

T11 Inversion using SVD and TSVD

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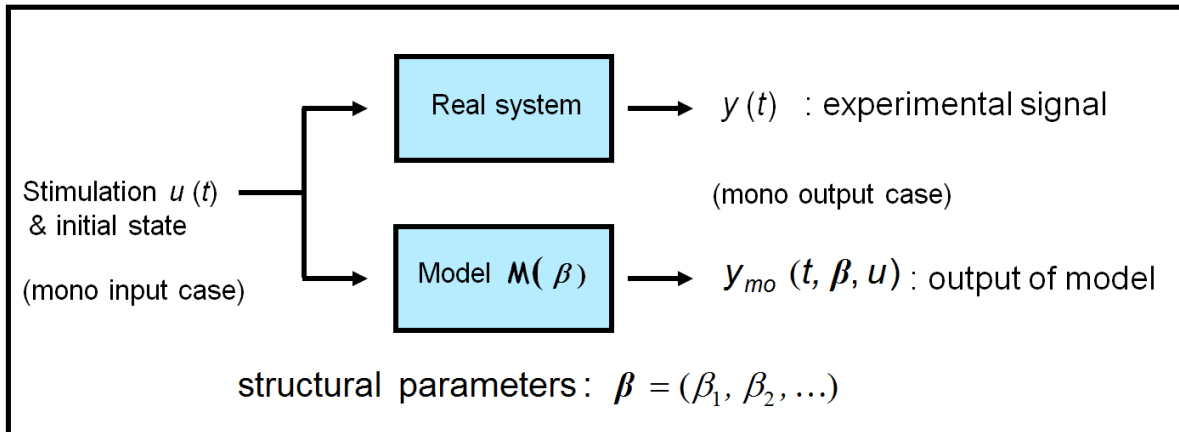
Abstract. Singular Value Decomposition (SVD) is a linear algebra process that allows to decompose any square or rectangular, real or complex, matrix into a product of three matrices, its central matrix being diagonal. Its diagonal coefficients are the singular values of the original matrix, which are all real and positive (or zero) numbers. This decomposition can be seen as a generalization of the eigenvalue decomposition that is valid only for square matrices. In this tutorial we will consider SVD either as a tool for calibrating a linear model (system identification) with a further use in inverse input problems, or for processing a large amount of space/time data that can be met when measuring temperatures using infrared thermography. In both applications, in order either to tackle the original ill-posed character of the original inverse problem (where the matrix at stake is the sensitivity matrix), or to perform some specific kind of data reduction (where the matrix at stake is the matrix of space/time data), the original SVD decomposition has to be modified. It gives rise to two types of regularization: Truncated SVD (TSVD) or Tikhonov regularization of zero order.

These two different problems, identification/inverse input problem and data reduction will be studied using two examples in this tutorial: a deconvolution problem by decomposition the sensitivity matrix and an initial temperature field reconstitution by decomposition of the space and time observable data.

11.1 Input estimation, identification and data reduction

We consider here three types of experimental inverse problems where Singular Value Decomposition (SVD) can be used :

- estimation of input $u(t)$, starting from the measurement of its output $y(t)$: this problem, where *the structure* of the model $\mathbf{M}(\beta)$ as well as its structural parameters β^{exact} are known is an *inverse input problem*;
- identification of a model, starting from experimental measurements of *both* input and output;
- data reduction or filtering, in case of multi-output time-space signal $y(\mathbf{P}, t)$ where \mathbf{P} can be any pixel on a surface field (case of infrared thermography measurements for example).



11.2 Introduction: the SVD decomposition

Any rectangular matrix (called \mathbf{K} here) with real or complex coefficients and of dimensions (m, n) with $m \geq n$ (SVD also exists in the case $m < n$, but it won't be dealt with here), can be written under the form:

$$\mathbf{K} = \mathbf{U} \mathbf{W} \mathbf{V}^t \text{ that is } \left[\begin{array}{c} \mathbf{K} \\ \mathbf{K} \end{array} \right] = \left[\begin{array}{c} \mathbf{U} \\ \mathbf{U} \end{array} \right] \left[\begin{array}{ccc} w_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & w_n \end{array} \right] \left[\begin{array}{c} \mathbf{V}^t \\ \mathbf{V}^t \end{array} \right] \quad (11.1)$$

where superscript t stands for the conjugate transpose of the corresponding matrix. If the coefficients of \mathbf{K} are real, it is simply its transpose.

This expression is sometimes called "thin" or "economy size" SVD and involves:

- \mathbf{U} , a unitary matrix (orthogonal if \mathbf{K} is real) of dimensions (m, n) : its column vectors (the *left* singular vectors of \mathbf{K}) 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 $\mathbf{K} \mathbf{K}^t$. Let us note that, in the general case, $\mathbf{U} \mathbf{U}^t \neq \mathbf{I}_m$.
- \mathbf{V} , a square unitary matrix (orthogonal if \mathbf{K} is real) 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 $\mathbf{K}^t \mathbf{K}$;
- \mathbf{W} , a square diagonal matrix of dimensions $(n \times n)$, that contains the n so-called *singular* values of matrix \mathbf{K} , ordered according to decreasing values: $w_1 \geq w_2 \geq \dots \geq w_n$. The singular values of matrix \mathbf{K} are defined as the square roots of the eigenvalues of matrix $\mathbf{K}^t \mathbf{K}$. If matrix \mathbf{K} is square and symmetric, its eigenvalues and singular values are the same.

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

$$\mathbf{K} = \mathbf{U}_0 \mathbf{W}_0 \mathbf{V}^t \quad \text{with} \quad \mathbf{U}_0 = \begin{bmatrix} \mathbf{U} & \mathbf{U}_{comp} \end{bmatrix}; \quad \mathbf{W}_0 = \begin{bmatrix} \mathbf{W} \\ \mathbf{0}_{(m-n) \times n} \end{bmatrix} \quad \text{and} \quad \dim(\mathbf{U}_{comp}) = m \times (m-n) \quad (11.2)$$

or:

$$\begin{bmatrix} \mathbf{K} \end{bmatrix} = \begin{bmatrix} \mathbf{U} & \mathbf{U}_{comp} \end{bmatrix} \begin{bmatrix} w_1 & & 0 \\ & \ddots & \\ 0 & & w_n \\ 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} \mathbf{V}^t \end{bmatrix} \quad (11.3)$$

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

$$\mathbf{U}_0^t \mathbf{U}_0 = \mathbf{U}_0 \mathbf{U}_0^t = \mathbf{U} \mathbf{U}^t + \mathbf{U}_{comp} \mathbf{U}_{comp}^t = \mathbf{I}_m \quad (11.4)$$

This singular value decomposition (11.4) can be implemented for any matrix \mathbf{K} , with real or complex value coefficients, for $m \geq n$.

11.3 Interest of the Singular Value Decomposition in linear parameter estimation

If all the n parameters in a parameter vector \mathbf{x} are looked for, for a linear model $\mathbf{y}_{mo}(\mathbf{x}) = \mathbf{S} \mathbf{x}$, where m noised measurements $\mathbf{y} = \mathbf{S} \mathbf{x} + \varepsilon$ are available, and if noise ε is independent and identically distributed (i.i.d.), that is $\text{cov}(\varepsilon) = \sigma_\varepsilon^2 \mathbf{I}_m$, its Ordinary Least Square (OLS) estimator can be written (see Lecture 3 of this Metti school):

$$\hat{\mathbf{x}}_{OLS} = (\mathbf{S}^t \mathbf{S})^{-1} \mathbf{S}^t \mathbf{y} \quad \text{with} \quad \mathbf{E}(\varepsilon) = \mathbf{0} \quad \text{and} \quad \text{cov}(\hat{\mathbf{x}}_{OLS}) = \sigma_\varepsilon^2 (\mathbf{S}^t \mathbf{S})^{-1} \quad (11.5)$$

Of course, in order for the inverse of the information matrix $\mathbf{S}^t \mathbf{S}$ to exist, matrix \mathbf{S} must not be singular, which means that its n sensitivity column vectors should form a free system of vectors (see lecture L8 in this series): the rank of \mathbf{S} should be equal to n .

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

We assume here that all the coefficients of \mathbf{x} have the same unit as all the coefficients of \mathbf{y} . This is the case for input estimation problems where \mathbf{y} is for example the vector of the sampled measured temperatures at m times t_i and \mathbf{x} the parameterized heat source $x(t)$ using a basis composed of n functions $g_j(t)$:

$$x(t) \approx x_{param}(t) = \sum_{j=1}^n x_j g_j(t) \Rightarrow x_{param}(t_i) = \mathbf{g}(t_i) \mathbf{x} \quad (11.6)$$

$$\text{with } \mathbf{g} = \begin{bmatrix} g(t_i) & g_2(t_i) & \cdots & g_n(t_i) \end{bmatrix} \text{ and } \mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}^t$$

In this parameterization a column-vector \mathbf{x} composed of n coefficients has replaced a function $x(t)$ of infinite continuous dimensions.

So, it is now possible to write the thin SVD decomposition of \mathbf{S}^* , which uses the notion of Euclidian norm of different true vectors, see equation (11.1):

$$\mathbf{S} = \mathbf{U} \mathbf{W} \mathbf{V}^t \quad (11.7)$$

It is now possible to calculate the amplification coefficient of the relative error k_r , see equation (1.7) in Lecture 1 of the same series:

$$k_r(\varepsilon) = \frac{\|\mathbf{e}_x\| / \|\mathbf{x}_{exact}\|}{\|\varepsilon\| / \|\mathbf{y}_{mo}(\mathbf{x}_{exact})\|} \quad \text{with} \quad \mathbf{e}_x = \hat{\mathbf{x}} - \mathbf{x}_{exact} \quad (11.8)$$

Using the properties of matrices \mathbf{U} and \mathbf{V} described in section 1, one can show:

$$\left. \begin{aligned} \|\mathbf{e}_x\| &= \|\mathbf{V} \mathbf{W}^{-1} \mathbf{U}^t \varepsilon\| \leq \|\mathbf{V} \mathbf{W}^{-1} \mathbf{U}^t\| \|\varepsilon\| \\ \|\mathbf{y}_{mo}(\mathbf{x}_{exact})\| &= \|\mathbf{S} \mathbf{x}\| \leq \|\mathbf{U} \mathbf{W} \mathbf{V}^t\| \|\mathbf{x}\| \end{aligned} \right\} \Rightarrow k_r(\varepsilon) \leq \|\mathbf{V} \mathbf{W}^{-1} \mathbf{U}^t\| \|\mathbf{U} \mathbf{W} \mathbf{V}^t\| = \|\mathbf{S}^+\| \|\mathbf{S}\| \quad (11.9)$$

One can recognize in the right-hand term of the last inequality (11.9) the product of the norms of two matrices. The second matrix is simply the SVD form of the reduced sensitivity matrix \mathbf{S}^* while the first one is just the pseudo inverse of \mathbf{S}^* , which is noted \mathbf{S}^+ here.

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

$$\|\mathbf{K}\|^2 = \text{Max}_{\|\mathbf{z}\|=1} (\mathbf{z}^t \mathbf{K}^t \mathbf{K} \mathbf{z}) = w_1^2(\mathbf{K}) \quad (11.10)$$

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

$$\|\mathbf{S}\| = w_1(\mathbf{S}) \quad \text{and} \quad \|\mathbf{S}^+\| = w_1(\mathbf{S}^+) = \frac{1}{w_n(\mathbf{S})} \quad (11.11)$$

So, it can be shown, using (11.8), (11.9) and (11.11) that the maximum value of the amplification coefficient of the relative error k_r , that is the criterion that assesses the ill-posed character of the OLS parameter estimation problem is equal to the condition number, noted $\text{cond}(\cdot)$ here, of the reduced sensitivity matrix:

$$k_r(\varepsilon) \leq \text{cond}(\mathbf{S}^*) = \frac{w_1(\mathbf{S})}{w_n(\mathbf{S})} \quad (11.12)$$

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

$$\hat{\mathbf{x}}_{\alpha}^{TSVD} = \mathbf{V} \mathbf{W}_{\alpha}^{-1} \mathbf{U}^t \mathbf{y} \quad (11.17)$$

Let us note that \mathbf{W}_{α} cannot be calculated since the $n-\alpha$ smallest singular values of \mathbf{S} , $w_{\alpha+1}, w_{\alpha+2}, \dots, w_{n-1}, w_n$, have been given an infinite level.

The TSVD solution (11.17) can be rewritten using the left and right singular column vectors \mathbf{U}_k and \mathbf{V}_k defined in section 1:

$$\hat{\mathbf{x}}_{\alpha}^{TSVD} = \begin{bmatrix} \mathbf{V}_1 & \mathbf{V}_2 & \dots & \mathbf{V}_{\alpha} \end{bmatrix} \begin{bmatrix} 1/w_1 & & & 0 \\ & 1/w_2 & & \\ & & \dots & \\ 0 & & & 1/w_{\alpha} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1^t \\ \mathbf{U}_2^t \\ \dots \\ \mathbf{U}_{\alpha}^t \end{bmatrix} \mathbf{y} = \sum_{k=1}^{\alpha} \frac{1}{w_k} (\mathbf{U}_k^t \mathbf{y}) \mathbf{V}_k \quad (11.18)$$

The discrepancy principle can be adopted for the choice of the optimal value for α :

$$J(\hat{\mathbf{x}}_{\alpha}^{TSVD}) < m\sigma_{\epsilon}^2 \text{ and } J(\hat{\mathbf{x}}_{\alpha+1}^{TSVD}) \geq m\sigma_{\epsilon}^2 \quad (11.19)$$

11.5.2 Tikhonov regularization of zero order

Another popular method of regularization is based on a penalization of the OLS sum (11.15) by an additive term that would prevent and explosion of the standard deviations of the different coefficients of \mathbf{x} . Tikhonov regularization of zero order consists in minimizing the following criterion:

$$J_{\mu}(\mathbf{x}) = \|\mathbf{y} - \mathbf{S}\mathbf{x}\|^2 + \mu \|\mathbf{x}\|^2 = (\mathbf{y} - \mathbf{S}\mathbf{x})^t (\mathbf{y} - \mathbf{S}\mathbf{x}) + \mu \mathbf{x}^t \mathbf{x} \quad (11.20)$$

The solution is explicit:

$$\hat{\mathbf{x}}_{\mu}^{Tik0} = (\mathbf{S}^t \mathbf{S} + \mu \mathbf{I}_n)^{-1} \mathbf{S}^t \mathbf{y} \quad (11.21)$$

This can be written using the SVD decomposition of \mathbf{S} :

$$(\mathbf{V} \mathbf{W}^2 \mathbf{V}^t + \mu \mathbf{I}_n) \hat{\mathbf{x}}_{\mu}^{Tik0} = \mathbf{V} \mathbf{W} \mathbf{U}^t \mathbf{y} \quad (11.22)$$

Using the fact that $\mathbf{V} \mathbf{V}^t = \mathbf{I}_n$, the preceding equation can be simplified:

$$\hat{\mathbf{x}}_{\mu}^{Tik0} = \mathbf{V} (\mathbf{W}^2 + \mu \mathbf{I}_n)^{-1} \mathbf{W} \mathbf{U}^t \mathbf{y} = \sum_{k=1}^n \frac{w_k}{w_k^2 + \mu} (\mathbf{U}_k^t \mathbf{y}) \mathbf{V}_k \quad (11.23)$$

Comparison of OLS (15), TSVD (11.18) and Tikhonov (11.23) estimates show that both OLS and regularized solutions can be written under the common form:

$$\hat{\mathbf{x}}_{reg} = \sum_{k=1}^n f_k (\mathbf{U}_k^t \mathbf{y}) \mathbf{V}_k \quad (11.24)$$

where coefficients f_k are called “filter factors, see [1] and are defined by:

- $f_k = 1$ for $k = 1$ to $n \leq m$ without any regularization (Ordinary Least Squares)
- $f_k = 1$ for $k = 1$ to $\alpha < n \leq m$ and $f_k = 0$ for $k = \alpha + 1$ to $n \leq m$ for TSVD regularization

$$- f_k = \frac{w_k^2}{w_k^2 + \mu} \text{ for } k = 1 \text{ to } n \leq m \text{ for Tikhonov regularization of zero order}$$

11.6 Application of regularization to a deconvolution problem

11.6.1 The convolution model in vector-matrix form

Classically, since the pioneering works of J.V. Beck the aim of the Inverse Problem of Heat Conduction (IHCP) consists in estimating the time variation of the heat flux starting from several internal temperature measurements.

Here we consider a slightly different IHCP where a heat flux (if $h_1=0$) or of the surface heat source (if $h_1 \neq 0$) $q(t)$ (in W/m^2) over the front face of a slab starting from the measurement of the transient temperature variations $T_s(t)$ from a sensor embedded at a depth $x = x_s$ inside the wall of thickness e , see figure 2. The two external heat transfer coefficients h_1 and h_2 with the surrounding environment at temperature T_∞ , the conductivity λ , the volumetric heat ρc are assumed as well as the dimensions x_s and e are assumed to be known.

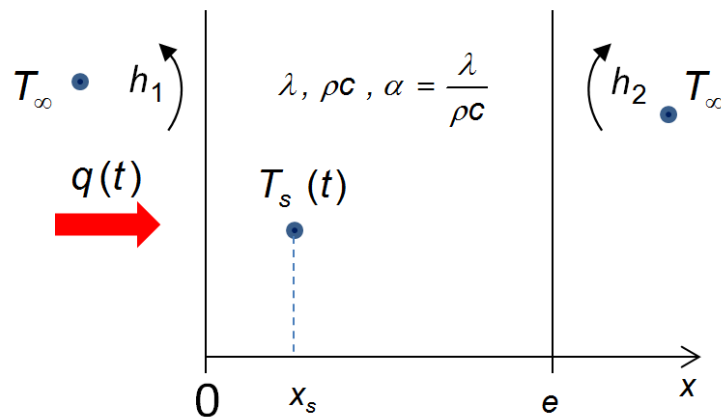


Fig. 2 Inverse Heat Conduction Problem for a homogeneous slab in 1 D

The initial temperature distribution in the slab is assumed to be uniform and equal to T_∞ . So, the solution of the direct problem consists in finding the response $T_s(t)$ of the sensor for a know thermal excitation $q(t)$.

Since the heat equation and all its boundary conditions are linear here:

$$\lambda \frac{\partial^2 \theta}{\partial x^2} = \rho c \frac{\partial \theta}{\partial t} \quad \text{with } \theta = T(x, t) - T_\infty \quad (11.25)$$

$$- \lambda \frac{\partial \theta}{\partial x} = q(t) - h_1 \theta \text{ at } x = 0; \quad - \lambda \frac{\partial \theta}{\partial x} = h_2 \theta \text{ at } x = e; \quad \theta = 0 \text{ for } t=0$$

(26)

with coefficients that do not depend on time, its solution in any point x (for example $x = x_s$) can be written under the form of a convolution product:

$$\theta_s(t) = z(t) * q(t) = \int_0^t z(t-t') q(t') dt' \quad (11.26)$$

This response can be easily calculated in the Laplace domain [2]:

$$\bar{\theta}_s(p) = \bar{z}(p) \bar{q}(p) \quad \text{with} \quad \bar{z}(p) = \frac{A_2}{C + (h_1 + h_2)A + h_1 h_2 B} \quad (11.27)$$

with the notation $\bar{g}(p) = \int_0^{+\infty} g(t) \exp(-pt) dt$

and where:

$$A = \cosh(e\sqrt{p/a}); B = \frac{\sinh(e\sqrt{p/a})}{\lambda\sqrt{p/a}}; C = \lambda\sqrt{p/a} \sinh(e\sqrt{p/a}); A_2 = \cosh((e-x_s)\sqrt{p/a}) \quad (11.28)$$

and where $\bar{z}(p)$ is the operational impedance and p the Laplace parameter.

Let us note that the inverse Laplace transform of $\bar{z}(p)$, to get values of $z(t)$ over a discrete time grid, can be made numerically (Stehfest algorithm [2, chapter 9]).

Here we assume that the measurements $\theta_s^{\text{exp}}(t_i)$ are made for discrete time values $t_k = k \Delta t$ over a $\left[t_0 = 0 \quad t_{\text{end}} = t_m = m\Delta t \right]$ time interval. So the temperature response of model (11.27) can be vectorized on the corresponding discrete time grid:

$$\Theta_s = \left[\theta_{s1} \quad \theta_{s2} \quad \dots \quad \theta_{sm} \right]^t \quad \text{with} \quad \theta_{si} = \theta_s(t_i) \quad \text{for} \quad i = 1 \text{ to } m \quad (11.29)$$

Parameterization of the flux $q(t)$ is made according to (11.6) for $x = q$, using the same number n of functions as the number of measurement times m :

$$q(t) \approx q_{\text{param}}(t) = \sum_{j=1}^m q_j g_j(t) \Rightarrow q_{\text{param}}(t_i) = \mathbf{g}(t_i) \mathbf{q} \quad (11.30)$$

where the basis functions $g_j(t)$ are *piecewise constant* (unit) *functions* over the $]t_{j-1}, t_j]$ interval. The interest of this parameterization is to keep the heat balance of the material system, since:

$$q_j = \frac{1}{\Delta t} \int_{t_{j-1}}^{t_j} q(t) dt \quad \text{for} \quad j = 1 \text{ to } m \quad (11.31)$$

A numerical quadrature of equation of equation (11.26) written at time $t = t_i$ yields:

$$\theta_s(t_i) = \sum_{j=1}^i z(t_i - t_{j+1}) q_j \Delta t = \sum_{j=1}^i z(t_{i-j+1}) q_j \Delta t \quad (11.32)$$

This quadrature does not derive from the trapezoidal rule since q_j is an integral value, see (11.31), and $z(t_{i-j+1})$ an instantaneous one.

Equation (11.32) can be put on a matrix/vector form:

$$\Theta_s = \mathbf{M}(\mathbf{z}) \mathbf{q} \text{ where } \mathbf{z} = \begin{bmatrix} z_1 & z_2 & \cdots & z_m \end{bmatrix}^t \text{ with } z_k = z(t_k) \text{ for } k=1 \text{ to } m \quad (11.33)$$

where $\mathbf{M}(\cdot)$ is a (square) matrix function of a column vector, here a Toeplitz matrix defined for any column vector \mathbf{x} by :

$$\mathbf{M}(\mathbf{x}) \equiv \Delta t \begin{bmatrix} x_1 & & & & \\ x_2 & x_1 & & & 0 \\ x_3 & x_2 & x_1 & & \\ \vdots & \vdots & \vdots & \ddots & \\ x_m & x_{m-1} & x_{m-2} & \cdots & x_1 \end{bmatrix} \text{ where } \mathbf{x} = \begin{bmatrix} x_1 = x(t_1) \\ x_2 = x(t_2) \\ x_3 = x(t_3) \\ \vdots \\ x_m = x(t_m) \end{bmatrix} \quad (11.34)$$

So, at the model level, convolution product (11.26) becomes the product of a square lower diagonal matrix by a column vector. It is this model $\mathbf{y}_{mo}(\mathbf{q}) = \boldsymbol{\theta}_s$ that has to be inverted (with regularization) starting from noisy measurements $\mathbf{y} = \boldsymbol{\theta}_s^{\text{exp}} = \boldsymbol{\theta}_s + \varepsilon$ of $\theta_s(t)$ after its sampling and parameterization of $q(t)$, to get an estimation of its parameter vector.

We simulate here the response for the following values of the different structural parameters:

$$h_1 = 0 ; h_2 = 10 \text{ W.m}^{-2}.\text{K}^{-1} ; \lambda = 1 \text{ W.m}^{-1}.\text{K}^{-1} ; \rho c = 3 \cdot 10^6 \text{ J.m}^{-3}.\text{K}^{-1} ; e = 0.2 \text{ m} ; x_s = e$$

Inversion of $\bar{z}(p)$ yields the following time impedance $z(t)$ that is plotted using $m = 200$ points on the $[0, t_{\text{final}} = 4 e^2/a]$ time interval in figure 3:

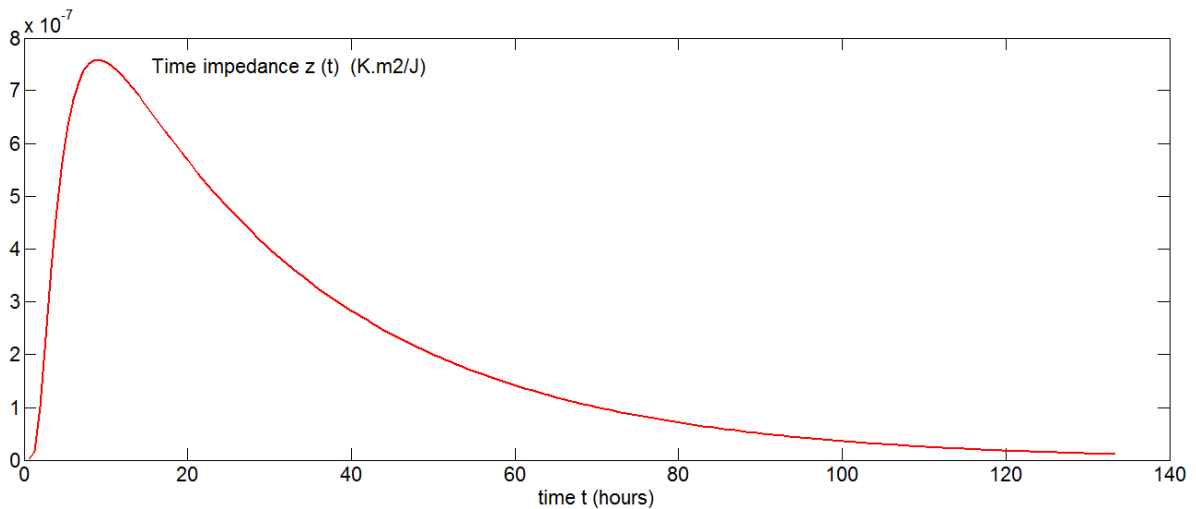


Fig. 3 – Transfer function ($x_s = e$)

11.6.2 Inverse input problem

So, the inverse problem input consists in solving (11.15), with $\mathbf{y} = \boldsymbol{\theta}_s^{\text{exp}} = \boldsymbol{\theta}_s + \boldsymbol{\varepsilon}$, $\mathbf{y}_{mo}(\mathbf{q}) = \boldsymbol{\theta}_s$ and $\mathbf{S} = \mathbf{M}(\mathbf{z})$. Here the exact and (simulated) noised temperature responses are plotted (for $t_{\text{final}} = 2 e^2/a$) in figure 4 for a i.i.d. normal noise of standard deviation $\sigma_\varepsilon = 0.1\text{K}$ and $m = 200$ points in time.

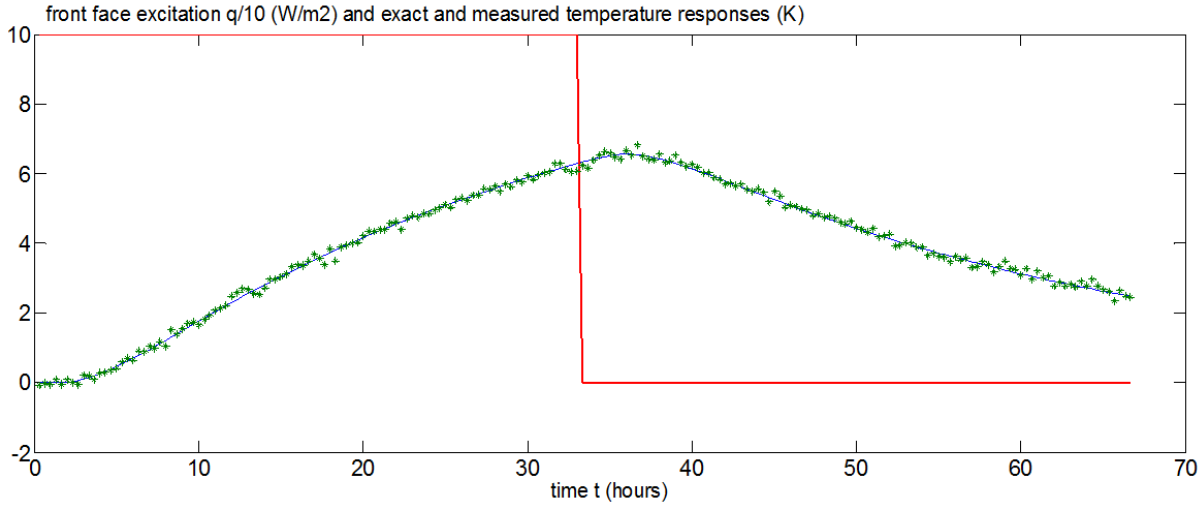


Fig. 4 – Excitation and response ($x_s = e$)

The inverse problem consists in finding a regularized estimation of the heat flux :

$$\hat{\mathbf{q}}_{reg} = \sum_{k=1}^n f_k \left(\mathbf{U}_k^t \boldsymbol{\Theta}^{\text{exp}} \right) \mathbf{V}_k = \mathbf{V} \mathbf{W}_{reg}^{-1} \mathbf{U}^t \boldsymbol{\Theta}^{\text{exp}} \quad \text{where } \mathbf{M}(\mathbf{q}) = \mathbf{U} \mathbf{W} \mathbf{V}^t \quad (11.35)$$

where \mathbf{W}_{reg}^{-1} is a filtered version of \mathbf{W}^{-1} , see equation (11.18)

11.6.3 Inverse identification and inverse input problems

Here we assume that the transfer function is unknown. So, in a first stage, we have to estimate it using a modified version of the convolution product (11.26) which is, under a vector/matrix for see (11.33):

$$\boldsymbol{\Theta}_s^{\text{calib}} = \mathbf{M}(\mathbf{q}_{\text{calib}}) \mathbf{z} \quad (11.36)$$

So a specific calibration experiment has to be run, where both excitation and response have to be measured, which yields an estimation $\hat{\mathbf{z}}$ of \mathbf{z} :

$$\mathbf{q}_{reg} = \sum_{k=1}^n f_k \left(\mathbf{U}_k^t \mathbf{y} \right) \mathbf{V}_k = \mathbf{V} \mathbf{W}_{reg}^{-1} \mathbf{U}^t \boldsymbol{\Theta}^{\text{exp}} \quad \text{where } \mathbf{M}(\mathbf{q}_{\text{calib}}) = \mathbf{U} \mathbf{W} \mathbf{V}^t \quad (11.37)$$

In a second stage, the inverse input problem of the experiment the inverter is interested into, can be considered (as in section 5.2 above, with the following model:

$$\boldsymbol{\Theta}_s = \mathbf{M}(\hat{\mathbf{z}}) \mathbf{q} \quad \Rightarrow \quad \hat{\mathbf{q}}_{reg} = \mathbf{V} \mathbf{W}_{reg}^{-1} \mathbf{U}^t \boldsymbol{\Theta}^{\text{exp}} \quad \text{where } \mathbf{M}(\hat{\mathbf{z}}) = \mathbf{U} \mathbf{W} \mathbf{V}^t \quad (11.38)$$

11.7 Data reduction using TSVD-Initial temperature field reconstitution by decomposition of the space and time observable data.

11.7.1 General remarks

The general 1-D problem of diffusion with initial condition, without internal source, in an infinite medium can be presented under the following system :

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2} \quad (11.39)$$

with at initial time :

$$T(x, t = 0) = f(x)$$

It is here assumed that the 1D medium is infinite and the temperature is zero for $T(x, t)$ and $f(x)$ when x tend to infinite.

Such a system is corresponding to a simple experiment. One illustration example is corresponding to the observation of the transient temperature response $T(x, t)$ to a pulse heating of a laser spot on a beam graduated following the x -direction.

Thanks to infrared thermography, the instantaneous temperature fields can be measured by infrared thermography at N_x different space steps x_i (lying between 0 and L) and at N_t different time steps t_j at N_t different time steps (lying between 0 and t_{max}). It is classically assumed that the measurement errors at each space and time step are uncorrelated, of zero mean and on uniform variance σ^2 or standard deviation σ . The processing of the observable temperature response: $\hat{T}(x, t)$ will be illustrated in this examples. The objective, is to use the great amount of data ($N_x \times N_t$ data) in order to filter the estimation of the initial temperature field $T(x, t = 0)$. The solution of the forward problem is considered first. The estimation of $T(x, t = 0)$ is then illustrated first by a Fourier transform method and then a TSVD directly applied on the observable field.

11.7.2 Solution by the Green's function approach

One way to consider the solution of the previous system is the « Green's function » approach. It can be presented with an integral form such as :

$$T(x, t) = \int_{-\infty}^{+\infty} K(x-s, t) f(s) ds \quad \text{or} \quad T(x, t) = \int_{-\infty}^{+\infty} K(x, s, t) f(s) ds \quad (11.40)$$

$K(x-s, t)$ is called the « Green's function », or the kernel defined as:

$$K(x-s, t) = \frac{Q}{\rho c} \frac{\exp\left(-\frac{(x-s)^2}{4at}\right)}{\sqrt{\pi at}} \quad \text{for } t > 0 \quad (11.41)$$

and:

$$K(x-s, t) = 0 \quad \text{for } t = 0 \quad \text{for any } x \quad (11.42)$$

The time variable t can be here fixed because such variable is non depending on x and s and non concerned with the inversion problem.

Such problem can also be presented under a general form such as:

$$\int_{\Omega} \text{system } X \text{ input } d\Omega = \text{output} \quad (11.43)$$

The expression (11.40) with variables x and s , is very near from the expression (11.26) with variables t et t' , except with the bounds ((11.40): integral equation of Fredholm and (11.26): integral equation of Volterra).

In a particular case, when $f(x)$ is a Dirac distribution, the output is directly the “Green’s function” expressed versus time and space. It is experimentally simple to get such realisation by considering the temperature response of a thin infinite 1D sample to a short pulse from a laser spot. The very localised initial condition can be considered at a “very short time” after the initial time.

In a general case ($f(x)$ is not a Dirac distribution but a continuous function), a numerical quadrature of the expression (11.40) or (11.43) and a linear system can be considered. A variant is to consider a space Fourier transform of the temperature field.

11.7.3 Fourier integral transform approach

An other way can be to consider the previous problem by implementing a space Fourier transform (see [7]):

$$\theta(\alpha_n, t) = \int_0^L T(x, t) \cos(\alpha_n x) dx \quad \text{with } \alpha_n = n\pi / L ; n > 0 \text{ or } = 0 \quad (11.44)$$

L is here assumed as a “large” bound of the x -domain, where the temperature is zero and no gradient is to be considered.

The system (11.39) becomes after Fourier transform:

$$-\alpha_n^2 \theta(\alpha_n, t) = \frac{1}{a} \frac{d\theta}{dt} \quad (11.45)$$

The initial condition becomes: $\theta(\alpha_n, 0) = F(\alpha_n)$

The solution of the forward problem is then:

$$\theta(\alpha_n, t) = \theta(\alpha_n, 0) \exp(-a\alpha_n^2 t) \quad \text{for every } n; \quad (11.46)$$

Or in the real space:

$$T(x, t) = \frac{1}{L} \left[\theta(0, 0) + \frac{1}{2} \sum_{n=1}^{\infty} \cos(\alpha_n x) \theta(\alpha_n, 0) \exp(-a\alpha_n^2 t) \right] \quad (11.47)$$

Or under vector-matrix form in the Fourier space:

$$\begin{bmatrix} \theta(\alpha_0, t) \\ \theta(\alpha_1, t) \\ \vdots \\ \theta(\alpha_n, t) \end{bmatrix} = \begin{bmatrix} \exp(-a\alpha_0^2 t) & & & \\ & \exp(-a\alpha_1^2 t) & & \\ & & \ddots & \\ & & & 0 & \ddots & \\ & & & & & \exp(-a\alpha_n^2 t) \end{bmatrix} \begin{bmatrix} \theta(\alpha_0, 0) \\ \theta(\alpha_1, 0) \\ \vdots \\ \theta(\alpha_n, 0) \end{bmatrix} \quad (11.48)$$

Or under condensed matrix-form in Fourier Space:

$$\Theta(t) = \text{diag}(\exp(-a\alpha^2 t)) \Theta(0) \quad (11.49)$$

The relation between the vectors $\Theta(t)$ and $\Theta(0)$ is linear. If the vector $\Theta(0)$ is truncated it is a vector of “parameters” to be estimated. $\Theta(t)$ can be observed at any time even the initial time. Generally, the “observed” vector (noted $\hat{\Theta}(t)$) is noisy and numerically computed from a discrete thermographic signal. The initial time is also observable noted as: $\hat{\Theta}(0)$, but also noisy. The noise affecting the “observed vector” is the Fourier transform of the “measurement noise” in x -space. It is here an orthogonal transform of a discrete signal (measured in x -space) regarded as a sequence of serially uncorrelated random variables with zero mean and finite variance. Such a “transformed noise” is also with zero mean and finite variance. It is here proposed to use the great amount of data obtained at the successive time steps in order to decrease the influence of the noise measurement on the observed $\hat{\Theta}(0)$ or directly in the real space: $T(x_i, t = 0)$.

Two ways are here possible. The Fourier method or the direct SVD decomposition on the observed temperature field which appears here as a matrix at different time and space steps.

11.7.4 Estimation of the initial temperature distribution with the Fourier method

With infrared thermography, it is possible to process a great number of temperature images at different time steps. The initial temperature vector can then be expressed from (11.48) and (11.49) as:

$$\begin{bmatrix} \Theta(0) \\ \Theta(t_1) \\ \vdots \\ \Theta(t_j) \end{bmatrix} = \begin{bmatrix} \mathbf{I} \\ \mathbf{diag}(\exp(-a\alpha^2 t_1)) \\ \vdots \\ \mathbf{diag}(\exp(-a\alpha^2 t_j)) \end{bmatrix} [\Theta(0)] = \mathbf{X1} [\Theta(0)] \quad (11.50)$$

The $\mathbf{X1}$ matrix is a sensitivity matrix. The initial vector to be estimated is here also directly observable but noisy. The great amount of data here given by the space and time observation can be exploited in order to reduce the influence of the measurement noise on the initial temperature field. The measured temperature vector in Fourier space $\hat{\Theta}(t_j)$ can be expressed versus the real vector $\Theta(t_j)$ by:

$$\hat{\Theta}(t_j) = \Theta(t_j) + \mathbf{e}_{\Theta(t_j)} \quad (11.51)$$

$\mathbf{e}_{\Theta(t_j)}$ is the vector where each component is a random variable called “measurement error”. Each component of such vector $[\mathbf{e}_{\Theta(t_0)} \mathbf{e}_{\Theta(t_1)} \dots \mathbf{e}_{\Theta(t_j)} \dots]^T$ has zero mean and the covariance matrix of this vector is diagonal and uniform (the Fourier transform is an orthogonal transform of the “measurement noise” in the x -space).

A new estimator of $\Theta(0)$ is then $\hat{\hat{\Theta}}(0)$ such as :

$$\hat{\hat{\Theta}}(0) = (\mathbf{X1}^T \mathbf{X1})^{-1} \mathbf{X1}^T [\hat{\Theta}(0) \hat{\Theta}(t_1) \dots \hat{\Theta}(t_j) \dots]^T \quad (11.52)$$

An other presentation of the previous expression is:

$$\hat{\theta}(\alpha_n, 0) = \frac{\sum_{j=0}^{N_t} \hat{\theta}(\alpha_n, t_j) \exp(-a\alpha_n^2 t_j)}{\sum_{j=0}^{N_t} \exp(-2a\alpha_n^2 t_j)} \quad (11.53)$$

The diagonal terms of the covariance matrix of the previous estimator are then:

$$\text{cov}\left(\hat{\theta}(0,0)\right) = \frac{\sigma^2 L^2}{N_x N_t} \quad \text{and} \quad \text{cov}\left(\hat{\theta}(\alpha_n, 0)\right) = \frac{\sigma^2 L^2}{N_x} \left(\frac{1}{\sum_{j=0}^{N_t} \exp(-2a\alpha_n^2 t_j)} \right) \quad \text{if } n \text{ non zero} \quad (11.54)$$

Then, the standard deviation of the estimator in the x -space (σ_E) are in the following interval:

$$\sigma / \sqrt{N_t} < \sigma_E < \sigma \quad (11.55)$$

It is necessary to remark that the processing of such amount of data is efficient if:

- The time steps related to the observation are near from 0.
- It is absolutely necessary to be sure of the forward model (diffusion with adiabatic boundaries) and to know exactly the thermal diffusivity: a .

The SVD approach is here presenting similarities with the Fourier approach (related to the orthogonality of the space transform) but will not require to know the exact physical model.

11.7.5 Estimation of the initial temperature distribution with the SVD

Several authors who are confronted to the challenge of the processing of great amount of data with IR cameras (see [3] Rajic, 2002, [4] Bamford et al, 2008) use SVD in order to obtain a suitable decomposition of the space and time temperature signal.

The observable discrete temperature fields $\hat{T}(x_i, t_j)$ measured by infrared thermography at N_x different space steps x_i (lying between 0 and L) and at N_t different time steps t_j at N_t different time steps (lying between 0 and t_{max}) can be decomposed as:

$$\hat{T}(x_i, t_j) = \sum_{r=1}^{r_0} U_r^x(x_i) W_r^x V_r^x(t_j) \quad \text{or} \quad \hat{\mathbf{T}} = \mathbf{U}_x \mathbf{W}_x \mathbf{V}_x^T \quad (11.56)$$

The properties of such a decomposition are not only containing a lot of the previously remarked properties (orthogonality of \mathbf{U} and \mathbf{V} , singular decreasing values in the diagonal matrix: \mathbf{W} , $r_0 = \min(N_x, N_t)$, ...); but also gives here a sum of “separated” terms depending on x and t (similarly as the Fourier method in expression (11.47)).

The truncation of the previous decomposition will allow to use her the “filtering” properties of the TSVD. The truncation is made at $r = r_{tx}$ such as the conserved singular values are greater than the variance of the temperature signal: σ^2 . It is then possible to obtain an estimation of the initial temperature without any consideration about the physical transfer model. Such a filter is generally better than a moving average filter taking only the local values of the temperature field.

By the same way a 2D problem can then be considered. Let us consider that the initial condition in a similar system as (11.39) is then depending on two space variables: x and y and that such initial condition is separable such as:

$$f(x, y) = f_x(x)f_y(y) \quad (11.57)$$

With the Fourier transform method, the solution of the 2D problem is then a product of two series depending on x and t and y and t , such as :

$$T(x, y, t) = \frac{1}{L} \left[\theta(0, 0, 0) + \frac{1}{2} \sum_{n=1}^{\infty} \cos(\alpha_n x) \theta(\alpha_n, 0, 0) \exp(-a\alpha_n^2 t) \right] \frac{1}{l} \left[\theta(0, 0, 0) + \frac{1}{2} \sum_{m=1}^{\infty} \cos(\beta_m y) \theta(0, \beta_m, 0) \exp(-a\beta_m^2 t) \right] \quad (11.58)$$

β_m is a spatial frequency related to the y -direction, equivalent to α_n related to the x -direction.

The expression (11.57) is then separable in the Fourier space such as:

$$\theta(\alpha_n, \beta_m, t) = \theta(\alpha_n, \beta_m, t=0) \exp\left(-a(\alpha_n^2 + \beta_m^2)t\right) \quad (11.59)$$

or:

$$\theta(\alpha_n, \beta_m, t) = \theta(\alpha_n, 0, t=0) \exp(-a\alpha_n^2 t) \theta(0, \beta_m, t=0) \exp(-a\beta_m^2 t) \quad (11.60)$$

The analogous estimator in the 2D Fourier space is also separable and gives by the same way as in expression (11.53):

$$\hat{\theta}(\alpha_n, \beta_m, 0) = \frac{\sum_{j=0}^{N_x} \hat{\theta}(\alpha_n, 0, t_j) \exp(-a\alpha_n^2 t_j) \sum_{j=0}^{N_y} \hat{\theta}(0, \beta_m, t_j) \exp(-a\beta_m^2 t_j)}{\sum_{j=0}^{N_x} \exp(-2a\alpha_n^2 t_j) \sum_{j=0}^{N_y} \exp(-2a\beta_m^2 t_j)} \quad (57-a)$$

instead of:

$$\hat{\theta}(\alpha_n, \beta_m, 0) = \frac{\sum_{j=0}^{N_x} \hat{\theta}(\alpha_n, \beta_m, t_j) \exp(-a(\alpha_n^2 + \beta_m^2)t_j)}{\sum_{j=0}^{N_x} \exp(-2a(\alpha_n^2 + \beta_m^2)t_j)} \quad (11.61)$$

In such a particular case where each instantaneous temperature field is separable versus the x -direction and y -direction, it is suitable to consider preliminarily a SVD, versus x and y at each time step such as:

$$\hat{T}(x_i, y_j, t) = \sum_k U_k(x_i, t) W_k(t) V_k(y_j, t) \quad (11.62)$$

Only the first term of such a decomposition is then to be taken into account. The order of magnitude of the second term must be much lower than the first one.

It is then suitable to consider a secondary decomposition vers the x and y directions such as:

$$U_1(x_i, t_j) = \sum_{r=1}^{r_0^x} U_r^x(x_i) W_k^x V_r^x(t_j) \quad \text{and} \quad V_1(y_j, t_j) = \sum_{r=1}^{r_0^y} U_r^y(y_j) W_k^y V_r^y(t_j) \quad (11.63)$$

The advantage of such a truncated double-decomposition is to operate a strong data reduction. For example, if $N_x = N_y = N_t = 1000$; the global number of data to be processed is 10^9 . But the successive

truncations allow to reduce the number of data to be considered to 12000 (if $r_0x=r_0y=3$). The measurement noise attenuation is than more than 100 times higher (see [5]).

One example where the Fourier methods are not necessarily well adapted even if the thermal diffusivity is perfectly known is the 2D temperature response to a punctual heat pulse in a semi-infinite medium such as:

$$T(x, y, t) = \frac{Q}{\rho c_p} \frac{\exp\left(-\frac{(x-x_0)^2}{4at}\right)}{\sqrt{\pi at}} \frac{\exp\left(-\frac{(y-y_0)^2}{4at}\right)}{\sqrt{\pi at}} \quad (11.64)$$

The figures 5-a to 5-c are illustrating that even when the noise level is of the same order of magnitude as the signal, the TSVD decomposition allows the detection of a very localised point source.

This argue in favour of the bolometric detection of localised radiative source of very low amplitude such as terahertz radiations (see [6]).

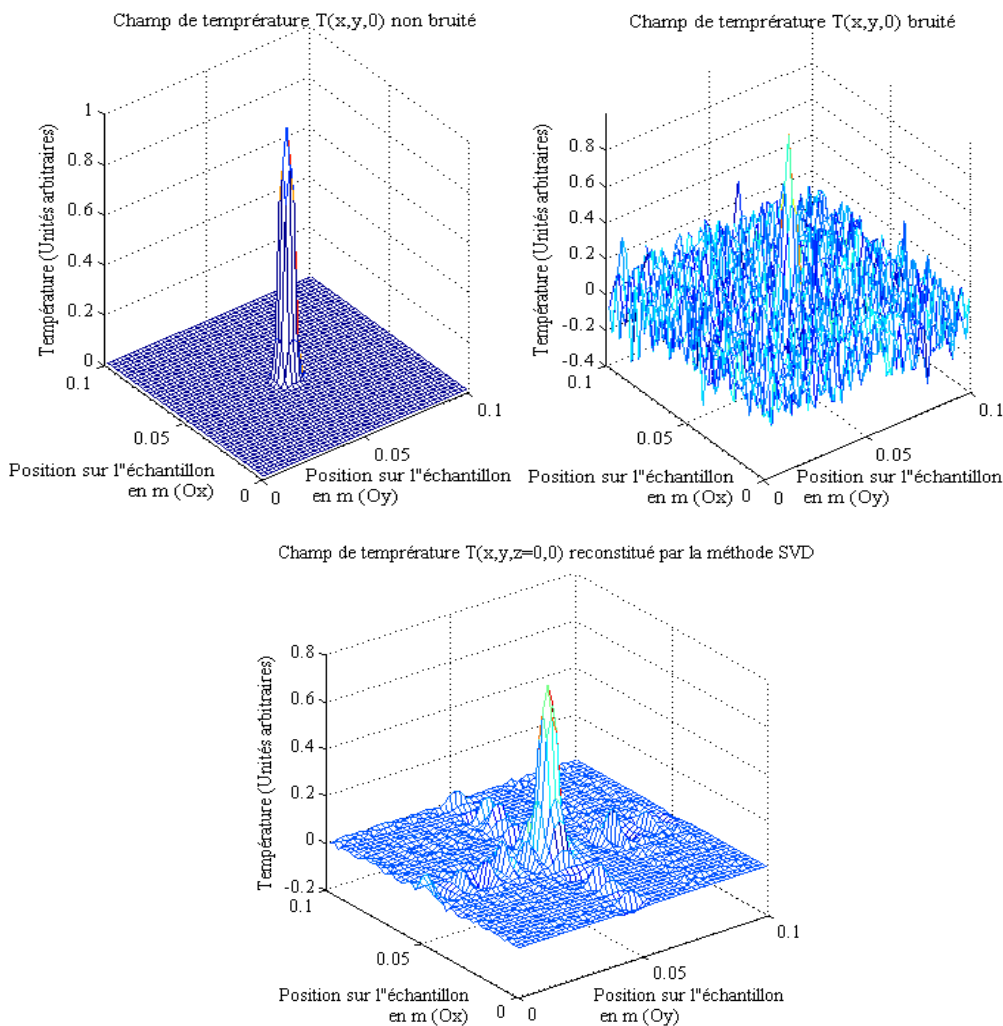


Fig 5 : Initial temperature field (expression (60) a-without noise, b-with a high noise/signal ratio, c-filtered and reduced by TSVD with $r_0=3$.

11.8 References

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