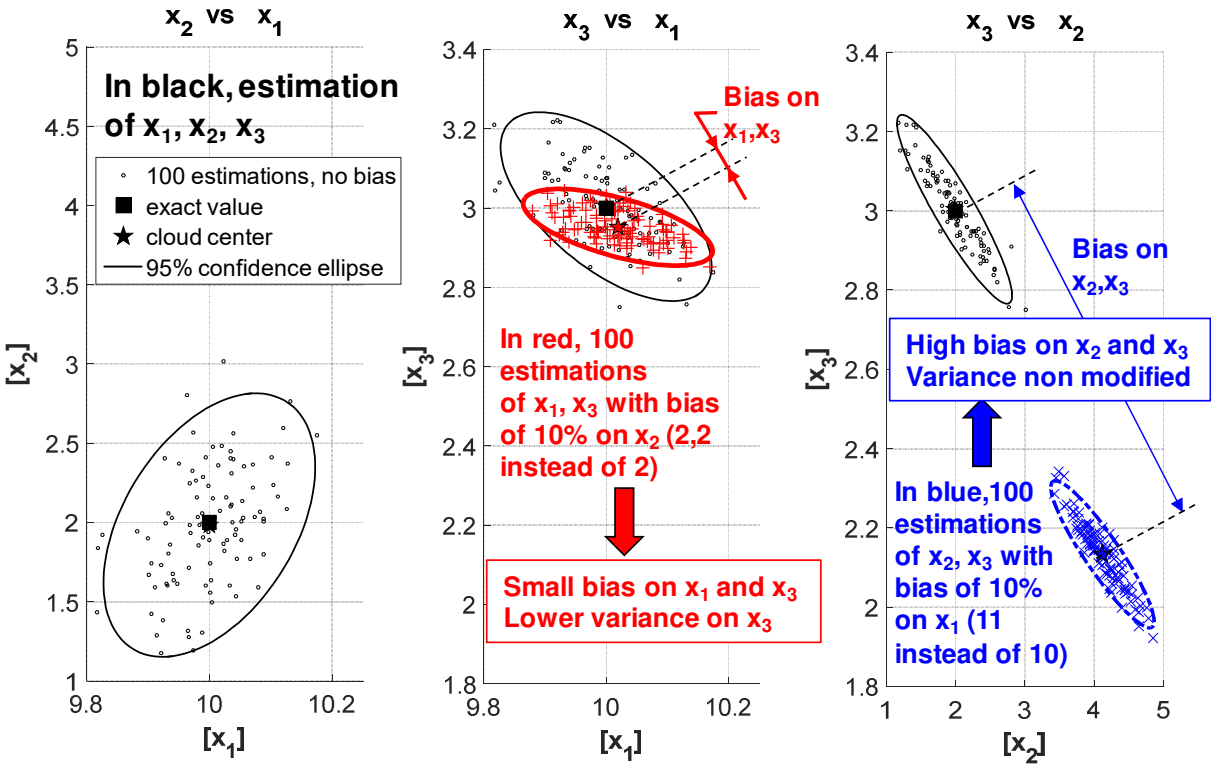

Figure 19*: *One parameter is blocked to a wrong ('biased') value, the two other are estimated (Monte Carlo run with 100 experiments). In black : no bias, same figure than Figure 17. In red (center plot), the parameter x_2 is blocked to a biased value (bias of +10%) and x_1 and x_3 are estimated and plotted in the x_3 vs x_1 plot. In blue (right plot), the parameter x_1 is blocked to a biased value (bias of +10%) and x_2 and x_3 are estimated and plotted in the x_3 vs x_2 plot. Exact values of (x_1, x_2, x_3) are (10, 2, 3). Centers of black, red and blue clouds are respectively (10.06, 1.998, 3.0003), (10.02, (2.2), 2.95) and ((11), 4.1, 2,1) where values between (.) are blocked values.

If x_2 is fixed to a wrong value (2.2 instead of 2, bias equal to +10%), then estimation of x_1 and x_3 is biased, see ***Figure 19*** (red center plot). But in that case, error due to fixed parameter (bias) is smaller than error due to noise measurement (variance). The condition number is small (equal to 9) for the simultaneous estimation of x_1 and x_3 and the amplification of bias (on x_2), given by Eq. (3.38) is here acceptable.

These behaviors can be related to the reduced sensitivities of ***Figure* 16**: the model is less sensitive to x_2 than x_1 during the chosen time range, then a bias on x_2 is less amplified than a bias on x_1. Last, according to Eq. (3.38), because of the inner product between S_r^t and S_c that amplifies the bias on fixed parameters e_c, one has interest to block parameters whose

sensitivity coefficient $\boldsymbol{S}_c$ is the most 'orthogonal' possible to the sensitivity coefficient of estimated parameters $\boldsymbol{S}_r^t$, or in other words, the least 'collinear', or the least 'similar'.

5. Conclusion

The example of a linear model with respect to its two parameters is rich enough to introduce many tools useful in the field of parameter estimation : the sensitivity coefficients that compose the sensitivity matrix are one of these tools. This matrix has to be inverted (or the corresponding linear system of normal equations has to be solved) in the estimation problem. The variance-covariance matrix (sometimes called more simply the covariance matrix) that helps to qualify the quality of the estimation (variance of each estimation, correlation between them, size of the confidence region if the stochastic law of the measurement noise is known), uses also these coefficients. In the non linear case, the problem is often solved by assuming a local linear behaviour of the objective function to be minimized (see lecture L7 of this series).

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