Lecture 1: Getting started with problematic inversions

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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 second hand member, case of a slab, in steady state regime, with either flux or 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 pinpoint the main crucial points in inverse measurement problems.
The last two lectures (L9 & L10) will be used to show how to solve them, with the help of the points studied in the lectures in between.

1. Introduction

Inverse problems are part of our daily practice, even if we do not know 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 precision, the phenomena at stake. The inverse use of this model gives rise to an inverse problem. Instead of introducing the different notions used for such problems, which will be progressively dealt with in the following lectures of this advanced school, we will present examples that correspond to an inverse use of a model, as well as the specific problems that appear concomitantly. These examples will correspond to *exact matching* between measurements and model outputs, with no use of a least square approach.

2. Example 1: square system of linear equations

Let us suppose we have a linear model that allows to get m output values $y_{mo1}, y_{mo2}, ..., y_{mom}$ for any values of the 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 only 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 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.

The example that will be studied here corresponds to the *m* = 2 case, 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 that is $\boldsymbol{y}_{mo}$ which 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 here. Each component of this noise represents less about 1 %, in absolute value, of the corresponding 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:

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

to recover an estimated value of the input

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

This means that an error of 53 % has been made for x_1 and of 77 % for x_2. This phenomenon is illustrated in figure 1: two far away values of $\boldsymbol{x}$, $\boldsymbol{x}^{exact}$ the exact value and $\hat{\boldsymbol{x}}$ the solution of (1.4), yield approximately the same values, within $\boldsymbol{\varepsilon}$, in the y_1 - y_2 plane. In this case, the determinant of matrix $\boldsymbol{S}$ is not very close to zero: its value is 9.

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 model (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, respectivelly can be introduced. Their values can be 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.

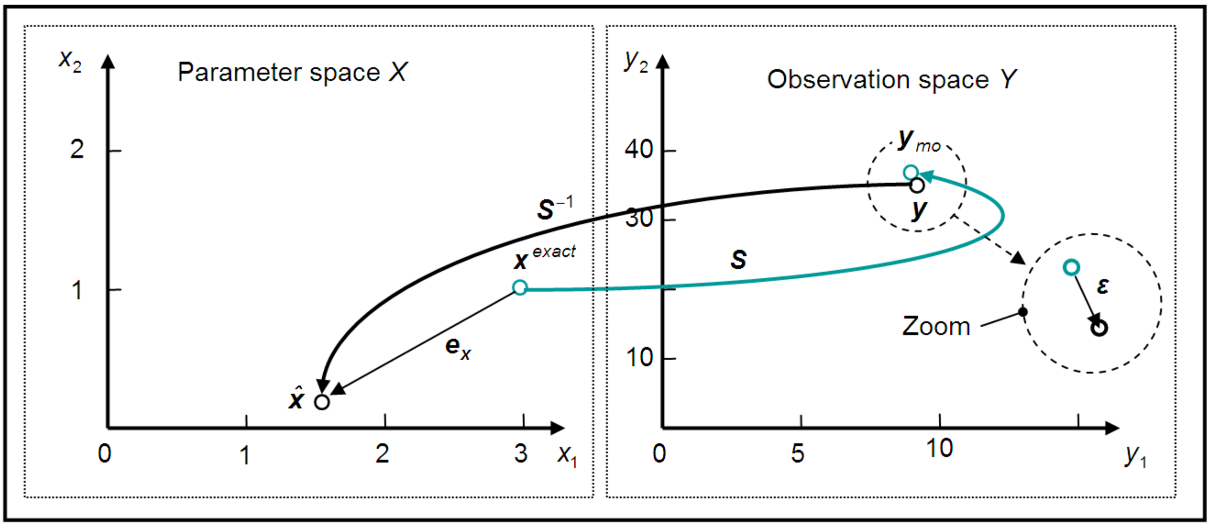

Figure 1 – Effect of the measurement error on parameter estimation through inverse mapping

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, calculation of these criteria, which requires a prior knowledge of the exact value $\boldsymbol{x}^{exact}$ of the unknown, is not possible. In order to analyze this stability problem, a condition number of matrix $\boldsymbol{S}$ shall be introduced, here for a square matrix.

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 unknows 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 $\|\boldsymbol{e_x}\| / \|\boldsymbol{x}^*\|$. The inverse process, where one starts from the measurement domain Y to get a value of the input in the parameters 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 1: Different inverse problems for steady state 1D heat transfer through a wall

3.1 Case of exact locations

The problem of one-dimension heat transfer through a homogeneous plane wall is considered now. Exact temperature T_e of the $x = e$ rear face 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 these two informations and the knowledge of the exact values of the conductivity λ and of the thickness *e* of the wall, three quantities can be looked for, see figure 2a:

- temperature T_0, of the other face (x = 0);
- the internal temperature distribution;
- flux *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:

$$y = T_e + \varepsilon \tag{1.10}$$

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

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

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 $\eta_1(\,.\,;\,...)$ 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:

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

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 in x_s :

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

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

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

The hat superscript $\hat{\alpha}$ over a α quantity designates here either an estimator of α, in the statistical sense, that is a random variable whose *realization* is an approximate value of the exact value of α, or its *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 :

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

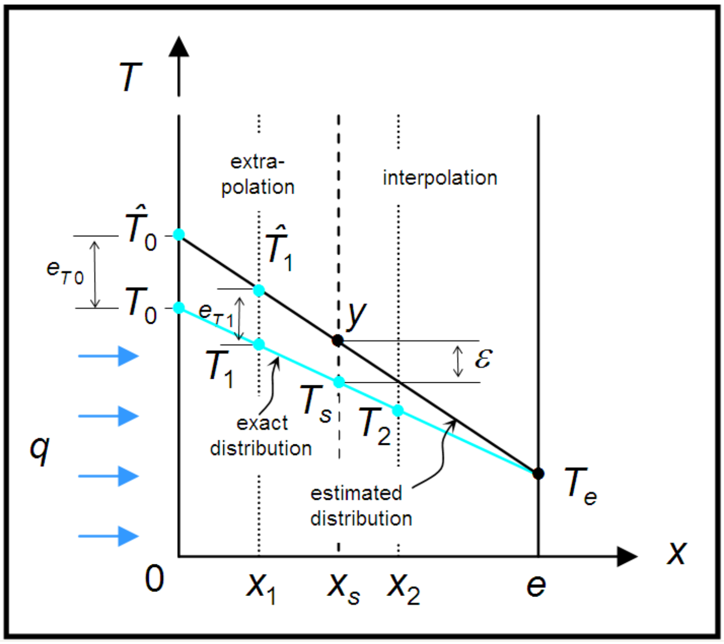

Figure 2a – Estimation of temperature/flux in a wall
Noised temperature measurement
Exact sensor location

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 the le $x = e$ 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 ($K \le 1$). 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 therfore to an amplification of the measurement noise ($K \ge 1$) : the inverse estimation temperature T_x problem is called *ill-posed* in this region.

Remark :

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 :

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

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 for 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 :

$$y = \eta_2\ (x_s\ /\ e,\ T_0,\ \ T_e) + \varepsilon = \eta_2\ (x_s^{nom}\ /\ e,\ T_0,\ T_e) + \varepsilon' \quad \text{with} \quad \varepsilon' = \delta\ (T_0\ - T_e)/e + \varepsilon \tag{1.19}$$

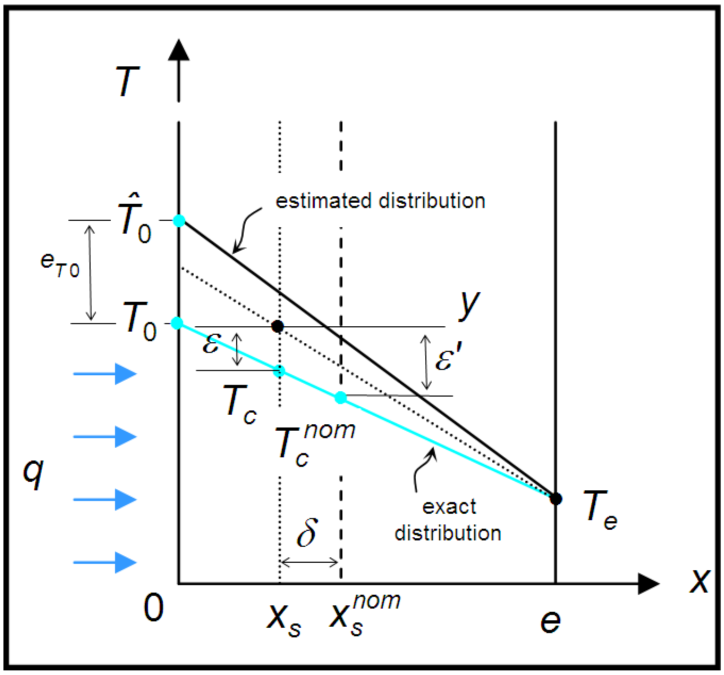

Figure 2b - Estimation of temperature/flux in a wall
Noised temperature measurement
Noised sensor location

If one assumes here that this position error δ is also a random variable, which is independent of temperature noise ε, of zero mean ($\text{E}\,(\delta) = 0$) 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' :

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

Contribution of this position error may become important in σ' and in all the statandard 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 non negligible 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:

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

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 :

$$\lambda^{nom} = \lambda^{exact} + e_\lambda \qquad (1.22)$$

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:

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

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 :

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

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:

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

If we consider the case given by (1.17) in section 3.1, with $R_{\text{pos}} = 0$ (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

$\lambda^{nom}=1$ W.m^{-1}.K^{-1}, with a standard deviation $\sigma_\lambda=$ 0.1 W.m^{-1}.K^{-1}) the error $\sigma_q \ /q^{exact}$ becomes equal to 10.1 % 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 L4 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. Conclusions

The first example that has been presented in this short lecture has been used to precise 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 lectures L2 and L4.

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.

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