

Lecture 8: Inverse problems and regularized solutions

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Abstract. The methods for solving inverse problems must propose some consistent solution despite it is ill-posed. Regularization is one of the important technic that yields the stabilization of the solution. We present in this lecture some generic examples as well as the main concepts within the linear estimation frame for the OLS estimator already studied in Lectures 1 and 3. The Singular Value Decomposition of the sensitivity matrix is used in order to analyse the solution. For such finite dimensional problems, the ill-posed behavior is indeed turned into a bad-conditioned matrix computation.

1. Introduction

The reader could see in Lecture 1, “Getting started with problematic inversions with three basic examples”, some examples of generic inverse problems, which gave rise to envision the main characteristics that make difficult to solved them. In Lecture 3, “Basics for linear inversion, the white box case”, the concepts and resolution of linear parameter estimation problems was presented, when using a direct model which computes the output from the knowledge of the input and some inner parameters used in the direct model.

The parameters to be recovered may be as well the passive structural parameters of the model (model identification), the parameters relative to the input variables, initial state, boundary conditions, some thermophysical properties, calibration, etc... For any of these cases in consideration, the output of the model can be properly computed if all the required information is available.

The problem is said to be well-posed, if, according to Hadamard (Hadamard 1923), three conditions are satisfied, such as

1- A solution exists

2- The solution is unique

3- The solution depends continuously in the data

Problems that are not well-posed in the sense of Hadamard are said to be ill-posed problems. Note that the simple inversion of a well-posed problem may be either a well-posed or an ill-posed problem.

The example of 1D steady heat conduction in a wall discussed in Lecture 1, shows how the interpolation problem (that is the computation of $T(x)$ between the sensor location and the well-known boundary condition) is a well-posed problem, while the extrapolation problem (computation of $T(x)$ between the unknown boundary condition to be retrieved and the sensor location) is an ill-posed problem, since the estimation error may increase drastically.

The example of searching the slope of a line with two or more data points, such as discussed in Lecture 3, may be either a well-posed or an ill-posed problem:

- a unique and stable solution exists if all the data points fit on the same line (no noise in the data), and the time zero has not been chosen for some noisy data point. In that very specific case, the problem of finding the slope is well-posed.
- If, due to the noise in the measurement points, the data do not fit on the same line, a solution does not exist and the corresponding inverse problem of finding the slope is ill-posed.
- If the values of time for taking the measurements are not properly chosen (mostly close to zero), the solution is unstable, since the errors in the measurement may increase drastically – see the absolute and relative amplification coefficients such as defined in Lecture 1, and the corresponding inverse problem is ill-conditioned and may be considered as ill-posed.

The parameter estimation problem stated by finding the vector of parameters by matching the measurements to the model is most often an ill-posed problem, since it is generally over-determined (because the number of measurements m is greater than the number of parameters n), and has no solution because $\mathbf{y} \notin \text{Im}(\mathbf{S})$. When the system is under-determined ($m < n$), it is also ill-posed because there is an infinity of solutions. Moreover,

when $m = n$, the problem may be well-posed if it were stable, but may also be unstable due to the effect of noise in the data.

In the present lecture, we will consider discrete inverse problems, where the number of parameters to be estimated is finite. When the magnitudes to be estimated are functions instead of discrete values, the corresponding problem is turned out to be a continuous inverse problem which may be fully ill-posed. However, in many cases, the searched functions can be parametrized and conveniently approximated by a discrete inverse problem. It was typically the case for the 1D transient inverse heat conduction example in section 4 of Lecture 1, where the wall heat flux was to be estimated as a function of time. The heat flux at each time t_i is represented by a stepwise function q_i .

The main challenge for such discrete function estimation problem is that the number of unknown is almost the same as the number of measurements, and the least squares approach is turned out to be quite close to an exact matching procedure where only one observation is available for one estimated value. In this case the solution is highly sensitive to any ill-conditioned behaviour of the sensitivity matrix.

2. Some examples of typical ill-posed problems

We give hereafter some typical examples of ill-posed problems, such as derivation and deconvolution of experimental data. These examples are typical of the case of a parameterized function estimation. Instead of having a low number of parameters to be estimated with a high number of measurements, as for the example in Lecture 3 of estimating the slope and intercept of a linear profile, the number of parameters to be estimated is herein very large and is quite of the same order as the number of observable data \mathbf{y} , which makes the problem highly sensitive to noise. Unfortunately, in this case the inversion is often also amplifying the measurement noise.

2.1 Derivation of a signal

The derivation of a signal is often required for data processing. It is the case of time dependent functions, for instance, when deriving the time evolution of the mass of a product during drying or deducing the velocity of a body from the measurement of its position. An

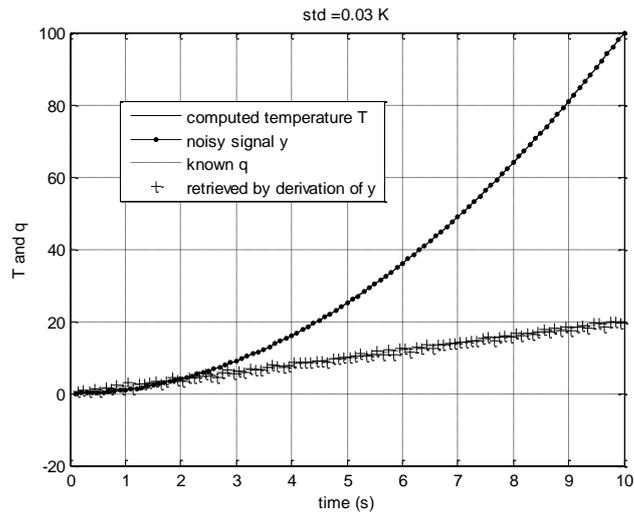
usual case in heat transfer is problem of estimating the heat flux $q(t)$ exchanged by a body with uniform temperature $T(t)$ and volumetric heat capacity C (lumped body approximation). The heat balance can be written as

$$C \frac{dT}{dt} = q(t) \quad \text{with the initial condition } t=0 \quad T=0 \quad (8.1)$$

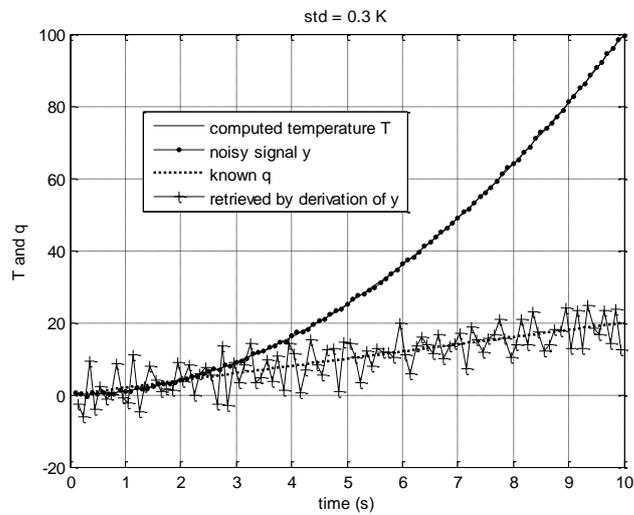
An inversion procedure is thought, for recovering an estimation of $q(t)$ from the measured temperature values $y(t_i)$, for different levels of the measurement noise, based on the following steps:

- a. Choose some heat flux function, such as $q(t) = 2t$ (arbitrarily chosen here)
- b. Compute the corresponding analytical solution $T(t) = t^2 / C$.
- c. Add some random error, in order to simulate some experimental data, such as $y(t) = T(t) + \varepsilon(t)$
- d. Retrieve the estimation by discrete derivation of the signal $\hat{q}(t) = C \frac{\Delta y}{\Delta t} \approx C \frac{dT}{dt}$
- e. Repeat for different values of the Signal-to-Noise Ratio (characterized by different levels of std)

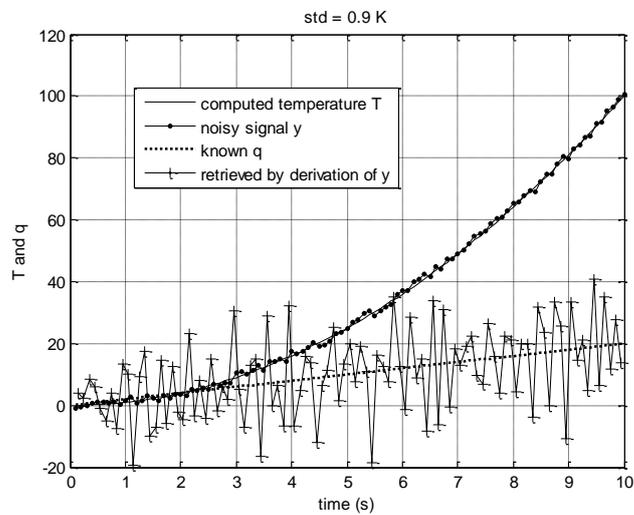
The results are depicted in Figure 1, assuming that $C = 1$. When the standard deviation (std) of the error is low, the heat flux is conveniently retrieved (Fig. 1a). For case (b), the noise on the signal y remains very low, in the sense it is still almost not visible in the corresponding curve. However, the heat flux is poorly computed. Increasing the level of noise, such as in Fig. 1c, where the std is 0.9 K, results in a drastically poor computation of the heat flux. Thus, the derivation of an experimental signal is an ill-posed problem, due to its unstable nature. The numerical derivation yields the computation of the difference of successive measurements, divided by the time step. The ill-posed character of the problem is more important as the time step decreases.



(a)



(b)



(c)

Figure 1 – Derivation of an experimental signal (a) std = 0.03 K (b) std = 0.3 K (c) std = 0.9 K

2.2 Deconvolution of a signal

The deconvolution of a signal is also an operation often required when processing experimental data, for instance when searching the transfer function of a system or sensor, in image processing, optics, geophysics, etc... We give again the heat transfer example of some heat capacity exchanging with convective heat losses with the surrounding medium, such as

$$C \frac{dT}{dt} = q(t) - hT \quad \text{with the initial condition } t = 0 \quad T = 0 \quad (8.2)$$

We assume here that $C = 1$, $T_\infty = 0$ and that the boundary surface of the body is 1.

Solving this equation by using the Laplace transform of the temperature and heat flux and inverting yields the solution in the form of the following product of convolution:

$$T(t) = \int_0^t q(t - \tau) \exp(-h\tau) d\tau \quad (8.3)$$

The same approach as in previous example is proposed herein, such as

- a. Choose some heat flux function, such $q(t)$
- b. Compute the corresponding analytical solution $T(t)$ as the convolution product above.
- c. Add some random error, such as $y(t) = T(t) + \varepsilon(t)$
- d. Retrieve the heat flux by inverting the product this signal (deconvolution)
- e. Repeat for different values of the Signal-to-Noise Ratio (different levels of std)

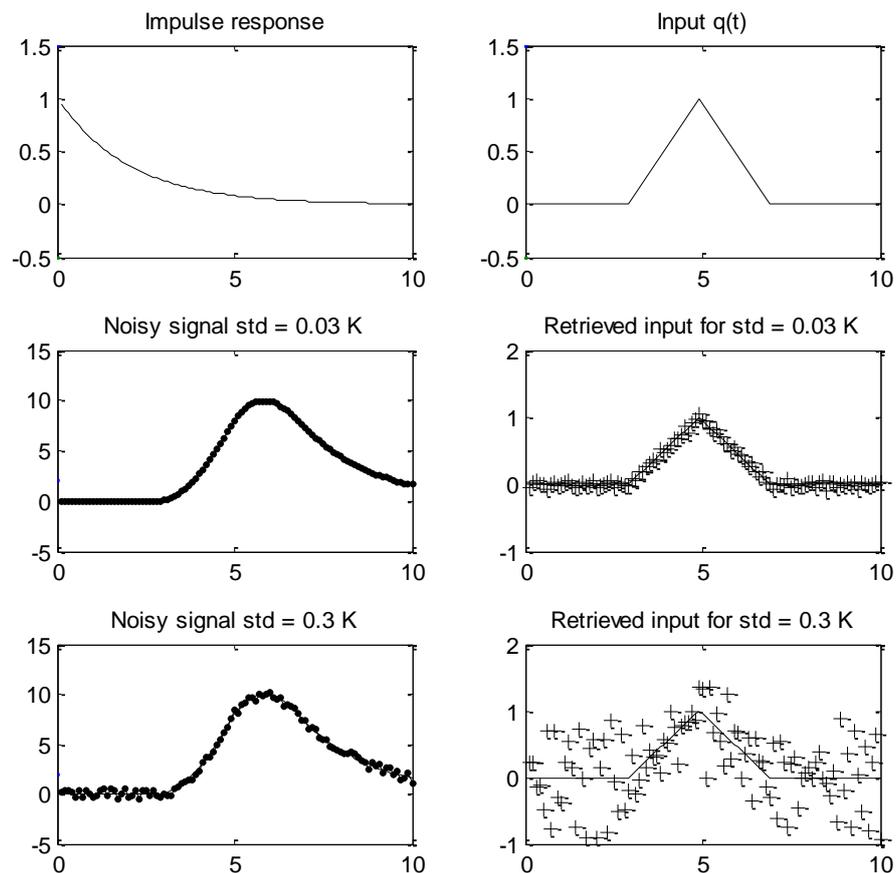


Figure 2 – Effect of the noise level on the deconvolution of a signal

The results are depicted in Figure 2. For a low standard deviation of the error ($\text{std} = 0.03 \text{ K}$), the heat flux is conveniently retrieved by the deconvolution operation. When increasing the noise level ($\text{std} = 0.3 \text{ K}$), the drastic amplification of the errors in the deconvolution operation makes the result absolutely inaccurate. The visual effect of the noise level in the curves where the temperature outputs are drawn shows that the increase of noise between the two situations which makes the solution accurate or unavailable is not significant. It is apparent with this example that the deconvolution of an experimental signal may be an ill-posed problem, depending on the functional form of the impulse response, due to its unstable nature.

3. Structure of the linear transform and stability

3.1 Singular Value Decomposition of the sensitivity matrix

It was already discussed that the existence, unicity and stability of the solution of the discrete linear parameter estimation problem, such as defined in Lecture 3 depend of the

characteristics and structure of the rectangular sensitivity matrix \mathbf{S} . Moreover, when the overdetermined problem $\mathbf{y} = \mathbf{S} \mathbf{x}$ is turned into the least squares problem given by the normal equations it appears that the structure of the square matrix $\mathbf{S}'\mathbf{S}$ is also important for the propagation of the errors between the observed data and the parameters. The anatomy of such linear transformation is very clearly discussed in the text of S. Tan & C. Fox (Tan 2006). One approach of interest in order to analyze this problem is to consider the Singular Value Decomposition of \mathbf{S} (SVD). We assume herein that $m > n$ (overdetermined system, there is more data than parameters) and that \mathbf{S} has only real coefficients.

The SVD of the matrix \mathbf{S} is then written as

$$\left[\begin{array}{c} \mathbf{S} \\ \end{array} \right] = \mathbf{U} \mathbf{W} \mathbf{V}^t = \left[\begin{array}{c} \mathbf{U} \\ \end{array} \right] \left[\begin{array}{ccc} w_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & w_n \end{array} \right] \left[\begin{array}{c} \mathbf{V}^t \\ \end{array} \right] \quad (8.4)$$

where

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

- \mathbf{V} , a square orthogonal matrix of dimensions (n, n) , : $\mathbf{V} \mathbf{V}^t = \mathbf{V}^t \mathbf{V} = \mathbf{I}_n$. Its column vectors (the *right* singular vectors of \mathbf{K}), are the n eigenvectors \mathbf{V}_k , ordered according to decreasing eigenvalues, of matrix $\mathbf{S}'\mathbf{S}$;

- \mathbf{W} , a square diagonal matrix of dimensions $(n \times n)$, that contains the n so-called *singular* values of matrix \mathbf{S} , ordered according to decreasing values: $w_1 \geq w_2 \geq \dots \geq w_n$. The singular values of matrix \mathbf{S} are defined as the square roots of the eigenvalues of matrix $\mathbf{S}'\mathbf{S}$.

In Lecture 3, the Singular value Decomposition of the reduced sensitivity matrix was used to prove that the condition number is a criterion that can be used to measure the degree of ill-posedness of the OLS estimator, through the analysis of the singular values of the sensitivity matrix, which is independent in that case of the noise level.

As previously seen in Lecture 3, the Ordinary Least Squares solution is obtained by minimizing the distance between the direct model $\mathbf{S}\mathbf{x}$ and the data \mathbf{y} , which is done by the

orthogonal projection of the data on the space spanned by the column vectors of \mathbf{S} . This is equivalent to minimize the objective function

$$J_{OLS}(\mathbf{x}) = \|\mathbf{y} - \mathbf{S}\mathbf{x}\|^2 = (\mathbf{y} - \mathbf{S}\mathbf{x})^t (\mathbf{y} - \mathbf{S}\mathbf{x}) \quad (8.5)$$

The minimization of $J_{OLS}(\mathbf{x})$ yields the OLS estimator, computed with Eq. (3.24) in Lecture 3. Applying the singular Value Decomposition to the sensitivity matrix yields

$$\hat{\mathbf{x}}_{OLS} = (\mathbf{S}^t \mathbf{S})^{-1} \mathbf{S}^t \mathbf{y} = \mathbf{V} \mathbf{W}^{-1} \mathbf{U}^t \mathbf{y} \quad (8.6)$$

In this case, if the standard statistical assumptions stand (see Lecture 3), the covariance matrix of the OLS estimator can be written as

$$\text{cov}(\mathbf{x}) = \sigma_\varepsilon^2 \mathbf{V} \mathbf{W}^{-2} \mathbf{V}^t \quad (8.7)$$

Eqs. (8.6) and (8.7) are valid if the sensitivity matrix \mathbf{S} is of full rank, which means that its smaller singular value w_n is strictly positive. The condition number is then defined as

$$\text{cond}(\mathbf{S}) = \frac{w_1}{w_n} \quad (8.8)$$

3.2 Spectral analysis of the OLS estimator

Applying SVD to the normal equations (see Eq. (3.23) in Lecture 3) in order to find the OLS estimator in the diagonal basis yields

$$\mathbf{S}^t \mathbf{S} \hat{\mathbf{x}}_{OLS} = \mathbf{S}^t \mathbf{y} \Rightarrow \mathbf{V} \mathbf{W} \mathbf{U}^t \mathbf{U} \mathbf{W} \mathbf{V}^t \hat{\mathbf{x}}_{OLS} = \mathbf{V} \mathbf{W} \mathbf{U}^t \mathbf{y} \quad (8.9)$$

where the estimation problem can be reconsidered now with the new parameter vector $\mathbf{b} = \mathbf{V}^t \mathbf{x}$ and a new observable vector : $\mathbf{z} = \mathbf{U}^t \mathbf{y}$, such as

$$\mathbf{W} \hat{\mathbf{b}}_{OLS} = \mathbf{z} \quad (8.10)$$

The unicity of the solution is confirmed here when the sensitivity matrix \mathbf{S} is of full rank, i.e. $r = n$, which is possible only if $m \geq n$ (more data than parameters). When $r < n$, the matrix has not full rank, and the parameters to be estimated must be reduced, or some parameters must be determined in an arbitrary form.

The linear transformation of the data \mathbf{y} also yields a new covariance matrix associated to the observable measurement noise. Hopefully, we can note that this operation does not affect the variance of the error of the transformed signal \mathbf{z} (here for the standard assumptions):

$$\text{cov}(\mathbf{z}) = \mathbf{U}^t \text{cov}(\mathbf{y}) \mathbf{U} = \sigma_\varepsilon^2 \mathbf{U}^t \mathbf{U} = \sigma_\varepsilon^2 \mathbf{I} \quad (8.11)$$

Hence the covariance matrix is computed by

$$\text{cov}(\hat{\mathbf{b}}_{OLS}) = \sigma_\varepsilon^2 \mathbf{W}^{-2} \quad \text{or} \quad \text{cov}(\hat{\mathbf{b}}_{OLS}) = \begin{bmatrix} \frac{\sigma_\varepsilon^2}{w_1^2} & \cdot & 0 \\ \cdot & \cdot & \cdot \\ 0 & \cdot & \frac{\sigma_\varepsilon^2}{w_n^2} \end{bmatrix} \quad (8.12)$$

The above equation shows that an effect of noise amplification appears due to the fact that the eigenvalues have a wide range of order of magnitude. It is of particular interest to note in Eq. (8.12) that the covariance matrix of the estimator in the diagonal basis is linking the square of the singular values to the variance of noise, that is to the level of uncertainty in the measurement errors.

A small perturbation applied to a single component k of \mathbf{z} , such as

$$\delta \mathbf{z} = \delta z_k \mathbf{U}_k \quad (8.13)$$

yields the following variation to the OLS estimator

$$\delta \hat{\mathbf{b}}_{OLS} = \frac{\delta z_k}{w_k} \mathbf{V}_k \quad (8.14)$$

which implies a relative variation corresponding to

$$\frac{\|\delta \hat{\mathbf{b}}_{OLS}\|}{\|\delta \mathbf{z}\|} = \frac{1}{w_k} \quad (8.15)$$

Thus the singular values indicate how the same perturbation yields different effects on the components of the estimator. Moreover, this relative variation may increase drastically when the singular values are close to zero. The relative variation between two components of respective index k and h is given by the ratio $\frac{w_k}{w_h}$. Hence the maximum relative variation

factor is obtained between the first and the last component, such as $\frac{w_1}{w_n}$, which is condition

number of the sensitivity matrix, as seen in Eq. (8.8). If $\text{cond}(\mathbf{S})$ is not too large, the problem is said to be well-conditioned and the solution is stable with respect to small variations of the data. Otherwise the problem is said to be ill-conditioned. It is clear that the separation between well-conditioned and ill-conditioned problems is not very sharp and that

the concept of well-conditioned problem is more vague than the concept of well-posed problem.

3.3 Example of a simple ill-conditioned matrix

$$\begin{bmatrix} 1 & 1 \\ 1 & 1.01 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{the inversion yields} \quad \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Let's give a perturbation of 1% on the second data point, such as

$$\begin{bmatrix} 1 & 1 \\ 1 & 1.01 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1.01 \end{bmatrix} \quad \text{the inversion yields} \quad \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Hence the resulting perturbation on the solution of the matrix inversion is surprisingly as far as possible from the original solution. The solution is quite unstable. Note immediately that the determinant is close to zero.

The eigenvalues are (2.005, 0.005), and the condition number is $402 \gg 1$.

4. Regularization

In the previous section it was shown how the ill-posed estimation problem is turned into an ill-conditioned problem by the least squares approach. Equations (8.6) and (8.7) show that the unstable behavior of the pseudo-inverse of the sensitivity matrix can be straightly addressed by the means of the singular values diagonal matrix \mathbf{W} . Regularization is relative to the search of some acceptable solution, by reducing the effect of measurement errors on the estimate. Several approaches may be used for this purpose. The main idea is to reduce the effect of the "small" singular values on the obtained solution, while trying to avoid that this "smooth" solution be quite different than the true-but-unknown solution. The two main approaches are

- (i) *Apply some prior information as a constraint*
The most usual methods are truncation of the diagonal basis and the parametrization of the solution (reduction of the number of parameters)
- (ii) *Apply some penalization to the objective function*
Some weighted prior information is included in the objective function

4.1 Truncated SVD

TSVD of order α is obtained when replacing in Eq. (8.6) the inverse of the matrix \mathbf{W} by the truncated inverse \mathbf{W}_α^{-1} where the smaller singular values are removed (their inverse put to zero), such as

$$\hat{\mathbf{x}}_{\mu}^{Tik0} = (\mathbf{S}^t \mathbf{S} + \mu \mathbf{I}_n)^{-1} (\mathbf{S}^t \mathbf{y} + \mu \mathbf{x}_{prior}) \quad (8.21)$$

Applying SVD to the sensitivity matrix \mathbf{S} and using $\mathbf{V} \mathbf{V}^t = \mathbf{I}_n$ yields :

$$\hat{\mathbf{x}}_{\mu}^{Tik0} = \mathbf{V} (\mathbf{W}^2 + \mu \mathbf{I}_n)^{-1} (\mathbf{W} \mathbf{U}^t \mathbf{y} + \mu \mathbf{V}^t \mathbf{x}_{prior}) \quad (8.22)$$

It is quite apparent in Eq. (8.22) how the regularization parameter will cancel the noise amplification effect of the smallest singular values in the diagonal matrix $(\mathbf{W}^2 + \mu \mathbf{I}_n)$ to be inverted. Nevertheless, the cost of this stabilization is also obvious, since the non-zero regularization parameter value yields that the information of the experimental data in \mathbf{y} is biased by the prior information (\mathbf{x}_{prior}). Hence let's point out that the regularized solution aims to balance accuracy and stability requirements.

4.3 Examples: Regularization for derivation and deconvolution

The experimental derivation and deconvolution examples given in section 2 by Equations (8.1) and (8.2) can be computed as linear estimation problem. These function estimation problem are highly sensitive to noise, since the number of unknown matches the number of function components to be retrieved (exact matching: the sensitivity matrix is a square matrix). Equation (8.22) is used for these two examples for different values of the regularization parameter.

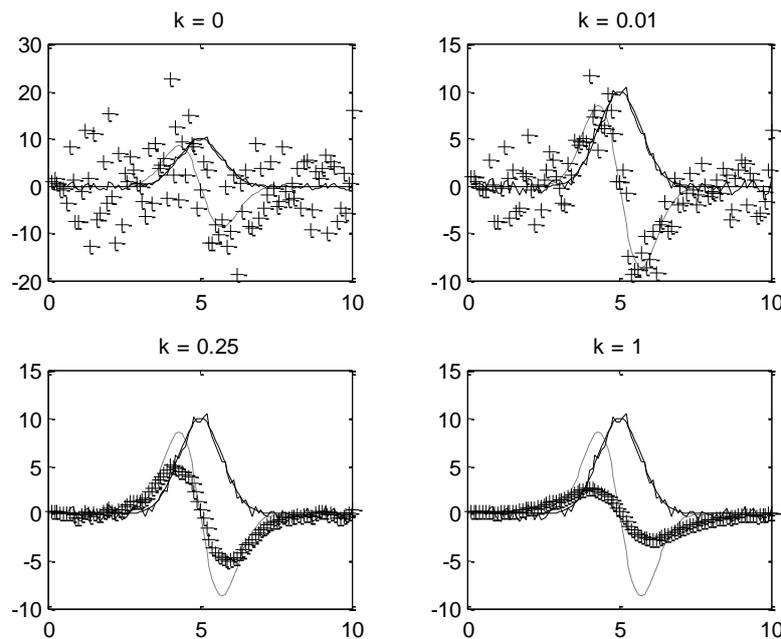


Figure 3 – Derivation and inversion with Tikhonov regularization

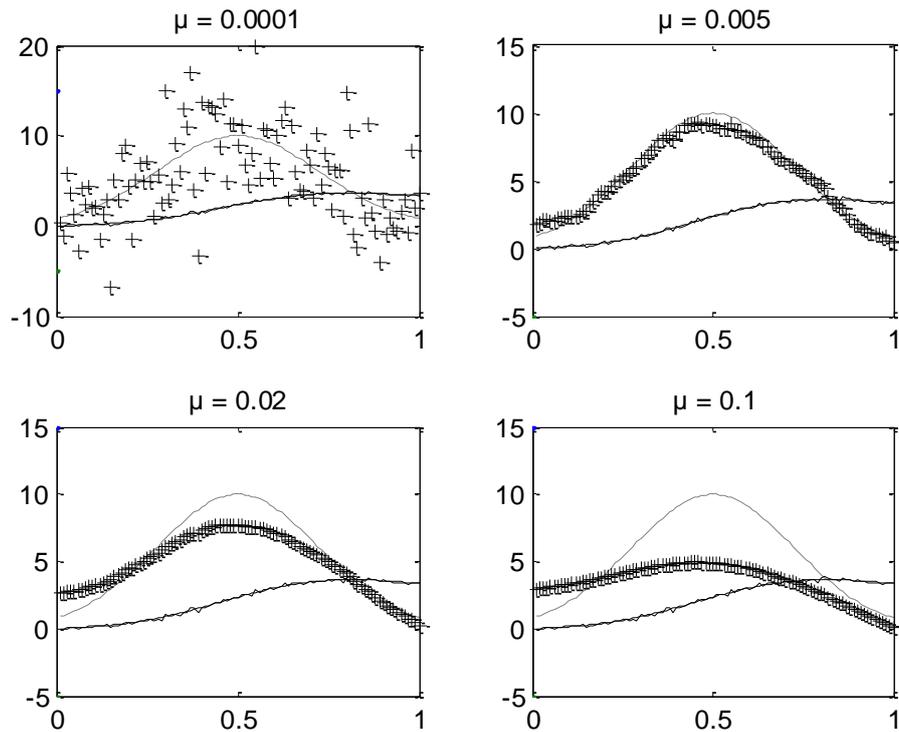


Figure 4 – Deconvolution and inversion with Tikhonov regularization ($\sigma_\varepsilon^2 = 0.01$)

Figures 3 and 4 show how increasing the value of the regularization parameter has a positive effect regarding the stabilization of the heat flux time history to be retrieved, while this effect is counter balanced by the apparition of a bias with the original solution. It is of great interest to point out in Figure 4 that the correct possible values of the regularization parameter μ are quite close to the variance of the measurement error (here $\sigma_\varepsilon^2 = 0.01$ K): stabilization is related to the signal-to-noise ratio.

The regularization of deconvolution Matlab code is given in appendix 1.

4.4 The regularization parameter

The convenient choice of the value of the regularization parameter is a nontrivial problem for which numerous solutions have been proposed. The L-curve method (due to Hansen,1992) has become a popular method, which is implemented by the graphical analysis of a log-log plot obtained by varying the value of the regularization parameter, as shown in figure 5. For each value of μ , the norm of the distance between the data and the model is reported on the horizontal axis, while the distance of \mathbf{x} to \mathbf{x}_{prior} is reported on the vertical axis. The L-curve selection criterion consists of locating the value which maximizes the curvature, that is the L-curve corner which separates the two regions: under-regularized on the left, over-regularized on the right.

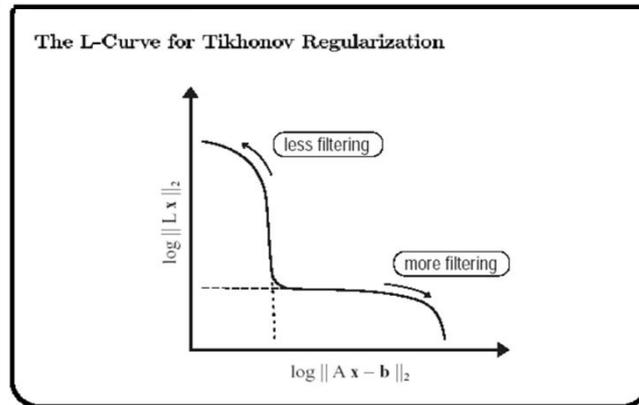


Figure 5 – Choice of the Tikhonov regularization parameter: L-curve

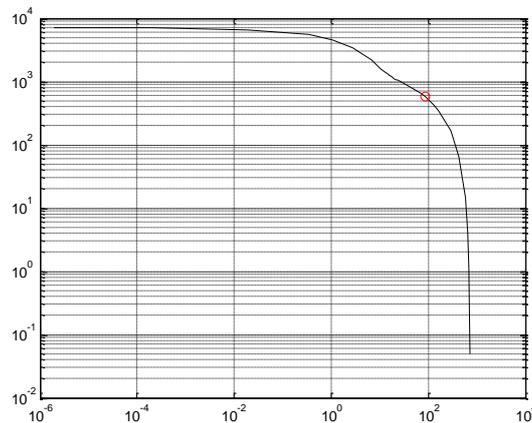


Figure 6 – L-curve obtained for the regularization of the deconvolution example

The L-curve is plotted for the regularized deconvolution example. The red circle is obtained when the regularization parameter μ has the same value as the standard deviation of the measurement noise. It is found to be quite close to the L-curve point.

6. Conclusions

Regularization is an important step for solving ill-posed problems. When the inverse problem is of finite dimension, which is the case for discrete estimation problems, the existence of solution is achieved by the least squares approach, and the problem is in fact ill-conditioned. For function estimation problems, the parametrization of the function to be retrieved tend to exact matching, where the number of experimental data is equal to the number of parameters. This case is generally highly sensitive to the measurement noise. Regularization stabilizes the solution by removing the effect of the smallest singular values which amplify the effect of these measurement errors. However the cost of regularization is that the stabilized solution is biased, hence the value of the regularization parameter (Tikhonov parameter or truncation order) must be carefully chosen.

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- Dossier AF 4516, pp. 1-24, janvier 2008.

Appendix 1

```
% Deconvolution and inversion with regularization
% fi=fi0*exp(-(t-t0)**2)
% dT/dt = fi - hT
% T=conv(fi,exp(-ht))
% Tr = T + bruit

N=100;dt=0.01;t0=dt*N/2;t=dt*(1:N);
fi0=10;h=1;fi=fi0*exp(-10*(t-t0).^2);

Q=sqrt(fi*fi');Amp=40;
% noise
bruit=0.1*randn(size(t));
cov(bruit)

k=[0.0001 0.005 0.02 0.1]; % Regularization parameter

X=dt*toeplitz(exp(-h*(t(1:N))), zeros(1,N)); % Sensitivity matrix

T=X*fi'; % Direct model (convolution)
Tr=T'+bruit;

for i=1:length(k)
    G=inv(X'*X+k(i)*eye(N));
    fir=G*X'*Tr';
    VI=eig(G);
    ki=k(i)
    cond_i=max(abs(VI))/min(abs(VI))
    p=i;
    subplot(2,2,p),plot(t,T,'k',t,Tr,'k',t,fi,'k:',t,fir,'k+',0,15,0,-5),
    title(['k = ',num2str(k(i))])
    figure(gcf);
end
```