## Lecture 9

# Inverse Problems - Part A: Regularized Solutions ${ }^{1}$ 

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#### Abstract

An important key feature of inverse problems, both theoretically and numerically, is their illposedness. It is important to construct special algorithms for their solutions. The main differences which are inherent to the formulation and the resolution of the direct and inverse problems are presented and the general linear inverse problem analysis (finite dimensional case) is detailed through the investigation of the Hadamard's conditions.Basic regularization processes which leads to build quasi-solutions satisfying some compromise between the accuracy and the stability requirements are briefly presented and illustrated by numerical results.


## 1.-Introduction

Research in heat transfer commonly involves experimentation, including design of experiments and mathematical modelling with associated numerical analysis and computation. Many problems in heat transfer can only be solved through the use of interactive computational-experimental procedures according to a specific methodology based on the resolution on Inverse Heat Transfer Problems (IHTP).

An important key feature of inverse problems, both theoretically and numerically, is their ill-posedness. They do not fulfill Hadamard's classical requirements of existence, uniqueness and stability, under data perturbations. Solutions of an inverse problem might not exists for all data, it might not be unique (which raises the practically relevant question of identifiability, i.e. the question if the data contain enough information to determine the unknown quantity), and it might be unstable with respect to data perturbations. The last aspect is of course especially important, since in real-world problems, measurements always contain noise (another source of noise being errors in numerical procedures), and approximation methods for solving inverse problems which are insensitive to noise as possible have to be constructed, so-called regularization methods.

Inverse problems in heat transfer have been the focus of a growing number of research efforts over the last 40 years [1]-[6]. These efforts led to a growing appetite in applications for posing and solving new inverse problems, which in turn stimulated new mathematical research e.g., on uniqueness questions and on developing stable and efficient numerical methods (regularization methods) for solving inverse problems [7]-[9].

Because most of inverse problems are ill-posed or ill-conditionned, it is very important to construct special algorithms for their solutions. This lecture will be devoted to present and to illustrate the main differences which are inherent to the formulation and the resolution of the direct and inverse problems. In the first section three examples of basic inverse heat transfer

[^0]problem are considered for a better understanding of the ill-posedness concept. In the second section, the analysis of the general linear inverse problem (finite dimensional case) is detailed and the three Hadamard's conditions are investigated. The third section is devoted to the presentation of basic regularization processes which leads to build quasi-solutions satisfying some compromise between the accuracy and the stability requirements. Numerical results are given to illustrate the efficiency of the different regularizing processes.

## 2- Ill-Posed Problems

Three basic examples of inverse heat transfer problems are briefly discussed in order to illustrate their ill-posedness.

## 2.1- Examples of linear inverse problems

### 2.1.1- Inverse initial state 1-D heat conduction problem

Consider the linear 1-D heat-conduction process, and the inverse initial state problem which consists in the determination of the temperature field $U(x)$ from the observation of the final state $Y(x)$ :

State equations

$$
\begin{gather*}
\frac{\partial T}{\partial t}(x, t)=\frac{\partial^{2} T}{\partial x^{2}}(x, t), \quad 0<x<1, \quad 0<t<t_{f}  \tag{1a}\\
T(0, t)=T(1, t)=0, \quad 0<t<t_{f}  \tag{1b}\\
T(x, 0)=U(x), \quad 0<x<1 \tag{1c}
\end{gather*}
$$

Output equation

$$
\begin{equation*}
Y(x)=T\left(x, t_{f}\right), \quad 0<x<1 \tag{1d}
\end{equation*}
$$

Let us introduce the function spaces $\mathbf{U}=\mathbf{Y}=\mathbf{L}^{2}(0,1)$ with the following norm

$$
\begin{equation*}
\|U\|_{\mathbf{U}}=\left[\int_{0}^{1} U^{2}(x) d x\right]^{1 / 2},\|\ldots\|_{\mathbf{U}}=\|. \ldots\|_{\mathbf{Y}} \tag{2}
\end{equation*}
$$

Then the inverse problem may be formulated under the generic form :
Determine $U \in \mathbf{U}$, such that $Y=A(U)$, from the given data $Y \in \mathbf{Y}$
Where $A($.$) is the operator to be inversed$
The solution of the direct problem is given by the method of separation of variables

$$
\begin{equation*}
T(x, t)=\sum_{n=1}^{\infty} c_{n} \cdot e^{n^{2} \pi^{2} t} \varphi_{n}(x), \text { where } \varphi_{n}(x)=\sqrt{2} \sin (n \pi x) \tag{3}
\end{equation*}
$$

So $Y(x)=\sum_{n=1}^{\infty} c_{n} \cdot e^{-n^{2} \pi^{2} t_{f}} \varphi_{n}(x)$ and $U(x)=\sum_{n=1}^{\infty} c_{n} \varphi_{n}(x)$. By using the orthogonal property of the eigenfunctions, $\left\langle\varphi_{n}, \varphi_{m}\right\rangle=\delta_{n m}$, it comes $c_{n}=. e^{n^{2} \pi^{2} t_{f}}\left\langle Y, \varphi_{n}\right\rangle$, which gives

The solution of the inverse problem

$$
\begin{equation*}
U=A^{-1}(Y)=\sum_{n=1}^{\infty} c_{n} \varphi_{n}=\sum_{n=1}^{\infty} e^{n^{2} \pi^{2} t_{f}} .\left\langle Y, \varphi_{n}\right\rangle \varphi_{n} \tag{4}
\end{equation*}
$$

The operator $A$ is linear, then the variation of the solution which results of any output error $\delta Y_{\varepsilon}=Y_{\ell}-Y$ is $\delta U=\sum^{\infty} e^{n^{2} \pi^{2} t_{f}}\left\langle\delta Y_{\varepsilon}, \varphi_{n}\right\rangle \varphi_{n}$. Suppose (for simplicity) that the error $\delta Y_{\varepsilon}$ is entirely supported by one eigenfunction, namely $\varphi_{N}: \delta Y_{\varepsilon}(x)=\varepsilon \sqrt{2} \sin (N \pi x),\|\delta Y\|_{\mathrm{Y}}=\varepsilon$ then $\delta U=\varepsilon e^{N^{2} \pi^{2} t_{f}} \varphi_{N}$, and $\|\delta U\|_{\mathbf{U}}=e^{N^{2} \pi^{2} t_{f}}\|\delta Y\|_{\mathbf{Y}}$.

This result means that any arbitrarily small output error, may induce a great variation on the solution $U$. The stability condition is violated, this inverse initial state heat conduction problem is illposed.

Numerical results: $U(x)=x^{2}(1-x) ; Y(x)$ is computed at $t_{f}=0.05$

```
% 1-D heat conduction
clear
nx=51;dx=1/(nx-1); x=0:dx:1;
nmax=5;tf=0.05;
u=x. *x. *(1-x);
plot(x,u);grid on;hold on
y=zeros(1,nx);
for n=1:nmax
fn=sqrt(2)*sin(n*pi.*x);
c(n)=dx*u*fn';
tn=n*n*pi*pi*tf;
y=y+c(n)*exp(-tn).*fn;
end
plot(x,y,'+')
```



Figure 1 : Initial $(t=0)$ and Final $\left(t_{f}=0.05\right)$ temperature fields for a 1-D heat conduction process

### 2.1.2- Inverse 1-D boundary heat source problem

A semi-infinite heat conducting body is submitted to a boundary heat flux density $U$ which is to be determined from the observed output $Y$ given by the temperature history at the sensor location $\mathrm{x}_{\mathrm{s}}$, on the time interval ( $\mathrm{o}, \mathrm{t}_{\mathrm{f}}$ ). The problem may be put under the generic form $Y=A(U), U \in \mathbf{U}, Y \in \mathbf{Y}$, by introducing the functional spaces $\mathbf{U}=\mathbf{Y}=\mathbf{L}^{2}\left(0, t_{f}\right)$, together with the following norm

$$
\|U\|_{\mathbf{U}}=\left[\int_{0}^{t_{f}} U^{2}(t) d t\right]^{1 / 2},\|\ldots\|_{\mathbf{U}}=\|\ldots\|_{\mathbf{Y}}
$$

and the linear operator $\mathrm{A}($.$) is defined by the convolution integral$

$$
\begin{equation*}
Y(t)=A(U)(t)=\int_{\dot{d}}^{t} f_{s}(t-\tau) U(\tau) d \tau, t \in\left(0, t_{f}\right) \tag{5a}
\end{equation*}
$$

where $\frac{1}{k}\left(\frac{\alpha}{\pi t}\right)^{0.5} \exp \left(-\frac{x_{s}^{2}}{4 \alpha t}\right)=f_{s}(t)$ is the impulse response.
The question of stability of the inverse solution for this kind of integral equation will be discussed later, but now suppose for simplicity, that the observed output is perturbed by an additive noise $Y(t)=\bar{Y}(t)+\delta Y(t)$, which is taken (for simplicity) under the simple periodic form $\delta Y(t)=\varepsilon \cdot \cos \omega_{n} t, \omega_{n}=2 n \pi / t_{f}$. From the linear property of the operator, it comes $A(\delta U)=\delta Y$. A frequential analysis leads to the periodic solution

$$
\begin{equation*}
\delta U(t)=\varepsilon . b \sqrt{\omega_{n}} \exp \left(x_{c} \sqrt{\left.\omega_{n} / 2 a\right)} \cdot \cos \left(\omega_{n} t+\Psi\right)\right. \tag{6}
\end{equation*}
$$

and consequently, it comes :

$$
\begin{gather*}
\|\delta U\|_{\mathrm{U}}=G\left(\omega_{n} ; x_{s}\right)\|\delta Y\|_{\mathbf{Y}}  \tag{7a}\\
G\left(\omega_{n} ; x_{s}\right)=b \sqrt{\omega_{n}} \exp \left(x_{s} \sqrt{\omega_{n} / 2 a}\right) \tag{7b}
\end{gather*}
$$

where the gain factor $G$ is an increasing function of both the sensor location and the frequency of the output error.

This results means that any arbitrarily small (periodic) output error, may induce a great (periodic) variation on the solution $U$. The stability condition is violated, this inverse boundary heat source problem is ill-posed. In practice, a specific data processing has to be performed on the observed output, especially for avoiding the amplification of the high frequency components of the output.

Numerical results : let $\omega_{\text {ref }}=\sqrt{\frac{2 a}{x_{s}^{2}}}\left[s^{-1}\right]$ and $G_{\text {ref }}=\frac{\lambda \sqrt{2}}{x_{s}}\left[W^{-2} K^{-1}\right]$, then the reduced gain factor is $G^{*}=\frac{G}{G_{\text {ref }}}=\omega^{*} \exp \left(\omega^{*}\right)$, with $\omega^{*}=\frac{\omega}{\omega_{\text {ref }}}$
\% semi-infinite heat conduction
\% reduced gain factor for the
\% IBHSP in the periodic case
w=logspace(-2,1,10);
$g=w . * \exp (w)$
plot (w, g)


Figure 2- Gain factor for the inverse boundary heat source problem versus the frequency of the periodical error

More generally, the unknown to be determined $U$ belongs to a functional space, whose size is infinite. But a finite approximation is straightforward. The time interval ( $\mathrm{o}, \mathrm{t}_{\mathrm{f}}$ ) is divided into $n$ sub-intervals $]_{t_{i-1}}, t_{i}[$, of length $\Delta t$. The linear convolution operator may be approximated by a matrix operator. This is not a practical way to solve the inverse problem, but this is to illustrate the ill-posedness of the problem.

$$
\begin{equation*}
Y\left(t_{i}\right)=\int_{o}^{t_{i}} f_{s}\left(t_{i}-\tau\right) U(\tau) d \tau \square \sum_{j=0, \ldots i-1} f_{s}\left(t_{i}-\tau_{j}\right) U\left(\tau_{j}\right) \Delta t, i=1, \ldots, n \tag{8}
\end{equation*}
$$

The problem is re-formulated under the generic form $Y=A(U), U \in \mathbf{U}, Y \in \mathbf{Y}$, by introducing the new vector spaces $\mathbf{U}=\mathbf{Y}=\mathbf{R}^{n}$ :

$$
\begin{equation*}
Y_{i}=\sum_{j=1, \ldots . . n} a_{i j} U_{j,} i=1, \ldots, n \tag{9a}
\end{equation*}
$$

$$
\begin{gather*}
\text { where }, U_{j}=U\left(\tau_{j-1}\right) \text { and } a_{i j}=\left\{\begin{array}{cc}
\Delta t \cdot f_{s}\left(t_{i}-\tau_{j-1}\right), j=1, \ldots, i \\
0, & j=i+1, \ldots, n
\end{array}\right\}  \tag{9b-c}\\
a_{i i}=\frac{1}{b} \sqrt{\frac{\Delta t}{\pi}} \exp \left(\frac{-x_{c}^{2}}{4 a \Delta t}\right), i=1, . ., n  \tag{9d}\\
\operatorname{det}(A)=\prod_{i=1}^{n} a_{i i} \tag{9e}
\end{gather*}
$$

The matrix A is square ( $n, n$ ), the (approximated) solution of the inverse problem is then $U=A^{-1}(Y)$. However, it must be noted that by decreasing the time step $\Delta t$, or by increasing the value of $n$, the determinant of the matrix $\operatorname{det}(A)$ goes to zero, hence the matrix becomes nearly singular, the numerical inversion process becomes ill-conditionned, and the unstable computed solution is very sensitive to the output error. There is some dilemma between accuracy and stability : by increasing $n$, the accuracy of the direct problem solution will increase but the stability of the inverse problem solution will decrease.

### 2.1.3- Inverse 2-D boundary heat source problem

Let us consider the solution of the 2-D steady-state heat-conduction process, described by the following set of equations (10). Numerical results of the direct problem, are plotted on figure 3 , they are computed with the following input data :
$T_{1}=0.5,0<y<1$
$q(y)=q_{0}\left(\sin \left(\frac{\pi y}{2}\right)-1\right), \quad 0<y<1$
Now suppose that the heat source boundary $q$ is unknown on $\Gamma_{4}$, and that the output $Y$ is observed on $\Gamma_{3}$. A 2-D inverse boundary heat source problem aims to the determination of the boundary heat flux $q$ from the data $Y$.

Steady-state equation
$\Delta T=0$ dans $\Omega$
$\left.\mathrm{T}\right|_{\Gamma_{1}}=T_{w}$
$\left.\frac{\partial T}{\partial n}\right|_{\Gamma_{2} \cup \Gamma_{3}}=0$
$-\left.\lambda \frac{\partial T}{\partial n}\right|_{\Gamma_{4}}=q$
Output equation
$Y=\left.T\right|_{\Gamma_{3}}$


Figure 3a : Spatial domain of the 2-D IBHP


Figure 3b Temperature field, solution of the Figure 3c Iso-values of the direct problem solution direct problem equations


Figure 3d : Boundary conditions on $\Gamma_{4}$


Figure 3e: Observed Output on $\Gamma_{3}$

The inverse problem may be formulated according to an internal lumped parameter model structure, obtained after the discretization of the spatial variable. It leads to the following state and output equations

$$
\begin{gather*}
{[A] T=\left[B_{1}\right] * T_{\mathrm{w}}+\left[B_{4}\right] q}  \tag{11a}\\
Y=[C] T \tag{11b}
\end{gather*}
$$

where $T$ is the state (temperature) vector , $q=\left[q\left(y_{i}\right)\right]_{i=1}^{n} \in \mathbf{R}^{n}$ is the heat source vector on $\Gamma_{4}, T_{w}=\left[T_{i}\right]_{i=1}^{n 1}$ is the fixed temperature on $\Gamma_{1}, \quad Y=\left[Y\left(x_{j}\right)\right]_{j=1}^{m} \in \mathbf{R}^{m}$ is the observed output vector and $[A],\left[B_{1}\right],\left[B_{4}\right],[C]$ are respectively $(N, N),(N, n 1),(N, n),(m, N)$ matrices. The size of the state vector, e.g. the number $N$ of nodes of the spatial grid, (without the nodes on the boundary $\Gamma_{1}$ ) defines the size of the square matrix $A$.
Finally the linear operator between the inputs (the heat source $q$, and the fixed temperature $T_{w}$ ) and the observed output takes the form of a linear matrix equation:

$$
\begin{equation*}
Y=[C][A]^{-1}\left(\left[B_{1}\right] * T_{w}+\left[B_{4}\right] q\right) \tag{12}
\end{equation*}
$$

The sensitivity analysis is an important step for evaluating the ill-posedness of the inversion process. It is based on the sensitivity equations

$$
\begin{align*}
\delta Y= & {[C][A]^{-1}\left[B_{4}\right] \delta q=[X] \delta q }  \tag{13a}\\
& {[X]=[C][A]^{-1}\left[B_{4}\right] } \tag{13b}
\end{align*}
$$

where the elements of sensitivity matrix are $X_{i j}=\frac{\partial Y_{i}}{\partial q_{j}}, \quad i=1, . . n ; j=1, . ., m$
It is clear in this example that the solution of the inverse problem will require the inversion of the matrix [X] whose size depends on two variables :

- the size $m$ of the observed output vector
- the size $n$ of the unknown heat source vector

Let us note that both the direct and the inverse problems are linear and leads to the inversion of matrices, respectively $[A]$ and $[\mathrm{X}]$, but the size of which may be quite different. It may noted too that the construction of the matrix $[\mathrm{X}]$ results of the spatial discretization of the distributed model into a lumped model structure (matrices $[A],\left[B_{1}\right],\left[B_{4}\right]$ ), but depends also on the sensors location (matrix $[C]$ ).

The analysis and the solution of this linear inverse problem is discussed in the next section.

## 2.2- The Hadamard conditions

A generic formulation of the three above inverse problems may be summarized as follows, they consist in solving the operator equation

$$
\begin{equation*}
Y=A(U) U \in \mathbf{U}, Y \in \mathbf{Y} \tag{2.1}
\end{equation*}
$$

where $\mathbf{U}, \mathbf{Y}$ are two metric spaces, $U$ is the unknown to be determined, $Y$ the observed output. More generally, the operator $A: \mathbf{U} \rightarrow \mathbf{Y}$ (linear or not), is assumed to be given. The domain and the set of values of the operator are respectively noted $D(A) \subset \mathbf{U}, R(A) \subset \mathbf{Y}$

Definition - The problem is well-posed in the sense of Hadamard, if
a) for any $Y \in R(A)$, there is a solution $U \in \mathbf{U}$, (existence condition)
b) the solution is unique within $\mathbf{U}$ (uniqueness condition)
c) the solution depends continuously on $Y$ (stability condition)

If at least one of the three conditions is not satisfied, the problem is said to be ill-posed. Efficient algorithms for solving the inverse problem cannot be developed without getting more insight of these questions.

The question of stability may be viewed as follows: which is the error $\delta U$ generated by the output data error $\delta Y$ ? When the stability condition is satisfied, small errors $\|\delta Y\|_{\mathrm{Y}}$ on the observed output, lead to small variations $\|\delta U\|_{\mathbf{U}}$ on the solution. Note that the norms $\|. . .\|_{\mathrm{U}}$ and $\|. . .\|_{\mathbf{Y}}$ of the spaces $\mathbf{U}, \mathbf{Y}$ have to be introduced to study this stability condition, the illposedness of the inverse problem may depend on the choice of these norms.

Quasi-solution - In practice the stability condition is essential, it leads to redefine the concept of solution for the inverse problems. The observed output are known approximately due to (additive or not) errors, then any element $U \in \mathbf{U}$ which can predict, through the operator $A$, the observed output $Y \in \mathbf{Y}$ with the tolerance level $\varepsilon$ of the errors, is an admissible solution for the inverse problem. It is possible that the problem, has no exact solution in the sense $U=A^{-1}(Y)$, but it have several or an infinite set of solutions which are acceptable within the tolerance $\varepsilon$, e.g. which satisy the inequality:

$$
\begin{equation*}
\|A(U)-Y\|_{\mathrm{Y}} \leq \varepsilon \tag{14}
\end{equation*}
$$

The elements $U \in \mathbf{U}$ which minimize the criterion $\|A(U)-Y\|_{\mathrm{Y}}$ are called quasi-solutions or solutions in the least square sense. Note once more, that the definition of this criterion leads to use the norm $\|. . .\|_{\mathrm{Y}}$ of the space Y .
«Inverse methods» are specific in the sense that they aim to take into account the error $\varepsilon$ on the observed output, in order to build a stable or "regularized" quasi-solution to the inverse problem. One way for building the quasi-solution, consists to consider a priori information, for example by introducing some a priori regularity constraints, or a priori estimate.

## 3.- Linear Inverse Problem Analysis

The three conditions of Hadamard are investigated for the linear inverse problem in the finite dimensional case. The mathematical analysis will show that the concept of quasisolution allows to satisfy the question of existence, but the uniqueness and stability conditions will remain unsatisfied. Then some regularization is needed to build a unique and stable quasi-solution.

## 3.1- Singular Value Decomposition

The linear inverse problem in the finite dimensional case consists in finding the vector $U \in \mathbf{R}^{n}$ solution of the matrix equation

$$
\begin{equation*}
Y=A . U \tag{15}
\end{equation*}
$$

where the output vector $Y \in \mathbf{R}^{m}$ and the matrix $A$ are given
When $m=n$, the matrix $A$ is squared, if the matrix is non singular and well conditionned, there is a unique and stable solution. The determination of $U=A^{-1} Y$ is done according to standard numerical methods which do not concern the "inverse techniques"discussed here.

When $m \neq n$, the matrix is rectangular and the analysis of the Hadamard's conditions is required. It is based on the singular value decomposition of the matrix $A$.

## Main results:

1. The square matrices $A A^{t}$ and $A^{t} A$ are both symetric matrices and they have the same set of real non negative eigenvalues
2. Let $r$ be the rank of these matrices, then $r \leq \inf (m, n)$
3. There is a set $\left\{\lambda_{1}, . ., \lambda_{r}\right\}$ of $r$ strictly positive real values, called singular values of $A$,
4. There is a set $\left\{V_{1}, \ldots, V_{n}\right\}$ of $n$ vectors within $\mathbf{R}^{n}$ such that

$$
A^{t} A V_{i}=\left\{\begin{array}{c}
\lambda_{i}^{2} V_{i}, i=1, . ., r \\
0 V_{i}, i=r+1, . ., n
\end{array}\right.
$$

5. There is a set $\left\{W_{1}, \ldots, W_{m}\right\}$ of $m$ vectors within $\mathbf{R}^{m}$ such that

$$
A A^{t} W_{i}=\left\{\begin{array}{c}
\lambda_{i}^{2} W_{i}, i=1, \ldots, r \\
0 W_{i}, i=r+1, \ldots, m
\end{array}\right.
$$

Let $\mathbf{V}=\left\{V_{1}, \ldots, V_{n}\right\}, \mathbf{W}=\left\{W_{1}, \ldots, W_{m}\right\}$ and $S$ the rectangular matrix such that

$$
S_{i j}=\left\{\begin{array}{c}
\lambda_{i}, \quad \text { if } i=j=1, . ., r \\
0, \text { otherwise }
\end{array}\right.
$$

then $\mathbf{V}$ and $\mathbf{W}$ are orthogonal matrices, $\mathbf{V V}^{\mathbf{t}}=\mathbf{I}_{\mathbf{n}}$ and $\mathbf{W}^{\mathbf{t}} \mathbf{W}=\mathbf{I}_{\mathbf{m}}$ are unitary matrices, and the singular decomposition of the matrix $A$ is

$$
\begin{equation*}
A=\mathbf{W} S \mathbf{V}^{t} \tag{16}
\end{equation*}
$$

## 3.2- Existence and uniqueness conditions

The new variables $Z=\mathbf{W}^{t} Y \in R^{m}$ and $X=\mathbf{V}^{t} U \in R^{n}$ are introduced. Tthen the linear inverse problem consists in finding the vector $X$ solution of the new uncoupled matrix equation

$$
\begin{equation*}
Z=[S] X \tag{17}
\end{equation*}
$$

where the vector $Z \in \mathbf{R}^{m}$ is given.
Example of SVD decomposition : $m=3, n=2$

| A |  | W |  |  | S |  | V |  |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 1 | 0 | 0.1826 | -0.8944 | -0.4082 | 2.4495 | 0 | 0.4472 | -0.8944 |
| -1 | 2 | -0.9129 | 0 | -0.4082 | 0 | 1.0000 | -0.8944 | -0.4472 |
| 0 | 1 | -0.3651 | -0.4472 | 0.8165 | 0 | 0 |  |  |

Consequently, there are $m$ algebraic equations to determine the $n$ components of the vector solution $X$ :

$$
\left\{\begin{array}{c}
\lambda_{i} X_{i}=Z_{i}, i=1, \ldots, r  \tag{18a}\\
\sum_{j=r+1, \ldots, n} 0 X_{j}=Z_{i}, i=r+1, . ., m
\end{array}\right.
$$

The condition of existence is clearly $Z_{i}=0, i=r+1, . ., m$.
More generally, $Z=\mathbf{W}^{t} Y \Rightarrow Z_{i}=\left\langle W_{i}^{*}, Y\right\rangle_{\mathbf{R}^{n}}$ and the subset of $\mathbf{R}^{m}$ generated by $\left\{W_{i}^{*} \in \mathbf{R}^{m}, i=1, . . r\right\}$ is called $\operatorname{Im}(A)$. Then the existence condition to the solution of the inverse problem is characterized by the orthogonal property equations :

$$
\begin{equation*}
Y \in \operatorname{Im}(A) \Leftrightarrow\left\langle W_{i}^{*}, Y\right\rangle=0, i=r+1, . ., m \tag{19}
\end{equation*}
$$

The uniqueness condition is clearly $r=n$, which is possible only if $m \geq n$

## 3.3- Quasi-solutions

The quasi-solutions are determined by introducing the least square criterion $J(\xi)=\|A \xi-Y\|_{\mathbf{R}^{m}}^{2}$ and by considering the vectors $U=\underset{\xi \in \mathbf{R}^{m}}{\arg \min } J(\xi)$ which minimize this criterion.

The differential of $J$ is $d J=2\left\langle A^{t} A \xi-A^{t} Y, d \xi\right\rangle_{\mathbf{R}^{m}}$, then the optimality condition $d J(U)=0, \forall d \xi$ leads to the matrix equation

$$
\begin{align*}
& A^{t} A U=A^{t} Y  \tag{20a}\\
& \text { or } \quad S^{t} S X=S^{t} Z \tag{20b}
\end{align*}
$$

Consequently, there are now $n$ algebraic equations to determine the $n$ components of the vector solution $X$ :

$$
\left\{\begin{array}{c}
\lambda_{i}^{2} X_{i}=\lambda_{i} Z_{i}, i=1, . ., r  \tag{21a}\\
\sum_{j=r+1, \ldots, n} 0 X_{j}=\sum_{j=r+1, ., m} 0 Z_{i}, i=r+1, . ., n
\end{array}\right.
$$

Thus, there is at least one quasi-solution, the existence condition is always satisfied. But, if $r<n$ (always true if $m<n$, sometime true otherwise), there are an infinite set of quasisolutions:

$$
\begin{equation*}
X=\sum_{i=1, \ldots, r} \frac{Z_{i}}{\lambda_{i}} \mathbf{V}_{i}+\sum_{i=r+1, \ldots, n} c_{i} \mathbf{V}_{i} \tag{22}
\end{equation*}
$$

where $\left\{c_{i}, i=r+1, . ., n\right\}$ is a set of arbitrary constant values.
One way to satisfy the uniqueness condition, consists in introducing some a priori estimate $X_{\text {est }}$ of the unknown solution. Then the set of arbitrary constant $\left\{c_{i}, i=r+1, . ., n\right\}$ is determined to get the closest solution $X^{*}$, e.g. the set of constant are searched for minimizing the distance $\left\|X^{*}-X_{\text {est }}\right\|$. The optimal quasi-solution $X^{*}$ associated to the a priori estimate $X_{\text {est }}$ satisfies the orthogonal properties $\left\langle\mathbf{V}_{i}, X_{i}^{*}-X_{\text {est }, i}\right\rangle=0, i=r+1, \ldots, n$, it is therefore :

$$
\begin{equation*}
X^{*}=\sum_{i=1, ., r} \frac{Z_{i}}{\lambda_{i}} \mathbf{V}_{i}+\sum_{i=r+1, \ldots, n} X_{e s t, i} \mathbf{V}_{i} \tag{23}
\end{equation*}
$$

The optimal quasi-solution $X^{*}$ associated to the $a$ priori estimate $X_{\text {est }}=\mathbf{0}$ is called the "minimal norm quasi-solution".

This mathematical analysis of the linear inverse problem $Y=A \cdot U$, where $A$ is a rectangular matrix ( $m \times n$ ), provides two main results

- If the observed output $Y \in \mathbf{R}^{m}$ does not belong to the subset of $\mathbf{R}^{m}$ generated by $\left\{W_{i}^{*} \in \mathbf{R}^{m}, i=1, . . r\right\}$, then $Y \notin \operatorname{Im}(A)$, there is no solution, but the resolution in the least square sense allows in any case to get at least one quasi-solution which minimizes the L-S criterion $J(\xi)=\|A \xi-Y\|_{\mathbf{R}^{m}}^{2}$.
- Then by introducing an a priori estimate $X_{\text {est }}$, it is possible to determine a unique quasi-solution.
This approach allows to satisfy both the existence and uniqueness conditions of Hadamard. The question of stability remains to be analyzed.


## 3.4- Stability condition and regularized solutions

3.4.1- The squared matrix case $m=n$

The matrix $A$ is assumed to be non singular and the observed output is corrupted by an additive noise :

$$
Y=Y_{e x}+\delta Y \text { with }\|\delta Y\|_{\mathbf{R}^{m}} \leq \varepsilon
$$

The matrix $\mathbf{W}^{\mathbf{t}}$ is orthogonal, then $\|\delta Y\|_{\mathbf{R}^{m}}=\|\delta Z\|_{\mathbf{R}^{m}} \leq \varepsilon$.
This error may affect all the components of $Z$. Suppose for simplicity that, the error corrupts only the component $k$, then : $\delta Z=\mathbf{W}^{t} \delta Y=\varepsilon W_{k}$, or $\delta Z_{k}=\varepsilon$,
The quasi-solution is

$$
\begin{equation*}
X=\sum_{i=1, ., n} \frac{Z_{i}}{\lambda_{i}} \mathbf{V}_{i} \tag{24}
\end{equation*}
$$

and $\delta X$ the error generated by $\delta Z_{k}=\varepsilon$, is $\delta X=\frac{\varepsilon}{\lambda_{k}} V_{k}$
e.g. the relative error variation is

$$
\begin{equation*}
\frac{\|\delta U\|_{\mathbf{R}^{n}}}{\|\delta Y\|_{\mathbf{R}^{m}}}=\frac{\|\delta X\|_{\mathbf{R}^{n}}}{\|\delta Z\|_{\mathbf{R}^{m}}}=\frac{1}{\lambda_{k}} \tag{25}
\end{equation*}
$$

This result means that an error $\varepsilon$ on the component $Z_{n}$ creates a perturbation on the solution which is $\lambda_{1} / \lambda_{n}$ times greater than the same error on the component $Z_{1}$. This ratio is called $\operatorname{cond}(A)$ the condition number of the matrix $A$. In practice, a large value for this ratio means that the solution will be very sensitive to the possible data errors.

### 3.4.2- The rectangular matrix case $m \neq n$

More generally, the matrix $A$ is rectangular ( $m \times n$ ), and the rank is $r \leq \inf (m, n)$. The sensitivity of the quasi-solutions to output data errors is characterized by the condition number of the matrix equation ():

$$
\begin{equation*}
\left[S^{t} S\right] \delta X=S^{t} \delta Z \tag{26}
\end{equation*}
$$

Note that even in the favorable case where $m \geq n$ and $r=n$, the value of $\operatorname{cond}\left(S^{t} S\right)$ is the ratio $\lambda_{1}^{2} / \lambda_{r=n}^{2}$ which is worst than cond(A), it means thar the last equation (26) is more badly conditionned than the original one (15)! To improve this ratio, the inversion process has to be "regularized".

## 4.- Regularization processes and stability condition

## 4.1- General ideas

There are several ways to regularize the inversion process. e.g. to make the quasi-solution less sensitive to the data errors and satisfy the stability condition. All of them consists in adding some a priori information. Two great approaches are briefly presented and illustrated:

- One approach consists in searching for a quasi-solution which satisfies some a priori constraints :

$$
\begin{equation*}
X_{c}=\arg \min _{X \in \chi}\|Z-S X\|^{2} \tag{27}
\end{equation*}
$$

Different possibilities are available for defining these constraints, the most usuals are the truncation of the basis $\left\{V_{i}^{*} \in \mathbf{R}^{n}, i=1, . . r\right\}$ or the parametrization of the solution

- An other approach is based on the "penalization" of the L-S criterion

$$
J(\xi)=\|S \xi-Z\|_{\mathbf{R}^{m}}^{2}
$$

Both of these approaches will lead to regularized but biased solutions. Then it may be underlined once more, that the regularization process aims to find some compromise between the accuracy and the stability requirements.

## 4.2- Regularization by truncation

The idea is to constrain the quasi-solution to belong to a sub-space $\chi \subset \mathbf{V}=\left\{V_{1}, \ldots, V_{n}\right\}$ where $\chi=\left\{V_{i} \in \mathbf{R}^{n}, i=1, . . p\right\}$ is obtained by truncation of the basis $\mathbf{V}$. The "regularizing parameter" is then the order $p<r$ of the truncation for which the condition number $\lambda_{1}^{2} / \lambda_{p}^{2}$ will become "acceptable".

In practice, this truncation means that the components of the output data $Y$ corresponding to the vectors $\left\{W_{i} \in \mathbf{R}^{m}, i=p+1, . . r\right\}$ will be eliminated in the inversion process, in order to avoid the amplification effect due to the smallest singular values. So the inversion process is performed on the modified output data

$$
\begin{align*}
& \tilde{Z}_{i}=\left\{\begin{array}{c}
Z_{i}, i=1, . . p \\
0, i=p+1, . . m
\end{array}\right.  \tag{28a}\\
& \tilde{Z}=\sum_{i=1, . . p} Z_{i} \mathbf{W}_{i} ; \text { with } Z_{\mathrm{i}}=\left\langle Y, \mathbf{W}_{i}\right\rangle_{\mathbf{R}^{m}} \tag{28b}
\end{align*}
$$

and the regularized solution is:

$$
\begin{equation*}
X_{c}=\sum_{i=1, \ldots p} \frac{\left\langle Z, W_{i}\right\rangle}{\lambda_{i}} \mathbf{V}_{i} \tag{30}
\end{equation*}
$$

Consequently, the inversion of the modified data instead of the original one will introduce a bias, e.g. a systematical error on the computed solution.

Numerical example : Consider the linear model equation $Y=A U$,
where $A=\left[\begin{array}{cccc}10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10\end{array}\right]$
The exact observed output ( without noise) is assumed to be $Y=\left|\begin{array}{llll}32 & 23 & 33 & 31\end{array}\right|^{t} ; \mid Y \| \approx 60$

The exact solution $U=A^{-1} Y$ is

$$
U=A^{-1} Y=\left|\begin{array}{llll}
1 & 1 & 1 & 1
\end{array}\right|^{t} ;\|U\|=2
$$

Introduce the additive error data

$$
\delta Y=\left|\begin{array}{llll}
0.1 & -0.1 & 0.1 & -0.1
\end{array}\right|^{t} ;\|\delta Y\|=\varepsilon=0.2
$$

Then the resulting error on $U$ is

$$
\delta \beta=A^{-1} \delta Y=\left|\begin{array}{llll}
8.2 & -13.6 & 3.5 & -2.1
\end{array}\right|^{t} ;\|\delta \beta\|=16.397
$$

and the amplification factor of the relative errors is

$$
G=\frac{\|\delta \beta\|}{\|\beta\|}\left[\frac{\|\delta Y\|}{\|Y\|}\right]^{-1}=2460.6!
$$

A spectral analysis confirms that the matrix $A$ is nearly singular .
Let $V$ and $D$ two matrices, where $V$ is orthogonal $\left(V^{-1}=V^{t}\right)$, and $D$ is diagonal, such that

$$
A V=V D \text { or } A=V D V^{t}
$$

Note that here $W \equiv V$. With MATLAB, they are found to be
[V,D]=eig(A)

| $\mathrm{V}=$ |  |  |  | $\mathrm{D}=$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0.5016 | -0.3017 | -0.6149 | 0.5286 |  |  |  |  |
| -0.8304 | 0.0933 | -0.3963 | 0.3803 |  | 0 | 0.8431 | 0 |
| 0 | 0 |  |  |  |  |  |  |
| 0.2086 | 0.7603 | 0.2716 | 0.5520 | 0 | 0 | 3.8581 | 0 |
| -0.1237 | -0.5676 | 0.6254 | 0.5209 | 0 | 0 | 0 | 30.2887 |

The ill-conditionness of the inversion operation is evaluated by the condition number of the matrix, it can be defined here by the ratio between the largest and the smallest eigenvalues

$$
\operatorname{cond}(A)=\frac{30.2887}{0.0102}=2.9841 e 3
$$

that is the same order of magnitude than the amplification factor.
The regularized solutions $U_{p}$ build by truncation of the basis $\mathbf{V}$ and the modified data $Y_{p}$ which results of the truncation are given in the following tables : the first column is the (exact) solution without noise on the $Y$ data, the following columns are computed with the
perturbed data: the second column is the solution without regularization $(p=0)$, the solutions in the columns three to five are obtained by taking respectively the truncation order $p=1,2,3$

| 1.0000 | 8.0000 | 1.1209 | 1.1090 | 1.0496 |
| :--- | :---: | :--- | :--- | :--- |
| 1.0000 | -10.600 | 0.7897 | 0.7934 | 0.7551 |
| 1.0000 | 3.9000 | 1.0397 | 1.0698 | 1.0960 |
| 1.0000 | -0.7000 | 0.9965 | 0.9740 | 1.0344 |
| p | 0 | 1 | 2 | 3 |

Table 1a: Exact and regularized solutions $U_{p}, p=0,1,2,3$ depending on the truncation order $p$

| 32.0000 | 32.1000 | 32.0302 | 32.0201 | 31.7910 |
| :--- | :--- | :--- | :--- | :--- |
| 23.0000 | 22.9000 | 23.0156 | 23.0187 | 22.8711 |
| 33.0000 | 33.1000 | 33.0710 | 33.0964 | 33.1976 |
| 31.0000 | 31.1000 | 31.1172 | 31.0982 | 31.3313 |
| p | 0 | 1 | 2 | 3 |

Table 1b: Exact and modified data $Y_{p}, p=0,1,2,3$ depending on the truncation order $p$
The norm of the deviations $\left\|Y_{p}-Y_{\text {exact }}\right\|$ between the modified data which results of the truncation process and the original one without noise are found to be :
$\left\|Y_{p}-Y_{\text {exact }}\right\|=\begin{array}{llll}0.2000 & 0.1412 & 0.1403 & 0.4573\end{array}$
and the norm of the deviations $\left\|U_{p}-U_{\text {exact }}\right\|$ between the regularized solution which results of the truncation and the exact solution are: $\left\|U_{p}-U_{\text {exact }}\right\|=\begin{array}{llll}13.9592 & 0.2459 & 0.2452 & 0.2699\end{array}$ They are plotted on the following figure versus ( $p+1$ ):

| $10^{2}$ |  |  |
| :--- | :--- | :--- |
| 10 | At the truncation order $p=3$, |  |
| we observe that |  |  |

Example 1 (see section 2.1.1) The application of the regularization process by truncation of the basis $\mathbf{V}$, to the first example of the inverse initial state problem is straightforward. By choosing a priori the order $p$ of truncation, the solution (eq.(4)) is "naturally" regularized and becomes:

$$
U_{c}=\sum_{n=1}^{p} \frac{\left\langle Y, \varphi_{n}\right\rangle}{\lambda_{n}} \cdot \varphi_{n} \text {, with } \lambda_{n}=e^{-n^{2} \pi^{2} t_{f}}
$$

## 4.3- Regularization by parametrization

The quasi-solution is constrained to belong to a sub-space $\chi=\mathbf{R}^{p}$, which is a priori given. By introducing a set of basis vectors $\left\{\omega_{i} \in \mathbf{R}^{p}, i=1, . . p\right\}$, the solution takes the parametrized form:

$$
\theta=\sum_{i=1, \ldots p} \theta_{i} \omega_{i}
$$

Example 3 (see section 2.1.3): application to the 2-D inverse heat source problem , eq.(12)

$$
Y=[C][A]^{-1}\left(\left[B_{1}\right] * T_{w}+\left[B_{4}\right] q\right)
$$

The unknown heat flux vector $q=\left[q\left(y_{i}\right)\right]_{i=1}^{n} \in \mathbf{R}^{n}$ is constrained to be determined under the parametrized form $q(y)=\sum_{j=1}^{p} \theta_{j} \omega_{j}(y)$. To choose the basis functions, a simple and usual approach consists in dividing the boundary $\Gamma_{4}=[0,1]$ into ( $p-1$ ) subintervals $\left[y_{k}, y_{k+1}\right], k=1, . . p-1$, and in constructing a set of $p$ linear piecewise functions (hat functions) such that : $\omega_{j}\left(y_{k}\right)=\delta_{j k}$. Then the linear mapping between the subspace $\chi=\mathbf{R}^{p}$ and the original space $\mathbf{R}^{n}$ is defined by a matrix equation $q=[M] \theta$, with $M_{i j}=\omega_{j}\left(y_{i}\right), i=1, . ., n ; j=1, . ., p$. More regular basis functions can be considered, like piecewise cubic polynomials (spline functions)...

Now the numerical conditionning of the linear inverse problem is characterized by the condition number of the new sensitivity equation :

$$
\delta Y=[C][A]^{-1}\left[B_{4}\right][M] \delta \theta=[X][M] \delta \theta
$$

The old sensitivity matrix [ $X$ ], eq.(13), is replaced by the new one $[X][M]$. The previous conditionning which was equal to cond $\left(X^{t} X\right)$, becomes cond $\left(M^{t} X^{t} X M\right)$.

## Numerical results

Let us compare the numerical values of the condition number for this inverse problem, cond $\left(X^{t} X\right)$ and cond $\left(M^{t} X^{t} X M\right)$, respectively before and after the regularization process by parametrization. The temperature field solution of the direct problem is computed with a $n \times n$ spatial grid. By taking $m=n-1$, the following values of the condition numbers are found:

| $n$ | 5 | 8 | 11 | 16 | 21 | 26 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\operatorname{cond}\left(X^{\prime} * X\right)$ | $9.2987 \mathrm{e}^{+}+004$ | $5.0208 \mathrm{e}+009$ | $2.3942 \mathrm{e}+014$ | $1.1284 \mathrm{e}+019$ | $4.7040 \mathrm{e}+020$ | $8.1567 \mathrm{e}+020$ |

Table 2.a - cond $\left(X^{t} X\right)$ before parametrization

| $\boldsymbol{n}$ | $\mathbf{1 6}$ | $\mathbf{2 1}$ | $\mathbf{2 6}$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{p}=5 \mathrm{yp}=[0 ; 0.25 ; 0.5 ; 0.75 ; 1.0]$ | $7.5950 \mathrm{e}+008$ | $6.5797 \mathrm{e}+008$ | $5.8852 \mathrm{e}+008$ |
| $\mathrm{p}=4 \mathrm{yp}=[0 ; 0.3 ; 0.6 ; 1.0]$ | $1.6898 \mathrm{e}+006$ | $1.6087 \mathrm{e}+006$ | $1.5596 \mathrm{e}+006$ |

Table $2 \mathrm{~b}-\operatorname{cond}\left(M^{t} X^{t} X M\right)$ after parametrization


This example shows the efficiency of this regularizing process: after parametrization of the function to be determined, the condition number of the inverse problem becomes independent of the mesh size of the spatial grid, then a good accuracy of the numerical solution of the direct problem can be reached without increasing the ill-conditionness of the inverse problem.

Some a priori information on the regularity of the function to be estimated has to be introduced to decide of the order $p$ of the parametrization.

## 4.4- Regularization by penalization

The linear inverse problem $Y=A . U$ was solved in the least square sense by searching $U=\underset{\xi \in \mathbf{R}^{m}}{\arg \min } J(\xi)$, with $J(\xi)=\|A \xi-Y\|_{\mathbf{R}^{m}}^{2}$, or equivalently after the SVD analysis of the matrix $A=\mathbf{W} S \mathbf{V}^{t}$, by minimizing $J(\xi)=\|S \xi-Z\|_{\mathbf{R}^{m}}^{2}$

The idea of the regularization process by "penalization" consists in considering a new L-S criterion which includes the a priori estimate $X_{\text {est }}$ and a positive parameter $\mu \in[0,1]$, socalled regularization parameter :

$$
\begin{equation*}
J_{\mu}(\xi)=(1-\mu)\|S \xi-Z\|_{\mathbf{R}^{m}}^{2}+\mu\left\|\xi-X_{e s t}\right\|_{\mathbf{R}^{n}}^{2} \tag{31}
\end{equation*}
$$

For each value of the parameter $\mu$, there is a unique solution $X_{\mu}^{*}=\arg \min _{\xi \in \mathbf{R}^{m}} J_{\mu}(\xi)$ which minimizes the penalized L-S criterion. The value $\mu=0$ leads to the L-S quasi-solution discussed above which is independent of the a priori estimate, and the value $\mu=1$ gives the solution $X=X_{\text {est }}$ which is independent of the output data. Thus the regularization parameter introduced to determine some compromise between the available data, will take into account the respective confidence of each data.

The optimality condition

$$
\delta J_{\mu}\left(X^{*}\right)=2\left\langle(1-\mu)\left(\left[S^{t} S\right] X^{*}-S^{t} Z\right)+\mu\left(X^{*}-X_{e s t}\right), \delta \xi\right\rangle_{\mathbf{R}^{n}}=0, \forall \delta \xi \in \mathbf{R}^{n}
$$

gives the "regularized" quasi-solution

$$
\begin{equation*}
X_{\mu}^{*}=\left[(1-\mu) S^{t} S+\mu I\right]^{-1}\left[(1-\mu) S^{t} Z+\mu X_{e s t}\right] \tag{32}
\end{equation*}
$$

The eigenvalues of the matrix $\left[(1-\mu) S^{t} S+\mu I\right]$ are equal to $(1-\mu) \lambda_{i}^{2}+\mu, i=1, . ., n$, they are strictly positive for any positive values of $\mu$. The components of the "regularized" quasisolution are

$$
X_{i}^{*}=\frac{(1-\mu) \lambda_{i} Z_{i}+\mu X_{i, \text { est }}}{(1-\mu) \lambda_{i}^{2}+\mu}, i=1, . ., n
$$

Changing $Z$ by $Z+\delta Z$ gives

$$
X_{i}^{*}+\delta X_{i}^{*}=\frac{(1-\mu) \lambda_{i}\left(Z_{i}+\delta Z_{i}\right)+\mu X_{i, \text { est }}}{(1-\mu) \lambda_{i}^{2}+\mu}, i=1, . ., n
$$

thus it comes

$$
\delta X_{i}^{*}=\frac{(1-\mu) \lambda_{i}}{(1-\mu) \lambda_{i}^{2}+\mu} \delta Z_{i}, i=1, . ., n
$$

and the continuity modulus given by

$$
\begin{equation*}
\rho(\mu)=\max _{i \leq r} \frac{\left|\delta X_{i}^{*}\right|}{\left|\delta Z_{i}\right|}=\max _{i \leq r} \frac{(1-\mu) \lambda_{i}}{(1-\mu) \lambda_{i}^{2}+\mu} \tag{33}
\end{equation*}
$$

is a decreasing function the parameter $\mu, \forall \mu \in] 0,1]$
The study of the influence of the regularization parameter on the condition number of the matrix $\left[(1-\mu) S^{t} S+\mu I\right]$ leads to similar results:

$$
\begin{equation*}
K(\mu)=\operatorname{cond}\left(\left[(1-\mu) S^{t} S+\mu I\right]\right)=\max _{j \leq r} \frac{(1-\mu) \lambda_{1}^{2}+\mu}{(1-\mu) \lambda_{j}^{2}+\mu} \tag{34}
\end{equation*}
$$

These results mean that the stability of the quasi-solution obtained with the "penalization" method will be improved by increasing the regularization parameter.
To answer the question of any practionner which want do know how to decide the value of the parameter $\mu$, let us recall that the introduction of the a priori estimate leads to biased solutions.

## Numerical example

It can be observed first by computating the residual $J\left(X_{\mu}^{*}\right)=\left\|S X_{\mu}^{*}-Z\right\|_{\mathbf{R}^{m}}^{2}$ as a function of $\mu$, that there is an optimal value $\mu_{\text {opt }}$ for which the residual is minimum.
Let us continue the numerical example studied in the previous section. We consider now the quasi-solution which minimizes the regularized LS criterion (eq. (31)):

$$
J_{\mu}(U)=\left\|Y_{\varepsilon}-A U\right\|^{2}+\mu\|U\|^{2}
$$

where the a prior estimate is equal to zero, $U_{\text {est }}=0$ and $Y_{\varepsilon}=Y+d Y,\|d Y\|=\varepsilon$
Note that here for simplicity (and without loss of generality), the scalar $\mu$ is used instead of $\mu /(1-\mu)$

The vector solution $U_{\mu, \varepsilon}$ which minimizes $J_{\mu}(U)$ is $U_{\mu, \varepsilon}=[A+\mu I]^{-1} Y_{\varepsilon}$;
The exact solution being known, the error estimate $d U$ can be computed. For a fixed noise level $\varepsilon$, this error depends on the scalar $\mu$ :

$$
d U=[A+\mu I]^{-1} Y_{\varepsilon}-A^{-1} Y
$$

With $\|\delta Y\|=\varepsilon=0.2$, the graphic representation of the norm $\|d U\|$ of the error estimate, versus the scalar $\mu$, shows an optimal value.

However in practice the exact solution (without noise $U=A^{-1} Y$ ) is unknown and this method is not practicable to determine the best value of $\mu$.


Figure 6 : Optimal value of the regularizing parameter

## The L-curve method

The correct choice of the regularization parameter is a nontrivial problem for which numerous solutions have been proposed. The L-curve method (due to Hansen ,1992) despite limitations has become a popular means of choosing a suitable value. One variant form of the method consists in a graphical analysis of a log-log plot :

$$
\begin{equation*}
\mathrm{x}(\mu)=\left\|S X_{\mu}^{*}-Z\right\|_{\mathbb{R}^{m}}^{2} \text { versus } \mathrm{y}(\mu)=\left\|X_{\mu}^{*}-X_{\text {est }}\right\|_{\mathbb{R}^{n}}^{2} \tag{35a}
\end{equation*}
$$

computed for different values of the parameter $\mu$. The curve $\mathrm{y}(\mathrm{x})$ shows an almost vertical part for very small values of $\mu$, while it is almost horizontal for larger values. The L-curve selection criterion consists of locating the $\mu_{K}$ value which maximises the curvature, that is the L-curve corner which separates two regions: for $\mu<\mu_{K}$, the solution is under-regularized, while for $\mu>\mu_{K}$, it is over-regularized.

## Numerical results

Let us continue the previous example. The L-curve is plotted for different values of the regularization parameter : $0.001<\mu<10$ (logarithmically equally spaced values). For each value, the regularized solution $X_{\varepsilon, \mu}$ is obtained according to the above equation (32) :

$$
\begin{aligned}
& X_{\varepsilon, \mu}=\left[D^{t} D+\mu I\right]^{-1} D^{t} Z \\
& Z=W Y_{\varepsilon}
\end{aligned}
$$

with the a priori estimate $X_{\text {est }}=0$. The L-curve corner where the curvature of the log-log plot is maximised is readily visible. It does not correspond to one specific value of the regularizing parameter but to some interval between $\mu=0.1$ and $\mu=1.0$


## Determination of the optimal value- Numerical results

For linear inverse problems, the penalized criterion, eq.(31), which is minimized to build the regularized solution is quadratic, then it possible to determine the optimal value of the regularization parameter.

Introduce the new variables $Z=V^{t} Y, X=V^{t} U$, then using the properties of the matrix $V$ : $V^{t} V=I$ and $\|V\|=1$, the LS criterion can be re-written as

$$
S_{\mu}=\|Z-D X\|^{2}+\mu\|X\|^{2}
$$

and the minimum $X^{*}$ of $S_{\mu}$ is reached for

$$
\left(D^{t} D+\mu I\right) X^{*}=D^{t} Z
$$

The components are $X_{i}{ }^{*}=\frac{\lambda_{i} Z_{i}}{\lambda_{i}^{2}+\mu}$
where $\lambda_{i}, \quad i=1,4$ are the eigenvalues of the matrix $A$

One way to determine the regularizing parameter $\mu$, for such quadratic case, consists in choosing the value for which the LS-residual will be equal to the noise level (discrepancy principle)

$$
\begin{equation*}
\|Z-D X\|^{2}=\varepsilon^{2} \tag{36}
\end{equation*}
$$

or $\mu$ solution of the algebraic equation

$$
\begin{aligned}
& \varphi(\mu)=\sum_{i}\left[Z_{i}-\frac{\lambda_{i}^{2} Z_{i}}{\lambda_{i}^{2}+\mu}\right]^{2}-\varepsilon^{2}=0 \\
& \text { or } \quad \varphi(\mu)=\sum_{i}\left[\frac{\mu Z_{i}}{\lambda_{i}^{2}+\mu}\right]^{2}-\varepsilon^{2}=0
\end{aligned}
$$

Numerical Solution computed with MATLAB

```
% optimal value of the function y=tikho(mu)
%regularizing parameter mu
[V,D]=eig(A)
Z=V'*(Y+dY);
ndy=norm(Y+dY) ;
muopt=fzero('tikho',1)
for i=1:4
X(i)=D(i,i)*Z(i)/(D(i,i)*D(i,i)
+muopt);
end
% regularized solution
U=V*X'
```

```
global D Z ndy
```

global D Z ndy
s=0;
s=0;
n=size(Z);
n=size(Z);
for i=1:n
for i=1:n
s=s+((mu*Z(i))/(D(i,i)*D(i,i)+mu))^2;
s=s+((mu*Z(i))/(D(i,i)*D(i,i)+mu))^2;
end
end
y=s-ndy*ndy;

```
y=s-ndy*ndy;
```

Zero found in the interval: [0.54745, 1.4525].
muopt $=1.4065$
$\mathrm{U}_{\text {opt }}=\left[\begin{array}{llll}1.1096 & 0.8013 & 1.0849 & 0.9391\end{array}\right]$
Note that for this example, the rule $\left\|Z-D X_{\mu_{o t t}}\right\|^{2}=\varepsilon^{2}$ adopted for determining the optimal value leads to a value located just after the L-curve corner, close to the over-regularized region.

## 4.5-The discrepancy principle and the conjugate gradient algorithm

For large scale linear inverse problems, or non linear problems, direct computation of the SVD can become non efficient or impracticable. In any case, the conjugate gradient method [1], [7] is well known to be among the most effective to compute regularized solution according to the discrepancy principle [6].

The method is based :
a) on the iterative computation of the gradient $\nabla J\left(U^{n}\right)$ of the the L-S criterion, at each iteration $n$ :

$$
\begin{aligned}
& J\left(U^{n}\right)=\left\|Y_{\varepsilon}-A U^{n}\right\|^{2} \\
& \nabla J\left(U^{n}\right)=-2 A^{t}\left[Y_{\varepsilon}-A U^{n}\right], n=0,1, . .
\end{aligned}
$$

b) in order to determine a new approximation of the solution :

$$
\begin{aligned}
& U^{n+1}=U^{n}+\gamma^{n} d^{n} \\
& d^{n}=-\nabla J\left(U^{n}\right)+\beta^{n} d^{n-1} \\
& \beta^{0}=0 ; \quad \beta^{n}=\left\|\nabla J\left(U^{n}\right)\right\|^{2} /\left\|\nabla J\left(U^{n-1}\right)\right\|^{2}
\end{aligned}
$$

where $\gamma^{n}=\underset{\gamma>0}{\operatorname{argmin}} J\left(U^{n}+\gamma d^{n}\right)$ is obtained by minimizing a scalar function,
c) and to use the regularizing discrepancy principle as a stopping rule :

$$
J\left(U^{n f}\right)=\left\|Y_{\varepsilon}-A U^{n f}\right\|^{2} \approx \varepsilon,
$$

where $\|\delta Y\|_{\mathbf{Y}}^{2}=\varepsilon$ is a measurement error computed in the $\mathbf{Y}$ space
Then, the last iteration index $n f$ is the regularization parameter in this method. Note that some a priori information on the noise level $\|\delta Y\|_{\mathrm{Y}}^{2}=\varepsilon$ of the output data has to be considered.

## Example-

The conjugate gradient algorithm is used for the determination of the quasi-solution of the inverse boundary heat source problem, example 2, section 2.1.2. It aims to determine the function $U$ over the time interval $\left[0, t_{f}\right]$, from the observed output data $Y_{\varepsilon}$ and the knowledge of the impulse function $f$, eq(5). It is based on the computation of the gradient of the LS-criterion.

The output $Y_{\varepsilon}$ is computed first, as the solution of the direct problem, with the input $U$ shown on the following plot. Additive noise will be consider later.

According to the method developed above, the determination of the quasi-solution of the inverse problem is based on the introduction of the LS-criterion $J(\xi)=\|A \xi-Y\|_{L^{2}}^{2}$ which here takes the form:

$$
J(U)=\frac{1}{2} \int_{0}^{t_{f}}\left[Y(t ; U)-Y_{\varepsilon}(t)\right]^{2} d t=\frac{1}{2}\left\|Y(U)-Y_{\varepsilon}\right\|_{L^{2}}^{2}
$$



Figure 8 : Input and output variables for the semi-infinite heat conducting body
Let us denote :

$$
\begin{aligned}
& Y(U)=f * U \quad \text { the convolution integral of the functions } f \text { and } U \text {, and } \\
& \langle\psi, u\rangle=\int_{0}^{t_{f}} \psi(t) u(t) d t \text { the inner product of the functions } \psi \text { and } U
\end{aligned}
$$

The optimality condition which characterizes the quasi-solution $U^{*}=\underset{\xi \in \mathrm{L}^{2}}{\arg \min } J(\xi)$ is

$$
d J=\left\langle\nabla J\left(U^{*}\right), \delta U\right\rangle_{\mathbf{L}^{2}}=0, \forall \delta U
$$

where $\nabla J\left(U^{*}\right)$ is the gradient of $J$ with respect to $U$.

Developping the differential of the the LS-criterion gives :

$$
d J=\left\langle Y(U)-Y_{\varepsilon}, f^{*} \delta U\right\rangle_{\mathbf{L}^{2}}
$$

To transform this last equation under the form above which involves the gradient, we denote $\psi=\left(Y(U)-Y_{\varepsilon}\right)$, and we start from the definition of the convolution integral:

$$
\langle\psi, f * \delta U\rangle=\int_{0}^{t_{f}} \psi(t) \int_{0}^{t} f(t-x) \delta U(x) d x d t
$$

Using the property of the function $f$ :

$$
x>t \Rightarrow t-x<0 \Rightarrow f(t-x)=0
$$

the last double integral becomes

$$
\langle\psi, f * \delta U\rangle=\int_{0}^{t_{f}} \delta U(x) \int_{0}^{t_{f}} \psi(t) f(t-x) d t d x
$$

then the gradient of $J$ is the function

$$
\begin{aligned}
& \nabla J(x)=\int_{0}^{t_{f}} \psi(t) f(t-x) d t, 0<x<t_{f} \\
& \nabla J(x)=\int_{x}^{t_{f}} \psi(t) f(t-x) d t, 0<x<t_{f}
\end{aligned}
$$

or, finally by noting $x$ the mute variable instead of $t$

$$
\begin{gathered}
\nabla J(t)=\int_{t}^{t_{f}} \psi(x) f(x-t) d x, 0<t<t_{f} \\
\nabla J(t ; U)=\int_{t}^{t_{f}}\left[Y(x ; U)-Y_{\varepsilon}(x)\right] f(x-t) d x, 0<t<t_{f}
\end{gathered}
$$

Then the gradient can be computed, and the conjugate gradient algorithm can be performed.
Numerical results
To compute $Y(t ; u)$ and $\nabla J(t ; U)$, the time variable is discretized

$$
t_{k}=k \Delta t, \quad \Delta t=\frac{t_{f}}{n f}
$$

where $n f$ is the number of time steps, and the integrals equation are put in the standard algebraic forms

$$
\begin{aligned}
& Y_{k}=Y\left(t_{k}\right)=\sum_{i=1}^{k} f_{k-i} U_{i}, k=1, . ., n f \\
& \nabla J_{k}=\nabla J\left(t_{k}\right)=\sum_{i=k+1}^{n f} f_{i-k} \psi_{i} \quad k=1, . ., n f
\end{aligned}
$$

with

$$
f_{n}=f\left(t_{n}\right)=f(n \Delta t)=\frac{1}{\sqrt{t_{n}}} \exp \left(-\frac{1}{\sqrt{t_{n}}}\right) \Delta t, \quad n=1, . ., n f
$$

The solution is computed over the time interval $\left[0, t_{f}=5\right\rfloor$, with $\Delta t=0.1$ and $n f=50$. An normally distributed noise is added to get the output data $Y_{\varepsilon}$. Two numerical experiments are performed with different noise level.

For both cases, the initial guess is taken equal to zero : $U_{i}^{(0)}=0, i=1 . . n f$, and the discrepancy principle is adopted to stop the iterative conjugate gradient algorithm which produces the following results shown on Figures 9 and 10.


Figure 9a: Exact input and computed solution after 5 iterations


Figure 9b : Output data and computed output after 5 iterations

$\varepsilon^{2}=\|\delta Y\|^{2}=53.30$
Figure 10a : Exact input and computed solution after 4 iterations


Figure 10b : Output data and computed output after 4 iterations

This example shows how the computation of the gradient of the LS criterion allows to construct the numerical solution of an inverse input problem formulated with an integral equation. Due to the linearity of the modelling equations, the criterion is quadratic, and the iterative conjugate gradient algorithm is very well adapted. The discrepancy principle is an efficient way to avoid the amplification of the data errors, and it is easy to implement.

This algorithm is widely used for solving more complex inverse heat transfer problems. Several examples with computational MATLAB codes can be found in the reference [7].

## 5.-Conclusion

A key feature of inverse problems is their ill-posedness. They do not fulfil Hadamard's classical requirements of existence, uniqueness and stability. Construction of quasi-solutions by minimizing an output least square criterion is a general approach for solving.

Some mathematical aspects of the resolution of linear inverse problems in the finite dimensional case, were given to analyse and to overcome their ill-posed characteristics. Basic algebra results led to efficient algorithms for the computation of regularized solutions. They are based on the singular value decomposition (SVD analysis) of the linear operator.

To make the quasi-solutions less sensitive to the data errors and satisfy the stability condition, e.g. to regularize the inversion process, some adding a priori information has to be considered. Two basic approaches were briefly presented and illustrated: one consists in searching for quasi-solutions which satisfy some a priori constraints, another one is based on the "penalization" of the L-S criterion. Finally the conjugate gradient algorithm to be known among the most effective method to compute regularized solution according to the discrepancy principle, was illustrated by solving the numerical solution of an inverse input problem formulated with an integral equation.

Other standard regularizing methods have not been discussed in this short lecture, most of them can be found in the Inverse Engineering Handbook [7].

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Appendix - Conjugate Gradient Algorithm for solving the linear inverse heat source problem

```
% Semi-infinite body
% Inverse input problem
% Integral Equation model
% Conjugate gradient algorithm
clear
dt=0.1;nf=50;
% the discretized heat flux
for n=1:nf
    axet(n)=dt*n;
    if n<11
                q(n)=n;
    elseif n<31
        q(n)=20-n;
    elseif n<41
            q(n)=-40+n;
    else
        q(n)=0;
    end
end
qexact=q;
% the output measurement
% with additive noise
for n=1:nf
    s=0;
    for i=1:n-1
        s=s+impulse(n-i)*q(i);
    end
    Y(n)=s;
end
A=0.2;
noise=A*randn(size(Y));Y=Y+noise;
eps=norm(noise)^2
% conjugate gradient algorithm
q(1:nf)=0;ls=1e9;iter=1;
while ls>eps
    iter
    % compute the LS-criterion
    for n=1:nf
        s=0;
        for i=1:n-1
            s=s+impulse(n-i)*q(i);
        end
        T(n)=s;psi(n)=Y(n)-T(n);
    end
    ls=0.5*norm(psi)^2
    lsw(iter)=ls;
```


[^0]:    ${ }^{1}$ Lecture given at Eurotherm Winter School, METTI 2005, Aussois, January 16-21,2005

