Transfer function identification through total least squares

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Abstract. When transient diffusion and/or advection occur in a physical system modelled by linear equations whose coefficients are time-invariant, the relationships between a source (a temperature or a thermal power) and its consequences (local temperatures) are convolution products. This study deals with identification of a transfer function when an additive noise not only corrupts the output (response) but also the input (excitation) in a calibration experiment. Regularization is implemented either through Truncated Singular Value Decomposition or by Total Least Squares.

1. Introduction

Inverse input estimation problems (source estimation) or model identification inverse problems (model calibration), based on measurements of the output in a corresponding experiment, are present in many engineering fields (mechanics, bio-physics, heat transfer, ...). If the transfer model they rely on is linear with time-invariant coefficients (LTI model), their common mathematical form is:

\[ A \ x = y \]  

where \( A \) is the matrix of the linear operator of size \( m \times n \), with \( m \geq n \), \( x \) the input column vector of size \( n \times 1 \) and \( y \) the output column vector of size \( m \times 1 \). We are interested here in the particular LTI model where system (1) is the discrete parameterized form of a convolution product in time. Before dealing with this problem, we will recall here the different ways of solving equation (1), here the discrete form of a Volterra integral equation of the first kind, where errors (noise) are present in both output \( y \) and matrix \( A \).

The field of application of this deconvolution type of problem is very large, from inverse heat conduction (surface heat flux estimation from interior temperature measurements) [3] to inversion of a seismometer signal for estimating a corresponding acceleration [1].

2. The different solutions of the inverse input problem, for a linear model

2.1 Regularized inversion in case of error in the output only
In the absence of regularization, the ordinary least squares (OLS) solution, consists in minimizing the following criterion based on the L2 (Euclidian norm) $\| \|$ of the output residual vector $r_y(x)$:

$$J_{OLS}(x) = \| r_y(x) \|^2 = r_y^T(x) r_y(x) \quad \text{with} \quad r_y(x) = y^{exp} - A x$$

(2a)

where superscript $T$ designates the matrix transpose and where the true version $A^{true}$ of matrix $A$ is available while the true value $y^{true}$ of the output is corrupted by an additive noise $\varepsilon_y$ of zero stochastic expectation (noted $E(\cdot)$ here), that is:

$$A = A^{true} \quad \text{and} \quad y^{exp} = y^{true} + \varepsilon_y \quad \text{with} \quad E(\varepsilon_y) = 0$$

(2b)

In this case the minimization of (2a) with respect to $x$ provides an explicit and unbiased estimation $\hat{x}_{OLS}$ of the true value $x^{true}$ of this vector:

$$\hat{x}_{OLS} = (A^T A)^{-1} A^T y^{exp} \quad \Rightarrow \quad E(\hat{x}_{OLS}) = x^{true}$$

(2c)

The following estimator can be given a strictly equivalent form using the Singular Value Decomposition (SVD) of matrix $A$, given here under its ‘full’ form version:

$$\hat{x}_{OLS} = V^T S^{−1} U^T y^{exp} \quad \text{where} \quad A = U' S' V'^T$$

$$\text{with} \quad U'^T U' = U' U'^T = I_m \quad ; \quad V'^T V' = V' V'^T = I_n \quad \text{and} \quad S' = \begin{bmatrix} \text{diag}(s'_1, s'_2, \ldots, s'_n) \\ 0_{(m-n) \times n} \end{bmatrix}$$

(2d)

where the singular values $s_k$ are positive (we suppose that matrix $A$ has a full rank here) and have subscripts in decreasing order ($s'_1 \geq s'_2 \geq \cdots \geq s'_n > 0$). $S'$ is a $m \times n$ matrix and diag($\cdot$) designates a square diagonal matrix whose diagonal is defined by its arguments. $U'$ and $V'$ are square orthonormal matrices of respective dimensions $m \times m$ and $n \times n$. $I_k$ designates the identity matrix of dimensions $k \times k$.

With the additional assumption that noise $\varepsilon$ is independent and identically distributed (i.i.d.), with a standard deviation $\sigma$, this estimator is the unbiased linear estimation of minimum variance, with a variance-covariance matrix equal to:

$$\text{cov}(\hat{x}_{OLS}) = \sigma^2 (A^T A)^{-1} = \sigma^2 V^T S^{−2} V'^T$$

(2e)

However, this solution corresponds to the inversion of a discrete form of an integral equation (a function estimation problem) that may be ill-posed if the condition number of $A$, equal to $s'_1/s'_n$, is too high, for a given value of the signal over noise ratio of the output.

So, a regularization of the inversion is compulsory. We only recall here the Truncated SVD (TSVD) regularization [1], even if many other regulation techniques are available (Tikhonov [2], Function specification method with future times for causal problems [3], …).

This TSVD regularization method consists in writing the SVD of $A$ using partitions of its matrices:
\[ A = U' S' V'^T = \begin{bmatrix} U'_{\alpha} & U'_{\beta} & U'_{\gamma} \end{bmatrix} \begin{bmatrix} S'_{\alpha} & 0_{\alpha \times \beta} & 0_{\alpha \times \gamma} \\ 0_{\beta \times \alpha} & S'_{\beta} & 0_{\beta \times \gamma} \\ 0_{\gamma \times \alpha} & 0_{\gamma \times \beta} & 0_{\gamma \times \gamma} \end{bmatrix} \begin{bmatrix} V'_{\alpha} \end{bmatrix} = U'_{\alpha} S'_{\alpha} V'_{\alpha}^T + U'_{\beta} S'_{\beta} V'_{\beta} \]  

(3a)

with \( \alpha + \beta = n \) and \( \gamma + n = m \)

where

\[ S'_{\alpha} = \text{diag} ( s'_1, s'_2, \ldots, s'_\alpha) \] and \( S'_{\beta} = \text{diag} ( s'_{\alpha+1}, s'_{\alpha+2}, \ldots, s'_{\alpha+n}) \)

(3b)

and

\[ \dim (U'_{\alpha}) = m \times \alpha \quad ; \quad \dim (U'_{\beta}) = m \times \beta \quad ; \quad \dim (U'_{\gamma}) = m \times \gamma \]

\[ \dim (V'_{\alpha}) = n \times \alpha \quad ; \quad \dim (V'_{\beta}) = n \times \beta \]

(3c)

and keeping only the first \( \alpha \) values (with \( 1 \leq \alpha < n \)) in the inversion (2d), that is:

\[ \hat{x}_{\text{T-OLS (\alpha)}} = V'_{\alpha} S'^{-1}_{\alpha} U'_{\alpha}^T y_{\text{exp}} \Rightarrow E (\hat{x}_{\text{TSVD (\alpha)}}) - x_{\text{true}} = -V'_{\beta} V'^T_{\beta} x_{\text{true}} \neq 0 \]  

(3d)

This estimator is biased, but since matrix \( A \) has been replaced by its first part \( U'_{\alpha} S'_{\alpha} V'^T_{\alpha} \) in (3a), its condition number has improved and is now \( s'_1/s'_\alpha < s'_1/s'_n \), which yields a more stable inversion.

The hyperparameter is chosen according to the discrepancy principle [4] that is, for an i.i.d. noise of standard deviation:

\[ J_{\text{OLS}} (\hat{x}_{\text{TSVD (\alpha)}}) \geq m \sigma^2 \quad \text{and} \quad J_{\text{OLS}} (\hat{x}_{\text{TSVD (\alpha+1)}}) < m \sigma^2 \]  

(3e)

2.2 Regularized inversion in case of error in the output and in the matrix of the model

We first consider, in this section that we have more data than unknowns, which means that model matrix \( A \) is \( m \times n \), with \( m > n \). We also assume that both output vector \( y \) and matrix \( A \) are corrupted by additive noises of zero expectations, noted \( \epsilon_y \) and \( \epsilon_A \) respectively:

\[ A_{\text{exp}} = A_{\text{true}} + \epsilon_A \quad \text{and} \quad y_{\text{exp}} = y_{\text{true}} + \epsilon_y \quad \text{with} \quad E (\epsilon_A) = 0 \quad \text{and} \quad E (\epsilon_y) = 0 \]  

(4a)

In the inverse analysis terminology, this type of assumption corresponds to an EIV (Error In Variable) model, where the structural parameters (matrix \( A \) here) are not errorless: not only the dependent variable (the output \( y \) here), but also the independent variables are corrupted by errors.

This inverse problem is solved by orthogonal regression, or Deming regression, or Total Least Squares (TLS) method. We assume that the physical units of all the the coefficients of \( A \) are the same and that they are identical to the units of \( y \), while the coefficients of \( x \) are dimensionless. So the sum to be minimized, the TLS criterion [5] is defined as:

\[ J_{\text{TLS}} (A, x) = \| r_y (A, x) \|^2_F = \| r_A (A) \|^2_F + \| r_y (A, x) \|^2_F \]  

(4b)

with

\[ G (A, x) = [A, A x] \quad ; \quad G_{\text{exp}} = [A_{\text{exp}}, y_{\text{exp}}] \quad ; \quad r_y (A, x) = G_{\text{exp}} - G (A, x) \]  

(4c)
or \( r_G(A, x) = [r_A(A), r_y(A, x)] \) with \( r_A(A) = A^{exp} - A \); \( r_y(A, x) = y^{exp} - Ax \) \( \quad \) (4d)

Subscript \( F \) designates the Frobenius norm of a matrix, that is the sum of the squares of all its coefficients, \( G \) is the "augmented" matrix, of size \( m \times (n+1) \), and \( r_G, r_A \) and \( r_y \) the residuals of the augmented matrix, of the system matrix, and of the output vector respectively. We can note here that the rank of matrix \( G \) is equal or smaller than \( n \).

The minimization of \( J_{TLS} \) with respect to \( A \) and \( x \) can be derived from the Eckart-Young theorem [6]. This one considers a matrix \( D^{exp} \) of size \( m \times n \), with \( m \leq n \) with its SVD decomposition given below:

\[
D^{exp} = U S V^T \quad \text{with rank} \ (D^{exp}) \geq r \quad \text{and} \quad U = [U_r, U_c] ; \ S = [S_r, S_c] ; \ V = [V_r, V_c]
\]

where

\[
\begin{align*}
\text{dim} \ (D^{exp}) &= \text{dim} \ (S) = m \times n ; \ \text{dim} \ (U) = m \times m ; \ \text{dim} \ (V) = n \times n \\
U^T U &= U U^T = I_m ; \ V^T V &= V V^T = I_n
\end{align*}
\]

and

\[
\begin{align*}
\text{dim} \ (S_r) &= m \times r ; \ \text{dim} \ (U_r) = m \times r ; \ \text{dim} \ (V_r) = n \times r
\end{align*}
\]

The best rank \( r \) approximation \( \hat{D} \) of \( D^{exp} \) corresponds to the first part of the partitioning of the above SVD [7]:

\[
\hat{D} = U_r S_r V_r^T \quad \text{and} \quad \| D^{exp} - \hat{D} \|_F = \min_{\text{rank}(D) = r} \| D^{exp} - D \|_F = \sqrt{s_{r+1}^2 + s_{r+2}^2 + \cdots + s_m^2}
\]

(5b)

where the \( s_k \)'s (for \( k = 1 \) to \( m \)) are the singular values of \( D^{exp} \) listed in descending order. The minimizer \( \hat{D} \) is unique if and only if \( s_{r+1} \neq s_r \).

Application of this theorem to matrix \( G^{exp} \), that is replacing \( D^{exp}, D \) and \( n \) by \( G^{exp}, G \) and \( n+1 \) respectively, yields:

\[
G = U S V^T = [U_A \ u_y] \begin{bmatrix} S_A & 0 \\ 0 & S_y \end{bmatrix} \begin{bmatrix} V_A & V_y \end{bmatrix} = U_A S_A V_A^T + s_{n+1} u_y v_y
\]

with

\[
\begin{align*}
\text{dim} \ (U) &= m \times (n+1) ; \ \text{dim} \ (S) = (n+1) \times (n+1) ; \ \text{dim} \ (V) = (n+1) \times (n+1) \\
\text{dim} \ (U_A) &= m \times n ; \ \text{dim} \ (S_A) = n \times n ; \ \text{dim} \ (V_A) = n \times n \\
S_A &= \text{diag} (s_1, s_2, \cdots, s_n) ; \ s_y = s_{n+1} \ \text{where} \ s_1 \geq s_2 \geq \cdots \geq s_n \geq s_{n+1} > 0
\end{align*}
\]

(5c)

Here the 'thin' SVD decomposition has been used, where matrix \( S \) is square and where matrix \( U \) is rectangular with the same dimensions as \( G^{exp} \), which means that only the \( n+1 \) original left singular vectors are present in \( U \).

The approximation of rank \( n \) of \( G^{exp} \) consists in discarding the second part of its decomposition (5c), that is taking \( r = n \) in (5b):

\[
\hat{G}_{TLS} = U_A S_A V_A^T
\]

(5d)
One can show [8, 9] that the corresponding TLS estimation of \( x \) is given by the coefficients of the last right singular vector \( v_y \), that is a \( n \times 1 \) vector \( v_{Ay} \) and a scalar \( v_{yy} \):

\[
\hat{x}_{TLS} = -\frac{1}{v_{yy}} v_{Ay} = (A^T A - S_{n+1} I_n)^{-1} A^T y^{exp} \quad \text{with} \quad V = \begin{bmatrix} V_A & v_y \end{bmatrix}
\]

(5e)

Let us note that in the case of a square \( A^{exp} \) matrix, \( m = n \) and the rank of the augmented matrix \( G^{exp} \) is equal to \( m \) and, as a consequence \( S_{n+1} = S_{\infty+1} = 0 \) and the OLS estimator (2c) and the TLS estimator (5e) are the same.

Since the variance of the components of the TLS estimator can be large, it is possible to get its regularized version by truncation, a regularization method called T-TLS here, by discarding more small singular values than the smallest one in (5c). The thin decomposition of \( G^{exp} \) is partitioned the following way:

\[
G^{exp} = U \Sigma V^T = \begin{bmatrix} U_\alpha & U_\beta \end{bmatrix} \begin{bmatrix} S_\alpha & 0 \\ 0 & S_\beta \end{bmatrix} \begin{bmatrix} V_\alpha & V_\beta \end{bmatrix}^T = U_\alpha S_\alpha V_\alpha^T + U_\beta S_\beta V_\beta^T \quad \text{with} \quad \alpha + \beta = n + 1 \quad \text{and} \quad \beta > 1
\]

(6a)

and the T-TLS estimator is given by:

\[
\hat{x}_{T-TLS} = -\frac{1}{\|V_2\|_2^2} V_1 \|V_2\|_2^2 \quad \text{with} \quad V = \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \quad \text{where} \quad \dim(V_1) = (n+1) \times \alpha \quad \dim(V_2) = (n+1) \times \beta
\]

(6b)

We will derive in the next section an exact form of model (1) for 1D heat diffusion in a slab, before considering the corresponding identification problem using both T-OLS and T-TLS.

3. Convolution model in a 1D heat diffusion case

3.1 Solution in Laplace domain

A homogeneous slab of thickness \( \ell \) is considered here. Its initial temperature is supposed to be uniform at a level \( T_i = T_{\infty} \), where \( T_{\infty} \) is the temperature of the ambient air that is supposed to be a constant. A surface heat source \( q(t) \), in W.m\(^{-2}\) is imposed over its front face \( (x = 0) \) at time \( t = 0^+ \), see fig. 1. The other (rear) face \( (x = \ell) \) exchange heat with the ambient air through a uniform and constant heat transfer coefficient \( h \). The slab is made out of a material of heat conductivity \( \lambda \), of volumetric heat \( \rho c \) and of heat diffusivity \( a = \lambda / (\rho c) \).

The heat equation, after the change of variable \( \theta (x, t) = T(x, t) - T_i \) is:

\[
\frac{\partial^2 \theta}{\partial x^2} = \frac{1}{a} \frac{\partial \theta}{\partial t}
\]

(7)

The initial and boundary conditions are:
Figure 1 – Slab with corresponding 1D boundary conditions
\[ \theta = 0 \text{ at } t = 0 \text{ for } 0 \leq x \leq \ell \quad (8) \]
\[ \varphi = -\lambda \frac{\partial \theta}{\partial x} = q(t) \text{ at } x = 0 \text{ for } t > 0 ; \quad \varphi = -\lambda \frac{\partial \theta}{\partial x} = h \theta \text{ at } x = \ell \text{ for } t > 0 \quad (9 - 10) \]

where \( \varphi (x, t) \equiv -\lambda \frac{\partial \theta}{\partial x} \) is the local \( x \)-component of the heat flux in the slab and \( \lambda \) is its conductivity.

This system is solved through integral time (Laplace) transformation of both temperature and flux [10]:
\[ \overline{\psi} (x, p) \equiv \int_0^t \psi(x, t) \exp(-pt) \, dt \quad \text{for } \psi = \theta \text{ or } \varphi \quad (11) \]

where \( p \) is the Laplace parameter. After this transformation, equations (2) and (5) become, with the introduction of the local flux \( \varphi \):
\[ \frac{\partial}{\partial x} \left[ \overline{\theta} \right] = - \left[ \begin{array}{cc} 0 & 1/\lambda \\ \lambda p/a & 0 \end{array} \right] \left[ \overline{\varphi} \right] \quad (12) \]

Integration of this ordinary differential equation system between \( x = 0 \) and \( x = \ell \) yields, after taking into account conditions (8) and (9):
\[ \begin{bmatrix} \overline{\theta}_1 \\ \overline{\theta}_2 \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} 1 & 0 \\ h & 1 \end{bmatrix} \begin{bmatrix} \overline{\theta}_1 \\ \overline{\theta}_2 \end{bmatrix} \text{ with } \begin{cases} A = D = \cosh (\eta \ell) \quad ; \quad \eta^2 = p/a \\ B = \lambda \eta \sinh (\eta \ell) \quad ; \quad C = \sinh (\eta \ell)/(\lambda \eta) \end{cases} \quad (13a, b) \]

The rear face temperature response \( \theta_2 \) at \( x = \ell \), is linked to the front face temperature response \( \theta_1 \) at \( x = 0 \) by a simple product involving a transfer function \( W \), called here a “transmittance”, in the Laplace domain:
\[ \overline{\theta}_2 (p) = \overline{W} \overline{\theta}_1 (p) \quad \text{with} \quad \overline{W} (p) = \frac{1}{A(p) + h B(p)} \quad (14a, b) \]

Return to the time domain makes a convolution product, noted “*” here, appear:
\[ \theta_2 (t) = W(t) \ast \theta_1 (t) \quad (15a) \]

or
\[ \theta_2 (t) = \int_0^t W(t-t') \theta_1 (t') \, dt' = \int_0^t W(t') \theta_1 (t-t') \, dt' \quad (15b) \]

One can consider the input to be either the surface power \( q(t) \) or the front face temperature \( \theta_1 (t) \) since this one is related to \( q \) by a transfer function, an impedance \( Z \) here, defined here:
\[ \overline{\theta}_1 (p) = \overline{Z} (p) \overline{q} (p) \quad \text{with} \quad \overline{Z} (p) = \frac{A(p) + h B(p)}{C(p) + h A(p)} \Rightarrow \theta_1 (t) = Z(t) \ast q(t) \quad (16a, b, c) \]
One cannot write the opposite \( q ( t ) = Y ( t ) \ast \theta _{1} ( t ) \), with \( \overline{Y} ( p ) = \frac{1}{Z} ( p ) \), since \( \overline{Y} ( p ) \) is not the Laplace transform of any time function: a transfer function has to be a monotonically decreasing function of the Laplace parameter \( p \), which is the case for \( Z ( p ) \) but is not true for its inverse \( \frac{1}{Z} ( p ) \).

### 3.2 Solution in finite dimensions

The commutative convolution integrals (15b) can be written after a numerical quadrature involving \( m \) discrete times \( t_1 = i \Delta t \) (for \( i = 1 \) to \( m \)), where \( \Delta t = t_f / m \) is the time step depending of the upper bound \( t_f \) of the time domain considered. This time step has to be very small with respect to the characteristic diffusion time \( \ell^2 / \alpha \) of the slab and with respect of the characteristic time of the temperature input function \( \theta _{1} ( t ) \). Under these conditions, one can write at any time

\[
\theta _{2} ( t_i) = \Delta t \sum _{k=1}^{i} W_{i-k+1} \theta _{1,k} \quad \text{or} \quad \theta _{2} ( t_i) = \Delta t \sum _{k=1}^{i} W_{i} \theta _{1,i-k+1}
\]

(17a, b)

Let us note that quadrature (17a or b) is not an application of the trapezoidal rule to equation (15b). In order to be unbiased \( \theta _{2} ( t_i) \) is an instantaneous sampled value of function \( \theta _{2} ( t) \), while both coefficients \( W_k \) and \( \theta _{1,k} \) are parameterized components of the corresponding functions \( W ( t) \) and \( \theta _{1} ( t) \) : they are their projections over a base of unit step functions. These are averaged values of each function over the \([ t_{k-1}, t_k \] interval that precedes time \( t_k \). This is due to the fact that the problem is causal and response \( \theta _{2} ( t) \) shall follow excitation \( \theta _{1} ( t) \) (and consequently \( W ( t) \), because of their symmetric form in convolution product (15a)). So, both functions \( \theta _{1} ( t) \) and \( W ( t) \) are piecewise constant functions:

\[
\theta _{1} ( t) = \sum _{j=1}^{m} \theta _{1,j} f_j ( t) \quad \text{and} \quad W ( t) = \sum _{j=1}^{m} W_j f_j ( t) \quad \text{with} \quad f_j ( t) = H(t-t_{j-1}) - H(t-t_j) \quad \text{for} \quad j = 1 \text{ to } m
\]

(18a, b)

where \( H ( t) \) is the Heaviside function and where:

\[
\theta _{1,j} = \frac{1}{\Delta t} \int _{t_{j-1}}^{t_j} \theta _{1} ( t) \, dt \quad \text{and} \quad W_j = \frac{1}{\Delta t} \int _{t_{j-1}}^{t_j} W ( t) \, dt
\]

(19a, b)

If all the observation times \( t_k \) over the \([ t_1, t_m = t_f \] are considered, equations (17) can be put under a matrix/column-vector form:

\[
\theta _{2} = M ( W ) \theta _{1} = M ( \theta _{1} ) W
\]

(20a, b)

Here \( M ( \cdot ) \) is a square matrix function, of dimensions \( m \times m \) whose argument is a column vector. It is a lower triangular Toeplitz matrix defined by:
The direct problem consists in calculating the output $\theta_2$ from a given known input $\theta_1$, if the structural parameters gathered in transmittance vector $W$ of the white box model (20a) are known. In order to estimate the components of $W$, that is to identify model (15a) of convolutive structure, two paths are available:

- either use a numerical inversion algorithm of the exact Laplace transform (14b) of the its transfer function, to calculate $W_j(t)$ at any time $t$: it is a model reduction procedure,
- or use a measurement of both input and output in a calibration experiment: since input and transmittance commute in the model in its form (20ab), it is an inverse input problem (very similar to the classical Inverse Heat Flux Conduction problem). So, it is also a model identification experiment, that can be polluted by the presence of noise on both output and input.

4. Inverse methods for convolutive model identification

We are interested in estimating the transmittance vector $W$ of model (15a) using measured values of both input $\theta_1^{exp}$ and output $\theta_2^{exp}$ of a potential calibration experiment. These experimental input and output differ from their exact value because of the presence of 2 random noises called $\epsilon_1$ and $\epsilon_2$ respectively. We assume that both noises have 0 mean and are independent and identically distributed (i.i.d), that is:

$$\theta_1^{exp} = \theta_1^{true} + \epsilon_1 \quad \text{with} \quad E(\epsilon_1) = 0 \quad \text{and} \quad \text{cov}(\epsilon_1) = \sigma_1^2 I_m \tag{22a, b, c}$$

$$\theta_2^{exp} = \theta_2^{true} + \epsilon_2 \quad \text{with} \quad E(\epsilon_2) = 0 \quad \text{and} \quad \text{cov}(\epsilon_2) = \sigma_2^2 I_m \tag{23a, b, c}$$

where $E(.)$ designates the expectation of a random vector, $\text{cov}(.)$ its variance-covariance matrix. We also assume that $\epsilon_1$ and $\epsilon_2$ are mutually independent (their covariance matrix, $\text{cov}(\epsilon_1, \epsilon_2)$, is equal to zero). In this paper we only consider a synthetized calibration experiment where the exact values of $\theta_1, W$ and $\theta_2$ are known.

4.1 Validation of the direct model and of its identification by Ordinary or Total Least Squares (OLS/TLS)

We consider a noiseless input $\theta_1$ that is defined by:

$$\theta_1(t) = \begin{cases} 
0 & \text{if } t \leq 0 \\
(1 - \exp(-t/\tau)) \theta_1^{\infty} & \text{if } t > 0 
\end{cases} \tag{24}$$

where $\tau$ is a constant and $\theta_1^{\infty}$ is the asymptotic (steady state value) of $\theta_1(t)$. The temperature response $\theta_2(t)$ on the rear face ($x = \ell$) has been calculated at the discrete times defined in section 3.2. The
values of the different quantities necessary for the solution of the discrete direct problem are given in Table 1.

Table 1 – Parameters of the simulation (direct problem)

| ℓ  | τ  | θ_{i_{0}} | t_{f} | Δt | h   | λ   | ρc |
|-----|----|------------|------|----|-----|-----|-----|
| (mm)| (s)| (K)        | (s)  | (s)| (W.m^{-2}.K^{-1}) | (W.m^{-1}.K^{-1}) | (kJ.m^{-3}.K^{-1}) |
| 50  | 30 | 30         | 700  | 0.5| 10  | 43  | 3666 |

In order to validate our input/output model, the commercial finite elements code COMSOL has been used to solve equations (7) to (10), and to simulate the output θ_2(t) using the input θ_1(t) given by (24). The corresponding plots are shown in Figure 2. Transmittance W, see (15a) and (15b) has been calculated using these synthetic θ_1(t) and θ_2(t) generated by COMSOL using either OLS or TLS and are shown in Figure 3. A numerical inversion of the analytical expression (14b) of the Laplace transform \( \hat{W} \) of \( W \) has been implemented, using the de Hoog’s algorithm [11] and the corresponding transmittance is shown in the same figure. This shows that without any noise, both OLS and TLS method yield the same estimation of the transmittance.

![Figure 2 – Input and numerical solution (COMSOL) of the output](image)

![Figure 3 – Analytic transmittance (numerical inversion of Laplace transform), and estimated transmittances identified by OLS and TLS without regularization, starting from inversion of noiseless input \( \theta_1 \) and noiseless output \( \theta_2 \) calculated by COMSOL as a direct model](image)

4.2 Identification of the transmittance starting from noisy input and output

Starting from the synthetic ‘true’ temperature distributions shown in Figure 2, a i.i.d. noise has been added on each input and output signal, see equations (22) and (23) and the transmittance has been estimated using truncated OLS (T-OLS) and truncated TLS (T-TLS) with an optimized truncation hyperparameter \( \alpha \) corresponding to the minimum Euclidian norm of the error \( \| \hat{W}_{\alpha} - W_{\text{true}} \| \). The results are shown for 3 cases: a noise of standard deviation 1 K on \( \theta_2 \), see Figure 4, the same noise on \( \theta_1 \) only, see Figure 5, and the same noise on both \( \theta_1 \) and \( \theta_2 \), see Figure 6.

We can notice that the two identification techniques (T-OLS and T-TLS) yield the same \( \hat{W}_{\text{optimal}} \) estimate, whatever the noise. A second remark is that the noise on the input has a smaller impact on the estimate that the noise on the output: this is due to its filtering by the system matrix, see section 4.3 further on.
In order to verify these results, inversions have been made for different values of the standard deviations \( \sigma_1 \) and \( \sigma_2 \). We define here the relative estimation error as:

\[
\epsilon^*_W = \frac{\| \hat{W}(\alpha_{\text{opt}}) - W_{\text{true}} \|}{\| W_{\text{true}} \|}
\]  

The corresponding results are presented in Table 2, in terms of the optimum value \( \alpha_{\text{opt}} \) of \( \alpha \), of the Signal over noise ratio SNR of each temperature signal, and of the relative estimation error \( \epsilon^*_W \), with the following definitions:

\[
\text{SNR}_k = \frac{\| \theta_k \|}{\| \epsilon_k \|} = \frac{\| \theta_k \|}{\sigma_k \sqrt{m}} \quad \text{for } k = 1 \text{ or } 2
\]

Table 2 – Relative error \( \epsilon^*_W \) and optimum hyperparameter \( \alpha_{\text{opt}} \) by T-OLS and T-TLS inversion for different standard deviations \( \sigma_1 \) and \( \sigma_2 \) of noise on input and/or output

| Configuration          | Case | \( \sigma_1 \) (K) | \( \sigma_2 \) (K) | SNR\(_1\) | SNR\(_2\) | T-TLS \( \epsilon^*_W \) (%) | \( \alpha_{\text{opt}} \) | T-OLS \( \epsilon^*_W \) (%) | \( \alpha_{\text{opt}} \) |
|------------------------|------|--------------------|--------------------|-----------|-----------|-----------------------------|----------------|-----------------------------|----------------|
| same noise for both signals | 1    | 0.01               | 0.01               | 2907      | 2563      | 3.7                         | 57             | 3.7                         | 57             |
|                        | 2    | 0.10               | 0.10               | 290.2     | 256.3     | 6.1                         | 28             | 6.1                         | 28             |
|                        | 3    | 1.00               | 1.00               | 29.3      | 25.6      | 19.3                        | 20             | 19.0                        | 20             |
|                        | 4    | 10                 | 10                 | 3.1       | 2.8       | 38                          | 4              | 37.9                        | 4              |
| different noise for each signal | 5    | 0.01               | 1.00               | 2907      | 25.6      | 18.6                        | 19             | 18.6                        | 19             |
|                        | 6    | 1.00               | 0.01               | 29.3      | 2563      | 5.9                         | 59             | 5.9                         | 59             |
|                        | 7    | 0.01               | 10                 | 2907      | 2.8       | 37.7                        | 4              | 37.3                        | 9              |
|                        | 8    | 10                 | 0.01               | 3.1       | 2563      | 17.1                        | 467            | 17.1                        | 467            |
| noise on one signal only | 9    | 0                  | 1.00               | \( \infty \) | 25.6      | 18.6                        | 19             | 18.6                        | 19             |
|                        | 10   | 0                  | 10                 | \( \infty \) | 2.8       | 37.7                        | 4              | 37.3                        | 9              |
|                        | 11   | 1.00               | 0                  | 29.3      | \( \infty \) | 5.5                         | 606            | 5.5                         | 606            |
|                        | 12   | 10                 | 0                  | 3.1       | \( \infty \) | 17.1                        | 492            | 17.1                        | 492            |
This table confirms that the two regularization techniques give nearly the same results, except for cases 3, 4 and 7, which can be explained by the numerical noise of the computer we used. This also shows that output noise degrades the quality of the inversion in a higher way than the input noise.

Since the results of T-OLS and T-TLS inversions are very close, we had a look on the distribution of the singular values of the two exact matrices \( A = M(\theta_1) \) and \( G = [M(\theta_1), \theta_2 = M(\theta_1)W] \) and of their noisy versions \( A^{\exp} = M(\theta_1^{\exp}) \) and \( G^{\exp} = [M(\theta_1^{\exp}), \theta_2^{\exp}] \). These are plotted in Figure 7.

![Figure 7 – Distribution of the eigenvalues of the matrices](image)

These plots show that the singular values of \( A \) and \( G \) are nearly the same. Presence of noise makes the intermediate singular values increase in the range \([100 < k < 1300]\) while they stay closer for the larger \( s_k \)’s, and it has the opposite effect in the last interval \([1300 < k < 1400]\) with an increase of the condition numbers of \( A \) and \( G \).

4.3 Identification modelling by a unique output noise in the case of noisy input and output

We assume here that i.i.d. noises corrupt both input and output of model (15b), see equations (22) and (23) and OLS are used to estimate transmittance vector \( W \). Since the dimensions of input and output are the same, the normal equation of the OLS problem can be written the following way:

\[
M(\theta_1 + e_i)(W + e_u) = \theta_2 + e_2
\]

(26)

where \( e_u = W - W^{true} \) is the estimation error. Subtracting (20b) from (26) yields:

\[
M(\theta_1) e_u = e_2 - M(W) e_1 = K e \quad \text{where} \quad K = [I_m, -M(W)]; \quad e = [e_2 \ e_1]^T; \quad \text{cov} (e) = \left[ \begin{array}{cc} \sigma_2^2 I_m & 0 \\ 0 & \sigma_2^2 I_m \end{array} \right]
\]

(27)

This has been obtained by neglecting second order terms, with the use of the commutativity of the convolution product and with the additional assumption of mutually independent noise. So, presence of noise \( e_1 \) on the input can be taken into account by replacing the output noise \( e_2 \) by a unique equivalent noise \( e_2' = K e \) that is not i.i.d. anymore. One easily shows:

\[
\text{cov} (e_2') = K \text{cov} (e) K^T = \sigma_2^2 \left( I_m + \frac{\sigma_2^2}{\sigma_2^2} M(W) M^T(W) \right) = \sigma_2^2 \Omega(W) \quad \text{with} \quad e_2' = K e
\]

(28)
This would mean that, before any regularization, a Gauss-Markov estimator, which minimizes the variance of each estimated parameter, within the framework of linear estimators, would be well suited. This estimator corresponds to the minimum of the following criterion

$$J_{GM}(W) = \left( \theta_2^{exp} - \mathbf{M}(\theta_1^{exp}) W \right)^T \Omega^{-1} \left( \theta_2^{exp} - \mathbf{M}(\theta_1^{exp}) W \right)$$

(29a)

whose solution is:

$$\hat{W}_{GM} = \left[ \mathbf{M}^T (\theta_1^{exp}) \Omega^{-1} \mathbf{M}(\theta_1^{exp}) \right]^{-1} \mathbf{M}^T (\theta_1^{exp}) \Omega^{-1} \theta_2^{exp}$$

(29b)

Unfortunately, when the linear model is square ($m = n$), this estimator, see (29b) in its unregularized version, degenerates into the OLS estimator. However, this deserves to be tested in the future for rectangular models with $m > n$.

5. Conclusions

We have shown, using an example of transient 1D heat diffusion in a wall, that identification of a temperature/temperature transfer function, when noise corrupts both input and output, could be regularized through truncated total least squares (T-TLS) based on a SVD decomposition of the augmented matrix. This TLS regularization of a deconvolution problem does not add anything new when compared to regularization of the ordinary least square problem, achieved here through truncated SVD. Even if the stochastic properties of an equivalent noise on the output only are known, it does not allow the construction of a better estimator than the two previous ones.

This unsuccessful performance of T-TLS here may stem from the fact that the reconstructed matrix, called $\hat{A}_n$ here does not possess the Toeplitz structure of a convolution matrix: this information, a constraint, is not present in the version of T-TLS we have used. Another perspective of this work is to change our target: instead of minimizing the relative (global) estimation error, called $\epsilon^W_1$, here, it can rather be more interesting to improve the estimation of transfer function $W(t)$ at the earlier times, that is up to its maximum: once this function estimated in the identification (calibration) experiment considered here, the quality of its early values conditions the quality of the reconstruction of the input, in a different inverse input experiment. This can be used in the design of a virtual sensor that allows to reconstruct here the front face temperature of a wall starting from measurement of the rear face temperature and of prior identification of the associated transfer function. As far as applications are concerned, not only inverse problems in diffusion, but also in advection-diffusion can be the subject of this type of identification through deconvolution, see [12] for example.

References

[1] R. C. Aster, B. Borchers, and C. H. Thurber, Parameter estimation and inverse problems, vol. 90. Academic Press, 2011.
[2] A.N. Tikhonov, V.Y. Arsenin, Solution of Ill-posed Problems, Winston & Sons, Washington, 1977.
[3] J.V. Beck, B. Balckwell, C.R. St.Clair Jr, Inverse Heat Conduction – Ill-Posed Problems, Wiley, New York, 1985.
[4] V.A. Morozov, Methods for Solving Incorrectly Posed Problems, Springer-Verlag, Berlin, 1984.
[5] G. H. Golub and C. F. Van Loan, “An analysis of the total least squares problem,” SIAM Journal on Numerical Analysis, vol. 17, no. 6, pp. 883–893, 1980.
[6] C. Eckart and G. Young, The approximation of one matrix by another of lower rank, Psychometrika, 1936, 1 (3), 211-8.
[7] R. D. Fierro, G. H. Golub, P. C. Hansen, and D. P. O’Leary, Regularization by truncated total least squares, SIAM Journal on Scientific Computing, vol. 18, no. 4, pp. 1223–1241, 1997.
[8] I. Markovsky, S. Van Huffel, Overview of total least squares methods. Signal Processing, vol. 87, pp. 2283–2302, 2007.
[9] H.P. Gavin and G.P. Zéhil, Total Least Squares, Course, Duke University, Sept. 10, 2013.
[10] D. Maillet, S. Andrè, J.-C. Batsale, A. Degiovanni, and C. Moyne, Thermal quadrupoles : solving the heat equation through integral transforms. Chichester : New York : Wiley., 2000.
[11] F. R. De Hoog, J. Knight, and A. Stokes, “An improved method for numerical inversion of Laplace transforms, SIAM Journal on Scientific and Statistical Computing, vol. 3, no. 3, pp. 357–366, 1982.
[12] W. Al Hadad, Y. Jannot, and D. Maillet, Characterization of a heat exchanger by virtual temperature sensors based on identified transfer functions, Journal of Physics : Conference Series, vol. 745 (http://iopscience.iop.org/article/10.1088/1742-6596/745/3/032089), p. 032089, IOP Publishing. October 21, 2016.