Lecture 1. Getting started with problematic inversions with three basic examples

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Abstract. Introduction to the inverse approach is made starting by simple examples (solution of a linear system of equations, with noised right-hand member, case of a slab, in steady state regime, with either heat flux or thermal conductivity estimation). The inverse terminology, the pitfalls of inversion (noise amplification effect), as well as the corresponding methodological approach are highlighted. The objective is not to solve these problems but to highlight the main crucial points in inverse measurement problems. Other lectures (L3 & L7 to L10) will be devoted to show how to solve them.

Introduction

Inverse problems are part of our daily practice, even if we do not know that they are inverse problems. We consider here a scientific field (heat transfer, mechanical or chemical engineering, physics...) where a quantitative model is available, that is a mathematical procedure which is able to simulate, with a good enough accuracy, the phenomena at stake. The inverse use of this model gives rise to an inverse problem. Instead of introducing the different notions associated to such problems, which will be progressively dealt with in the following lectures of this advanced school, we will present examples that correspond to the inverse use of a model, as well as the specific problems that appear concomitantly. These examples will correspond to *exact matching* between measurements (noted y or Y further on) and model outputs (noted y_{mo} or T or ΔT further on). The term "*exact matching"* means that inversion is made through solving an equation where both model outputs and measurements are equal, which is only possible when the number of unknowns is equal to the number of measurements. Consequently, the least square sum is not only minimum but equal to zero.

2. Example 1: square system of linear equations

Let us suppose that we have a linear model that allows to get m output values y_{mo1}, y_{mo2}, ..., y_{mom} for any values of the m input values x_1 , x_2 , ..., x_m . Note that we assume here that both numbers of input and output values are the same and that the output values are subscripted by the index "*mo*" to remind us that it is derived from a model. It is very convenient to use here column vectors to represent this linear relationship under the form:

$$\boldsymbol{y}_{mo} = \boldsymbol{S}\ \boldsymbol{x} \tag{1.1}$$

where $\boldsymbol{y}_{mo}$ and $\boldsymbol{x}$ are both (m, 1) matrices (column vectors) composed of the y_{mo}'s and of the x's values and $\boldsymbol{S}$ a square (m, m) matrix, which is called a « *sensitivity matrix* » in the inverse problem terminology.

In the direct problem input $\boldsymbol{x}$ is known and $\boldsymbol{y}_{mo}$, the output of the model, is calculated.

Let us consider the following example that corresponds to m = 2, with:

$$\boldsymbol{S} = \begin{bmatrix} 10 & -21 \\ 39 & -81 \end{bmatrix} \qquad \boldsymbol{x} = \boldsymbol{x}^{exact} = \begin{bmatrix} 3 \\ 1 \end{bmatrix} \ \Rightarrow \ \boldsymbol{y}_{mo} = \boldsymbol{S}\ \boldsymbol{x}^{exact} = \begin{bmatrix} 9 \\ 36 \end{bmatrix} \tag{1.2}$$

We have supposed here that, in the given problem, we know the exact value $\boldsymbol{x}^{exact}$ of the input vector $\boldsymbol{x}$.

Conversely, if $\boldsymbol{y}_{mo}$ is known, solution of system (1.2), or inversion of matrix **S**, provides the true value of the input:

$$\boldsymbol{x}^{exact} = \boldsymbol{S}^{-1}\boldsymbol{y}_{mo} \tag{1.3}$$

We have therefore solved the *inverse problem* using exact data $\boldsymbol{x}$.

Let us now assume that the output, that is the data, corresponds to some measurements of $\boldsymbol{y}_{mo}$ which are corrupted by an additive noise $\boldsymbol{\varepsilon} = \begin{bmatrix} 0.1 & -0.3 \end{bmatrix}^T$ (superscript T designates the transpose of a matrix). Each component of this noise is about 1% of each component of the exact output $\boldsymbol{y}_{mo}$:

$$\boldsymbol{y} = \boldsymbol{y}_{mo} + \boldsymbol{\varepsilon} = \begin{bmatrix} 9{,}1 \\ 35{,}7 \end{bmatrix} \tag{1.4}$$

The natural idea for retrieving an approximate solution of the inverse problem is to replace the exact model output $\boldsymbol{y}_{mo}$ by its measured value $\boldsymbol{y}$ in (1.4), or to solve linear system (1.1) $\boldsymbol{S}\ \boldsymbol{x} = \boldsymbol{y}$ with this noised right-hand member:

$$\begin{bmatrix} 10 & -21 \\ 39 & -81 \end{bmatrix} \boldsymbol{x} = \begin{bmatrix} 9.1 \\ 35.7 \end{bmatrix} \tag{1.5}$$

By inverting $\boldsymbol{S}$, it is found the value of the input vector as:

$$\hat{\boldsymbol{x}} = \boldsymbol{x}^{exact} + \boldsymbol{e}_{\boldsymbol{x}} = \begin{bmatrix} 1.40 \\ 0.233 \end{bmatrix} \tag{1.6}$$

In this relation, $\boldsymbol{e}_{\boldsymbol{x}}$ is the error on the $\hat{\boldsymbol{x}}$ estimate relatively to the exact value.

This means that an error of 53 % has been made for x_1 (1.40 instead of 3) and of 77% for x_2 (0.233 instead of 1). This phenomenon is illustrated in figure 1: considering two very different values of $\boldsymbol{x}$ from $\boldsymbol{x}^{exact}$, yields approximately to the same values for $\boldsymbol{y}$. Let us note that the determinant of matrix $\boldsymbol{S}$ is 9, thus nonzero value.

Let us note that, in this particular case, this solution $\hat{\boldsymbol{x}}$ of system $\boldsymbol{S}\ \boldsymbol{x} = \boldsymbol{y}$ is also an ordinary least squares solution of equation (1.1) with noisy data $\boldsymbol{y}$.

In order to analyse the possibly "pathological" character of the solution of $\boldsymbol{S}\ \boldsymbol{x} = \boldsymbol{y}$, two global criteria, the amplification coefficients of the absolute and relative errors, k_a and k_r, respectively, can be used. Their values are calculated using the Euclidian norm L_2:

$$k_a\ (\boldsymbol{\varepsilon}) = \frac{\|\boldsymbol{S}^{-1}\boldsymbol{\varepsilon}\|}{\|\boldsymbol{\varepsilon}\|} = \frac{\|\boldsymbol{e}_x\|}{\|\boldsymbol{\varepsilon}\|} = \frac{1.774}{0.316} = 5.61 \quad \text{with} \quad \|\boldsymbol{u}\| = \left(\sum_{j=1}^{2} u_j^2\right)^{1/2} \quad \text{and} \quad \boldsymbol{e}_x = \hat{\boldsymbol{x}} - \boldsymbol{x}^{exact}$$

$$\text{and} \qquad k_r\ (\boldsymbol{\varepsilon}) = \frac{\|\boldsymbol{S}^{-1}\boldsymbol{\varepsilon}\| / \|\boldsymbol{S}^{-1}\boldsymbol{y}_{mo}\|}{\|\boldsymbol{\varepsilon}\| / \|\boldsymbol{y}_{mo}\|} = \frac{\|\boldsymbol{e}_x\| / \|\boldsymbol{x}^{exact}\|}{\|\boldsymbol{\varepsilon}\| / \|\boldsymbol{y}_{mo}\|} = \frac{1.774 / 3.16}{0.316 / 37.11} = 65.8 \tag{1.7}$$

Figure 1 shows the amplification effect of the measurement noise in the above example.

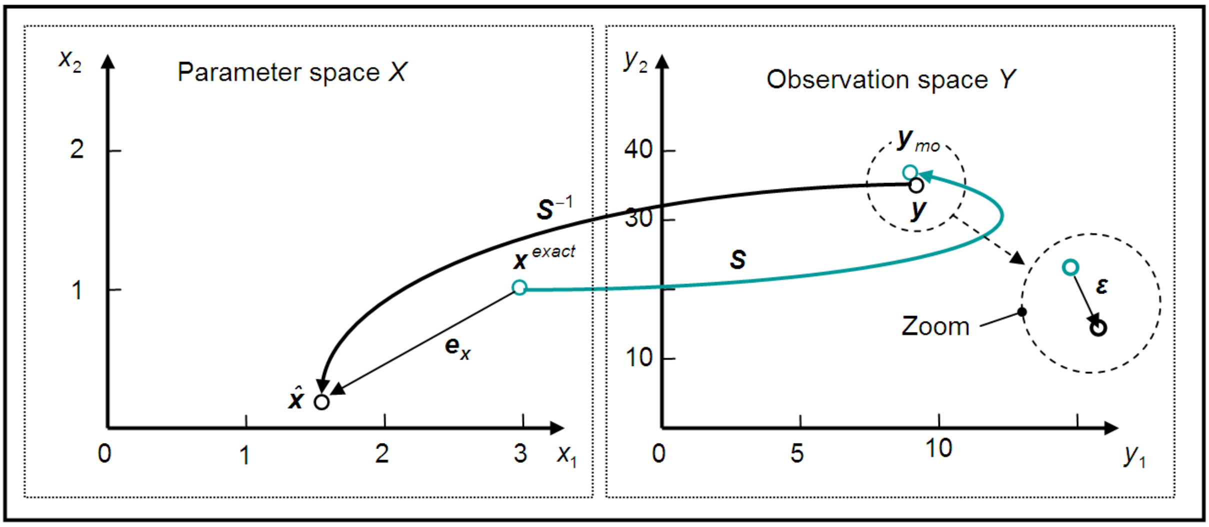


Figure 1 – Effect of the measurement error on parameter estimation through inverse mapping

Criteria (1.7), which measure the amplification effect of the measurement noise $\boldsymbol{\varepsilon}$ allow to quantify the unstable character of the solution. In practice, calculations of these criteria, which require a prior knowledge of the exact value $\boldsymbol{x}^{exact}$ of the unknown, is not possible. In order to analyse this stability problem, a condition number of matrix $\boldsymbol{S}$ shall be introduced.

Remark 1

In figure 1, the exact $\boldsymbol{x}^{exact}$ and estimated $\hat{\boldsymbol{x}}$ values of parameter vector $\boldsymbol{x}$ are shown in the left-hand side, in the two-dimension vector space of the *parameters* X (also called *input* space), where an orthonormal basis that corresponds to the components (x_1, x_2) of these vectors has been chosen. In the right-hand side, the output $\boldsymbol{y}_{mo}$ of the model, and measurements $\boldsymbol{y}$ are shown in the *observation* space Y where a corresponding orthonormal coordinates system (y_1, y_2) has been selected. The two norms present in the definition of k_a are the lengths of the vectors of the estimation error $\boldsymbol{e_x} = \hat{\boldsymbol{x}} - \boldsymbol{x}^{exact}$ and of the measurement noise $\boldsymbol{\varepsilon} = \boldsymbol{y} - \boldsymbol{y}_{mo}$. The other extra norms present in the definition of k_r are the lengths of the vectors representing the exact values $\boldsymbol{x}^{exact}$ (model input) and $\boldsymbol{y}_{mo}$ (model output).

Remark 2

The norms used in (1.7) are not necessarily the same in spaces X and Y. For example, coordinates (x_1, x_2) can be expressed in W.m^{-2}, if the unknowns are fluxes and coordinates (y_1, y_2) can be temperatures (Kelvin). However, in order to define such norms in each space, x_1 and x_2 should have the same units as well as y_1 and y_2. If it is not the case a scaling has to be implemented in both domains.

Remark 3

Coefficient k_r does not depend on the physical dimensions in X and Y: it explains the transformation of the noise/signal ratio $\|\boldsymbol{\varepsilon}\| / \|\boldsymbol{y}_{mo}\|$ into a relative estimation error $\|\boldsymbol{e_x}\| / \|\boldsymbol{x}^{exact}\|$. The inverse process, where one starts from the measurement domain Y to get a value of the input in the parameter domain X, corresponds to the inverse linear mapping $\boldsymbol{S}^{-1}$. Passage from Y space into X space is associated with a high amplification of the error: this problem is therefore ill-conditioned.

Remark 4

The high value $k_r(\boldsymbol{\varepsilon}) = 65.8$ of the relative amplification coefficient is not the highest possible here, things can become even worse. This maximum value of this coefficient is the condition number (see lecture L2) of $\boldsymbol{S}$, that can be reached for a specific value of noise $\boldsymbol{\varepsilon}$:

$$k_r(\boldsymbol{\varepsilon}) \leq \text{cond}(\boldsymbol{S}) = 958 \qquad (1.8)$$

3. Example 2: Different inverse problems for steady state 1D heat transfer through a wall

3.1 Case of exact sensor locations

The problem of one-dimension heat transfer through a homogeneous plane wall is considered. Exact temperature T_e at the rear face ($x = e$) is assumed to be known while a sensor located at a depth x_s inside the wall allows the measurement of a temperature y.

Using those two information and the knowledge of the exact values of the thermal conductivity λ as well as the thickness e of the wall, three quantities can be seek (see figure 2a):

- the temperature T_0, of the front face ($x = 0$),
- the internal temperature distribution,
- the heat flux density q that flows through the wall.

One temperature is *observed*:

$$T_s = \eta_1\,(x_s\,;\; q,\, T_0\,,\lambda) \tag{1.9}$$

However, its measurement y by the sensor is supposed to be corrupted by an additive *noise* ε of zero mean and of standard deviation σ:

$$y = \;T_s + \varepsilon \tag{1.10}$$

The observed temperature T_e can be considered as a particular output of the model η_1 of temperature distribution, at location $x = e$ with:

$$T_x = \eta_1\,(x;\, q,\, T_0\,,\lambda) \equiv T_0 - q\; x/\lambda \tag{1.11}$$

In the parameter estimation terminology:

- T_x is the dependent or output variable,
- x is the explanatory or independent variable,
- q, T_0 and λ are the parameters,
- and function η_1 (**.** ; **...**) is the model structure.

Parameters q, T_0 have a special status: they are also called *input* variables (or *solicitations*), because if they are both equal to zero, the wall temperature field is equal to zero. They correspond respectively to the right-hand members of the two boundary conditions of the second and first kinds for the heat equation whose model (1.11) is the solution of what is called a *direct problem*:

$$\frac{\mathrm{d}^2 T}{\mathrm{d}x^2} = 0 \qquad \text{with} \qquad -\lambda \left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{x=0} = q \qquad \text{and} \qquad \left.T\right|_{x=e} = T_e \tag{1.12}$$

We will see later on that this direct problem, whose solution (1.11) is the internal temperature field *in between* the two boundaries ($x = 0$ and $x = e$), is *a well-posed problem*.
The wall conductivity λ is called a *structural* parameter: if its value changes, the material system also changes.

As a consequence of model (1.11), the known value of the rear face temperature verifies:

$$T_e = \,T_0 - q\; e/\lambda \tag{1.13}$$

Elimination of q between the two equations (1.11) and (1.13) yields a second model η_2 for the output of the sensor located at x_s:

$$T_s = \eta_2\,(x_s/e,\, T_0,\, T_e) = \left(1 - \frac{x_s}{e}\right) T_0 + \frac{x_s}{e}\, T_e \tag{1.12}$$

Inversion of this second model is straightforward, replacing T_s by its measured value *y*:

$$\hat{T}_0 = \frac{1}{1 - x_s^*}\, y - \frac{x_s^*}{1 - x_s^*}\, T_e \qquad \text{with} \qquad x_s^* = x_s / e \tag{1.13}$$

The hat superscript $\hat{\alpha}$ over a α quantity is either an estimator of α (that is a random variable whose *realization* is an approximate value of the exact value of α) or an *estimated* (observed) value.

This allows the calculation of the *estimation* error for T_0, $e_{T0} = \hat{T}_0 - T_0$, which is a random variable proportional to ε, of zero mean (symbol E (.) is used here for the mathematical expectancy of a random variable), with its own standard deviation σ_0:

$$e_{T0} = \varepsilon\,/(1 - x_s^*) \qquad \Rightarrow \qquad \mathrm{E}\,(e_{T0}) = 0 \qquad \text{and} \qquad \sigma_0 = \sigma\,/(1 - x_s^*) \tag{1.14}$$

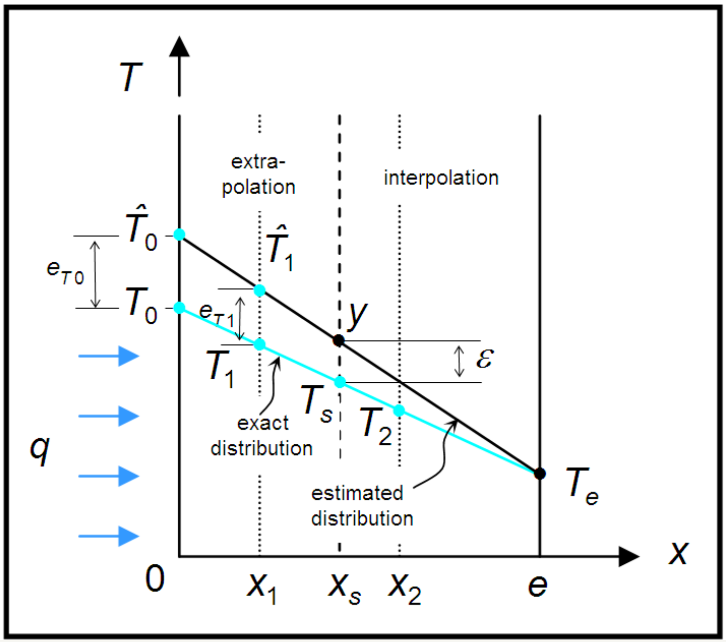


Figure 2a – Estimation of temperature/flux in a wall
Noised temperature measurement
Exact sensor location

A direct consequence of (1.14) is that estimation of T_0 is unbiased, $\mathrm{E}\,(\hat{T}_0) = T_0$, and its standard deviation $\sigma_{T0} = \sigma_0 = \sigma\,/(1 - x_s^*)$ is an increasing function of the relative depth x_s^* of the sensor inside the wall.

An obvious property of the linear extrapolation related to the straight line model (1.12) can be highlighted:

- error on T_0, measured by its standard deviation σ_0, becomes infinite if the sensor is located at $x = e$ (rear face). It reaches a minimal value for a measurement at the $x = 0$ face;

The estimated temperature distribution that derives from $\hat{T}_0$, also called *recalculated* distribution, is given by $\eta_2\,(x\,/\,e,\,\hat{T}_0,\,T_e)$:

$$T_{\text{recalce}}\,(x) = \eta_2\ (x^*,\,\hat{T}_0,\,T_e) = \hat{T}_x = \frac{1 - x^*}{1 - x_s^*}\ y + \frac{x^* - x_s^*}{1 - x_s^*}\ T_e \quad \text{with} \quad x^* = x\,/\,e \qquad (1.15)$$

The random error $e_{Tx} = \hat{T}_x - T_x$ for temperature T_x at any depth x, can be assessed by the same type of derivation, as well as its standard deviation σ_{Tx}:

$$e_{Tx} = K\,\varepsilon \qquad \Rightarrow \qquad \sigma_{Tx} = K\,\sigma \qquad \text{with} \quad K = \frac{1 - x^*}{1 - x_s^*} \qquad (1.16)$$

Two regions can be distinguished inside the wall (see figure 2a):

- the external layer, between x_s and e, that is the layer whose points x_2 are located in between boundaries where temperature boundary conditions (1rst kind) are either approximately (y) or exactly (T_e) known: going from y to $\hat{T}_x$ corresponds to a graphical *interpolation* with a reduction of the estimation error with respect to the noise ($K \leq 1$). The inverse temperature T_x estimation problem is *well-posed* in this region.

- layer in between 0 et x_c, with *external* points x_1, where the same operation consists in making an extrapolation. This corresponds therefore to an amplification of the measurement noise ($K \geq 1$) : the inverse problem of estimation of temperature T_x is *ill-posed* in this region.

Remark 5:

This partition of the space domain into two zones, an internal one located between limits where noised boundary conditions are available, and an external one, beyond these limits, leads to ill-posed problems as soon as the temperature field, or its derivative, is looked for in the external zone. This is true not only in this 1D steady state type of diffusion problem, but also in transient regime, whatever the space dimension (1 to 3D) of the geometrical domain.

An estimation $\hat{q}$ of heat flux q can be given here, as well as an assessment of its error e_q and of its standard deviation σ_q (a statistical quantification of what is called « absolute » error) and of its relative standard deviation $\sigma_q\ /q$ (a statistical quantification of what is called « absolute » error):

$$\hat{q} = \lambda \frac{y - T_e}{e - x_s} \Rightarrow e_q = \frac{\lambda}{e - x_s}\varepsilon \Rightarrow \sigma_q = \frac{\lambda}{e - x_s}\sigma \Rightarrow \sigma_q / q = \frac{1}{1 - x_s^*}\ \frac{1}{SNR}$$

(1.16a, b, c, d)

Let us note that the relative standard deviation of the estimated flux (1.16d) depends on the temperature signal/noise ratio $SNR = (T_0 - T_e)/\sigma$ and on the relative depth x_s^* of the sensor.

We consider a numerical example here. The wall is 0.2 m thick with a thermal conductivity equal to 1 W.m^{-1}.K^{-1}, with a 30°C temperature difference between its faces and a 0.3 °C value for the standard deviation of the temperature noise for a measurement in $x_s = 0.18$ m :

$$q = \lambda \frac{T_0 - T_e}{e} = 1\ \frac{30}{0.2} = 150\ \mathrm{W.m^{-2}} \qquad \text{and} \qquad SNR = (T_0 - T_e)/\sigma = 30/0.3 = 100 \qquad (1.17)$$

This yields a 10 % error (relative standard deviation) for $\hat{q}$ (see equation 1.16d). A mid-slab measurement ($x_s = 0.1$ m) would have given a 2 % error for this flux: the location of the measurement is therefore a key parameter.

3.2 Case of imprecise sensor locations and errors for parameters "assumed to be known"

Measurement noise is not the only cause of the estimation error: in numerous practical experimental situations, where a sensor has to be embedded in a material, the precise location of its active element (the hot junction of a thermocouple, for example) is not precisely known. So a different type of error has to be taken care of.

Let us assume that, in the above example, the objective is the same (estimation of the front face temperature T_0, of the inner temperature distribution T_x and of the heat flux *q*), but the sensor which was thought to be positioned at a *nominal* location x_s^{nom} is actually located at depth x_s, with:

$$x_s^{nom} = x_s + \delta \qquad (1.18)$$

see figure 2b. So, the noised output *y* of the sensor stems from the error δ in its depth, see figure 2b:

$$y = \eta_2\ (x_s / e, T_0,\ T_e) + \varepsilon = \eta_2\ (x_s^{nom} / e, T_0, T_e) + \varepsilon' \quad \text{with} \quad \varepsilon' = \delta\ (T_0 - T_e)/e + \varepsilon$$

(1.19)

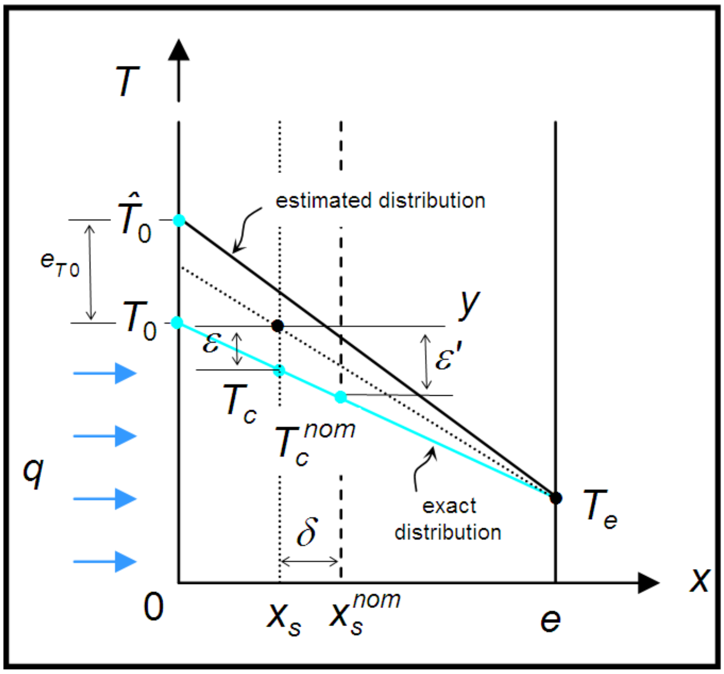


Figure 2b - Estimation of temperature/flux in a wall
Noised temperature measurement
Noised sensor location

If one assumes here that this position error δ is also a random variable, which is independent of temperature noise ε, of zero mean ($E(\delta) = 0$) and of standard deviation σ_{pos}, we find the same type of error as in section 3.1, simply replacing σ by a standard deviation σ':

$$\sigma'^2 = var(\varepsilon') = \sigma^2 + ((T_0 - T_e)/e)^2 \sigma_{pos}^2 = \sigma^2 \left(1 + SNR^2 / R_{pos}^2\right) \quad \text{with} \quad R_{pos} = e/\sigma_{pos} \tag{1.20}$$

Contribution in σ' of this position error may become important as well as in all the standard deviations of the subsequent estimation errors (σ_{T0}, σ_{Tx} an σ_q) considered in section 3.1, as soon as the signal/position error R_{pos} ratio becomes low with respect to the signal/temperature noise ratio SNR.

Let us go back to the numerical application (1.17), with the additional assumption of a position error of standard deviation 2 mm. These two ratios become:

$$R_{pos} = e/\sigma_{pos} = 200/2 = 100 \quad \text{and} \quad SNR = (T_c - T_e)/\sigma = 30/0.3 = 100 \tag{1.21}$$

So, in this case, the presence of the position error is equivalent to a 41 % increase of the temperature measurement noise ($\sigma' / \sigma = \sqrt{2}$ here). The consequence would be a 14.1 % error for the estimated flux (for $x_s = 0.18$ m).

This problem of *error in the dependent variable* in parameter estimation problems can be solved using *total least squares* [1, 2] or *Bayesian* estimation techniques. The interested reader can also refer to [3, 4, 5].

Let us note that this type of error belongs to a broader class of errors not directly linked to the measurement noise: it concerns the '*parameters supposed to be known*' (but not estimated generally) in a parameter estimation problem.

Such a problem arises if, in the preceding example, thermal conductivity λ is not precisely known. We can assume than a 'nominal' value λ^{nom} is known, but it differs from the exact value λ^{exact} by an error e_λ:

$$\lambda^{nom} = \lambda^{exact} + e_\lambda \tag{1.22}$$

If we refer to the derivations made in section 3.2, this conductivity error will not have any additional effect on the errors on T_0 and T_x. However, estimation (1.16) of flux q has to be revisited:

$$\hat{q} = \lambda^{nom} \frac{y - T_e}{e - x_s} = \frac{\lambda^{exact} + e_\lambda}{e - x_s} \left(T_s - T_e + \varepsilon\right) = \frac{\lambda^{exact} \left(T_s - T_e\right)}{e - x_s} \left(1 + \frac{e_\lambda}{\lambda^{exact}}\right) \left(1 + \frac{\varepsilon}{T_s - T_e}\right) \tag{1.23a}$$

In the case of a small relative error $e_\lambda / \lambda^{exact}$ for the conductivity and for large signal over noise ratio SNR, the preceding equation can be linearized, which yields the relative error e_q / q^{exact} for the estimated flux:

$$q^{exact} + e_q \approx q^{exact} \left(1 + \frac{e_\lambda}{\lambda^{exact}} + \frac{\varepsilon}{T_s - T_e}\right) \quad \Rightarrow \quad \frac{e_q}{q^{exact}} = \frac{e_\lambda}{\lambda^{exact}} + \frac{1}{SNR\,(1 - x_s^*)} \frac{\varepsilon}{\sigma} \tag{1.23b}$$

To go further on, it is necessary to assume that λ^{exact} is a random variable of mean equal to λ^{nom} and of standard deviation σ_λ. Taking the variance of equation (1.21b) yields:

$$\frac{\sigma_q}{q^{exact}} \approx \left(\frac{\sigma_\lambda^2}{\left(\lambda^{exact}\right)^2} + \frac{1}{SNR^2\ (1 - x_s^*)^2} \right)^{1/2} \tag{1.23c}$$

If we consider the case given by (1.17) in section 3.1, with $R_{pos} = 0$ (no position error, with $x_s = 0.18$ m), and an error of 10 % for the conductivity, that is e_λ of zero mean around

λ^{nom}=1 W.m^{-1}.K^{-1}, with a standard deviation σ_λ = 0.1 W.m^{-1}.K^{-1}) the error σ_q / q^{exact} becomes equal to 14.1 % instead of 10 % for an exact conductivity. This error caused by the supposed to be known conductivity can even become dominant error if the sensor is better located (x_s=0.10 m).

The interested reader can refer to lecture L3 in this school to gain a deeper insight onto the effects of the errors on the parameters that can not be estimated thanks to temperature measurements and that are 'supposed to be known' in thermophysical characterization problems.

4. Example 3: Inverse problem for unsteady state 1D heat transfer through a wall

4.1 Presentation of the direct problem:

We consider a semi-infinite 1D material with constant thermal properties (λ = 43 W.m^{-1}.K^{-1}, a = 1,18.10^{-5} m^2.s^{-1}) submitted to a heat flux depending on time. We can compute the temperature for several depths in the material (z = 0, 1, 1.5, 5, 10 mm) by a direct calculation (Finite Element Method, thermal quadrupoles, analytical solution).

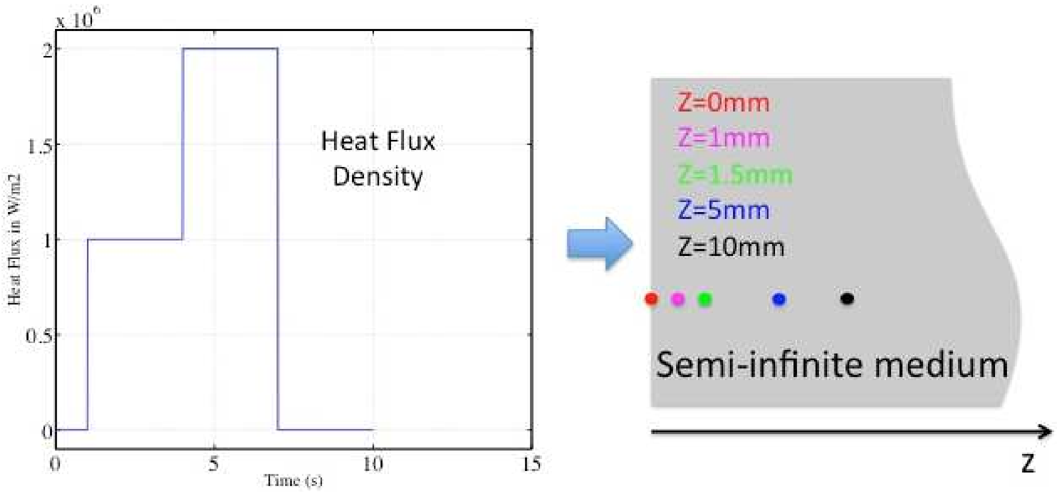


Figure 3a - Heat flux applied to the semi-infinite medium, for several temperature sensor positions

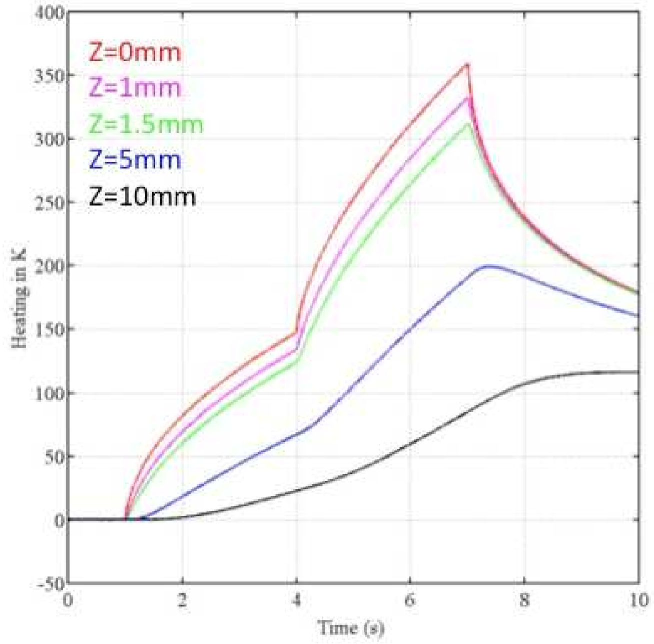
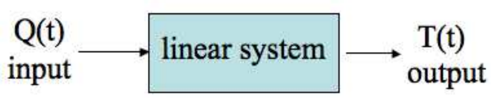


Figure 3b - Corresponding temperature responses for several positions

4.2 Deconvolution procedure, description:

The system is modelled by a linear system subjected to a prescribed heat flux $Q\,(z = 0,\ t)=Q\,(t)$ leading to the temperature rise $T\,(z,\ t)$. The linear system theory allows to write the temperature $T\,(z,\ t)$ as the convolution of $Q\,(t)$ with the impulse response $h(z,\ t)$ of the system, (i.e. the material temperature response to a delta function, that is a Dirac distribution, of power density applied to the surface). We assume that the initial temperature distribution in the material (at $t = 0$) is uniform.



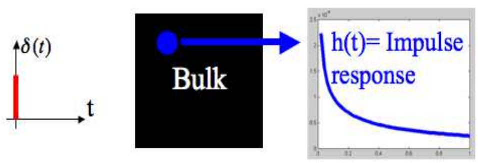


Figure 4 - Linear System

Figure 5 - Impulse response in the bulk

The temperature response T at time t and depth z is:

$$T\,(z,\,t) = T\,(z,\,t{=}0) + Q(t)^{*}\ h\,(t) = T\,(z,\,t{=}0)\ + \int_0^t Q(\tau)\ h\,(t-\tau)\ \mathrm{d}\tau \qquad (1.24)$$

The impulse response $h(z,\ t)$ of the system is the first time derivative of its step response $u(z,t)$. So, we approximate (1.24) by finite differences which leads to the expression of the temperature at each time step F in matrix form: where ***X*** is a triangular lower square matrix (of order F) assembled with the components $\Delta u(z,F) = u(z,F) - u(z,F-1)$ [6]:

$$\begin{bmatrix} \Delta T(z,1) \\ \Delta T(z,2) \\ \vdots \\ \vdots \\ \vdots \\ \Delta T(z,F) \end{bmatrix} = \begin{bmatrix} \Delta u(z,1) & 0 & \cdots & \cdots & \cdots & 0 \\ \Delta u(z,2) & \Delta u(z,1) & \cdots & \cdots & \cdots & 0 \\ \Delta u(z,3) & \Delta u(z,2) & \ddots & . & . & 0 \\ & & \ddots & \ddots & . & \vdots \\ & & . & \ddots & \ddots & \vdots \\ \Delta u(z,F) & \Delta u(z,F-1) & \cdots & \cdots & . & \Delta u(z,1) \end{bmatrix} \cdot \begin{bmatrix} Q(z=0,1) \\ Q(z=0,2) \\ \vdots \\ \vdots \\ \vdots \\ Q(z=0,F) \end{bmatrix} \tag{1.25}$$

$\Updownarrow$

$$\Delta \boldsymbol{T} = \boldsymbol{X}.\boldsymbol{Q} \tag{1.26}$$

In order to simulate experimental data, a noise is added to the calculated values as:

$$\boldsymbol{Y} = \Delta \boldsymbol{T} + \boldsymbol{\varepsilon} \tag{1.27}$$

Y is the experimental data, $\Delta \boldsymbol{T}$ is the output of model (1.26) and $\boldsymbol{\varepsilon}$ is a zero mean Gaussian noise with a constant standard deviation of 0.1 K. All three preceding quantities are written here in a column-vector form of size (F x 1). The deconvolution procedure consists in inverting Eq. (1.26), i.e. expressing surface heat fluxes with measured surface heating:

$$\boldsymbol{Q} = \boldsymbol{X}^{-1}\,\boldsymbol{Y} \tag{1.28}$$

In the case of the deconvolution from surface temperature (z = 0), the inverse problem is stable and the inversion of matrix ***X*** does not cause any problem (see Fig. 6a).

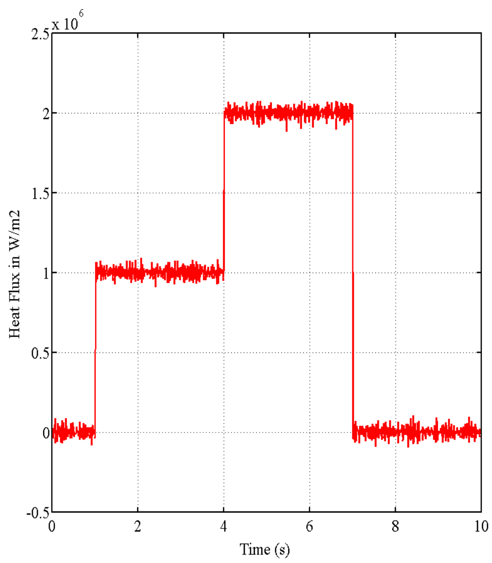


Figure 6a – Estimated heat flux, starting from noisy measurements at z = 0

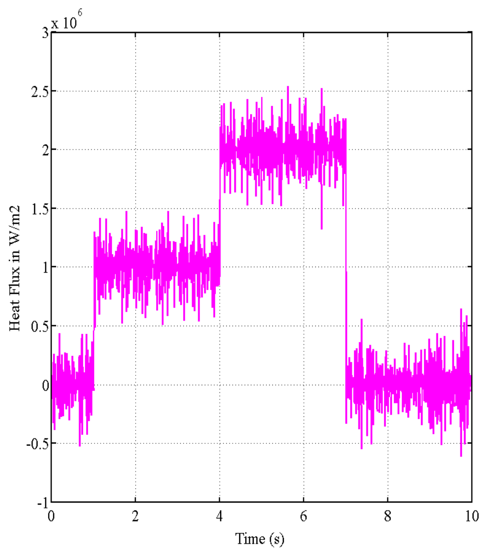


Figure 6b – Estimated heat flux, starting from noisy measurements at z = 1 mm

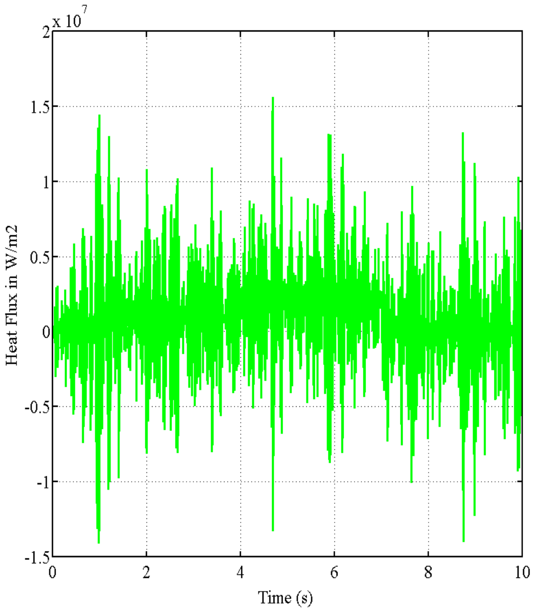


Figure 6c - Estimated heat flux, starting from noisy measurements at z = 1.5 mm

However, in the case of the deconvolution of the temperature measured by a buried sensor (*z* >0), the inverse problem becomes difficult to solve with a good precision because the conditioning of ***X*** gets wrong. The deeper the sensor is located, the more unstable the problem becomes. Clearly, it means that matrix ***X*** becomes difficult to invert because of the presence of very small coefficients (in absolute value) in its diagonal: the result does not respect the stability criterion because the noise in ***Y*** is amplified. In figure 6b the heat flux estimated with the temperature at *z* = 1 mm is plotted. The inversion is possible, but the estimated heat flux is very noisy. The heat flux estimated using the temperature at z = 1.5 mm (see Fig. 6c), is too noisy to be exploited: a regularization procedure is needed to find a more stable "quasi solution".

4.3 Regularization procedure

The solution vector $\hat{\boldsymbol{Q}}$, is very sensitive to measurement errors contained in the vector of temperature measurements ***Y***. In order to obtain a stable solution, we use a regularization procedure. For example, we can use the Tikhonov regularization method [7]. The regularized solution becomes:

$$\hat{\boldsymbol{Q}}_{reg} = (\boldsymbol{X}^t\boldsymbol{X} + \gamma \boldsymbol{R}^t\boldsymbol{R})^{-1}\boldsymbol{X}^t\boldsymbol{Y} \qquad (1.29)$$

- $\hat{\boldsymbol{Q}}_{reg}$ is the regularized solution (an estimation of ***Q***)
- γ is the regularization parameter
- ***R*** is the regularization *matrix* depending on the type of information that we want to impose.

In our case, we want a solution with a minimal norm of the solution (0 order) $\left\|\hat{Q}_{reg}\right\|$, so we will take $\boldsymbol{R} = \boldsymbol{I}_d$. An optimal value of the regularization parameter can be found using the "L curve" technique [8]. This type of representation allows to choose the best compromise - which is situated at the bending point of the 'L-curve' - between a stable solution, with a low value of $\left\| \boldsymbol{R}\hat{\boldsymbol{Q}}_{reg} \right\|$ and an accurate solution, with low residuals $\left\| \boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{Q}}_{reg} \right\|$. Another possibility is to use the "discrepancy principle", that is to choose γ such as the root mean square of the residuals gets the same order of magnitude as the measurement noise, that is $\left\| \boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{Q}}_{reg} \right\| \approx \sqrt{m}\,\sigma$, m being the number of measurement times.

Considering the case of the temperature deconvolution at z = 1.5mm (with noise):

- For low values of γ (Fig. 7a.), the solution is unstable with low residuals
- For strong values of γ (Fig. 7b.), the solution is stable but departs from the exact solution.
- For the best compromise of the γ value (Fig. 8) the heat flux is stable and can be used.

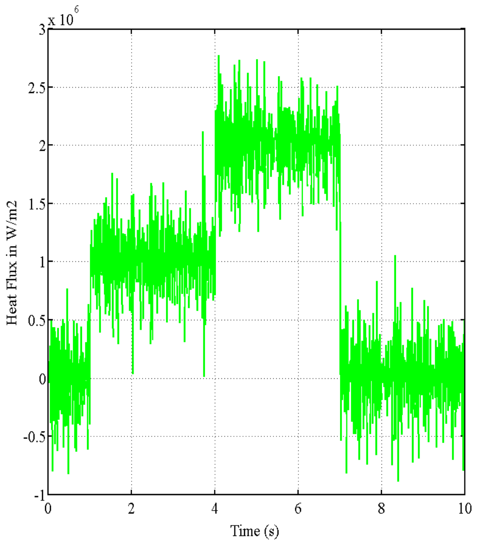


Figure 7a - Heat flux estimation with a low γ

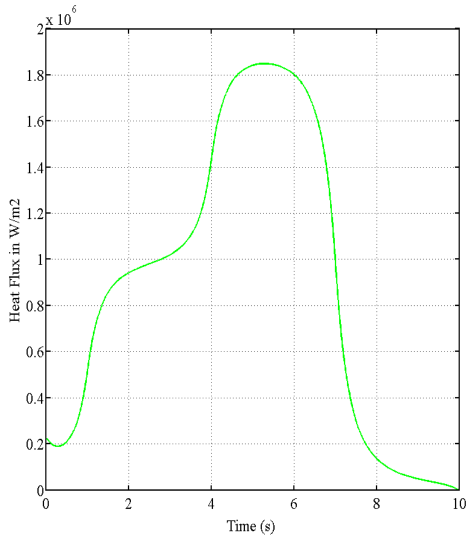


Figure 7b - Heat flux estimation with a large γ.

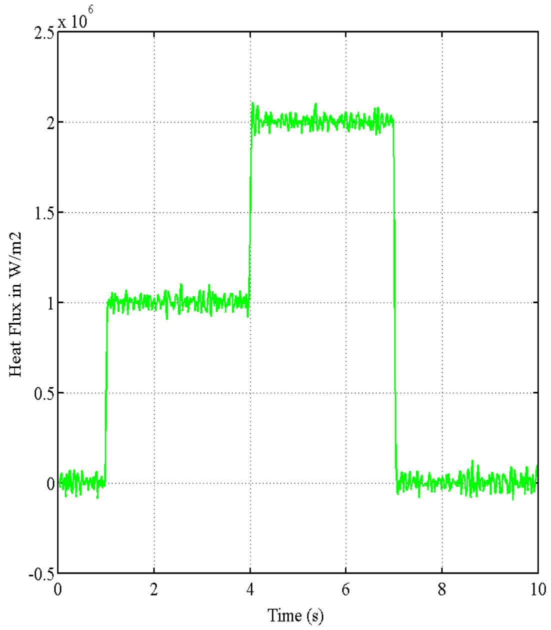


Figure 8 - Heat flux estimation with the best compromise of γ=5.10^{-13} K^2.m^4.W^{-2}.

One can note that the value γ depends on the level of the noise, the time resolution and the depth of the measurement.

5. Conclusions

The first example presented in this short lecture has been used to introduce the notion of an ill-posed problem: under certain circumstances, a small error in the right-hand member of a linear system of equations, which can correspond to noised measurements, can yield a very large error in the solution.

Study of the condition number of the corresponding matrix allows to assess the severity of this effect. The reader can refer here to the *Singular Value Decomposition* of this matrix, on which the condition number relies (see further lectures).

In the second example, the inverse 1D steady state input problem has been considered. The very important effect of the location of the temperature sensor on the estimation of the temperature distribution and of the flux through a wall has been highlighted. It has been shown that the temperature noise is not the unique source of error in the estimates.

Errors on the location of the sensor, as well as more generally the effect of the parameters 'supposed to be known', have also to be studied with great care in order to get reliable estimations.

In the third example, the temperature of an “in depth” measurement can be used for a heat flux estimation (an inverse problem of function estimation) depending on time. With a regularization procedure, a quasi solution can be obtained using a regularization parameter depending on the depth of the measurement, the noise, and the time resolution. One can note that the transfer function of the material can be modelled, computed or measured.

References

[1] S. Van Huffel and P. Lemmerling. 2002. *Total Least Squares and Errors-in-Variables Modeling: Analysis, Algorithms and Applications*. Dordrecht, The Netherlands: Kluwer, Academic Publishers.

[2] http://en.wikipedia.org/wiki/Total_least_squares

[3] Denis Maillet, Thomas Metzger, Sophie Didierjean, Integrating the error in the independent variable for optimal parameter estimation, Part I : Different estimation strategies on academic cases, e *Inverse Problems in Engineering*, vol. 11, n°3, juin 2003, pp. 175-186.

[4] Thomas Metzger, Sophie Didierjean, Denis Maillet, Integrating the error in the independent variable for optimal parameter estimation, Part II : Implementation to experimental estimation of the thermal dispersion coefficients in porous media with not precisely known thermocouple locations, *Inverse Problems in Engineering*, vol. 11, n°3, juin 2003, pp. 187-200.

[5] Thomas Metzger, Denis Maillet, Multisignal least squares: dispersion, bias, regularization, Chapter 17, *Thermal Measurements and Inverse Techniques*, Editors**:** Helcio R.B. Orlande; Olivier Fudym; Denis Maillet; Renato M. Cotta, Publisher: CRC Press, Taylor & Francis Group, Bocca Raton, USA, 779 pages, May 09, 2011, pp. 599-618.

[6] H.S. Carslaw, J.C. Jaeger, *Conduction of Heat in Solids*, Oxford University Press, 1959.

[7] A.N. Tikhonov, V.Y. Arsenin, *Solutions of Ill-Posed Problems*, V.H. Winston&Sons, Washington, D.C., 1977,

[8] P. Hansen, D. O'Leary, SIAM, The use of the L-curve in the regularization of discrete ill-posed problems, *J. Sci. Comput* 14 (1993) 1487-1503.