ON A WEIGHTING METHOD IMPROVING IDENTIFIABILITY OF DISTRIBUTED PARAMETER SYSTEMS

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1. INTRODUCTION

1.1 Motivations

The output least-square estimation problem of the coefficient of an elliptic or parabolic problem is generally ill-conditionned (Chavent [1], Kunisch [4]). Even with a performing quasi-Newton minimization method like BFGS this leads to a very slow convergence and to highly oscillating estimated coefficents. In this paper we present a method for improving the conditionning of the problem by including in the error function a time dependent weighting factor. This weighting is designed in order to improve the convergence of the minimization algorithm that is to have a condition number of the hessian of the error function as small as possible. The method can also be applied to the estimation problem for ordinary differential equations.

The method is specially intended for evolution equation where the number of observation is large compared to the number of parameter to estimate.

Locally after linearization and discretization, the output least square estimation problem for parabolic equations is an ordinary least square problem. For the sake of simplicity we present our weighting method within this framework.

1.2. The basic example : identification of diffusion coefficients

As a reference problem let us consider the following system

$$\begin{cases} \dfrac{\partial u}{\partial t} - \sum\limits_{i=1}^{n} \dfrac{\partial}{\partial x_i}\left[\tau(x)\dfrac{\partial u}{\partial x_i}\right] = f(x,t) & \text{in } \Omega\times(0,T) \\ u(x,t) = 0 \quad \text{on } \Gamma \text{ the boundary of } \Omega \\ u(x,0) = u_0(x) \end{cases} \tag{1.1}$$

where $\tau(.) : \overline{\Omega} \rightarrow \mathbb{R}$ is a continuous fonction ($\tau(x) \geq \underline{\tau} > 0$), which is the "parameter" (here the diffusion coefficient) to be identified.

If we consider the simple case of a distributed observation, this corresponds to the following criterion

$$J(\tau) = \int_0^T \int_\Omega |u(x,t;\tau) - z(x,t)|^2 \, dx \, dt = \int_0^T \| u(\tau) - z\|^2_{L^2(\Omega)} \, dt \tag{1.2}$$

The identification problem consists in minimizing the functionnal (1.2) under the constraint $\tau \geq \underline{\tau}$.

1.3. Orthonormalization of sensitivity functions

The main goal of this study is to introduce a weighting term in (1.2) :

$$J_W(\tau) = \int_0^T < W(t)(u(t;\tau) - z(t)), u(t;\tau) - z(t) >_{L^2(\Omega)} \, dt \tag{1.3}$$

where $W(t) \in \mathcal{L}(L^2(\Omega);L^2(\Omega))$ such that the hessian of J_W is well conditionned. An ideal case would be to determine a new scalar product in $L^2(0,T;L^2(\Omega))$ such that the sensitivity functions are orthonormal for this product.

We first recall classical facts in least square estimation. Then we turn to problems where the observation is time dependent and we present our method in that case. Then we apply it to the OLS estimation problem for parabolic equations. We end by some numerical experiments.

2. WEIGHTED LINEAR LEAST SQUARE PROBLEMS

2.1 Least-square estimator

We consider the following problem : let $A \in \mathcal{M}_{p,q}(\mathbb{R})$ be a matrix with $\mathrm{rank}(A) = q \leq p$, the classical *least square problem* consists in finding $\hat{\theta} \in \mathbb{R}^q$ such that

$$|A\hat{\theta}-b| \leq |A\theta-b| \quad ,\forall \theta \in \mathbb{R}^q, \tag{2.1}$$

where $b \in \mathbb{R}^p$ represents a vector of "measurements" of the form

$$b = A\bar{\theta} + v \tag{2.2}$$

where $\bar{\theta}$ is the "true" value of parameters and v is a given noise with zero mean and covariance matrix R.

It is well known that the least square estimator is given by

$$\hat{\theta} = (A^T A)^{-1} A^T b,$$

with a covariance matrix of error of estimation

$$\mathbb{E}\ [(\theta-\bar{\theta})(\theta-\bar{\theta})^T] = P = (A^T A)^{-1} A^T R A\ (A^T A)^{-1}$$

The classical weighted form of (2.1) consists in modifying the least square criterion

$$\begin{cases} \text{for } W \in \mathcal{S}_p(\mathbb{R}),\ W > 0, \text{ find } \hat{\theta}_W \text{ such that :} \\ |A\hat{\theta}_W - b|_W \leq |A\theta-b|_W \quad \forall \theta \in \mathbb{R}^q, \end{cases} \tag{2.3}$$

where $|x|_W^2 = x^T W x$, and ($\mathcal{S}_p(\mathbb{R})$ is the space of symmetric matrices of order p)

Then $\hat{\theta}_W$ is given by

$$\hat{\theta}_W = (A^T W A)^{-1} A^T W b.$$

The covariance of the error of this estimator is then

$$P_W = (A^T W A)^{-1} A^T W R W A\ (A^T W A)^{-1} \tag{2.4}$$

2.2 The minimum variance estimator

It is classical that if we look for the minimum variance linear estimator of $\bar{\theta}$, then the estimator $\hat{\theta}_{MV}$ is given by

$$\hat{\theta}_{MV} = (A^T R^{-1} A)^{-1} A^T R$$

and the corresponding covariance matrix of the error is

$$P = (A^T R^{-1} A)^{-1}.$$

In that conditions it is clear that if we want to determine the weighting matrix W in order to minimize the variance of the error, the optimal choice for W is

$$W = R^{-1}, \tag{2.5}$$

and in this case both estimators are identical, i.e. : $\hat{\theta}_{R^{-1}} = \hat{\theta}_{MV}$.

2.3 Introduction of a "Newton type" weighting

The basic idea is to reduce the weighted least-square problem (2.3) to a simple one in which the projection on Range (A) is trivial. It is clear that a convenient choice is to select W such as

$$A^T W A = I \quad , \text{I identity matrix in } \mathbb{R}^q. \tag{2.6}$$

But there is (at least in the case $q < p$) non uniqueness of such a W. A possible idea consists in adding a condition, for instance we impose to $\hat{\theta}_W$, to realize the minimum variance of the error. From (2.4) we have

$$\text{var} \{ \hat{\theta}_W - \bar{\theta} \} = \text{tr}\, P_w = \text{tr}\, (A^T W A)^{-1} A^T W R W A\, (A^T W A)^{-1} = \text{tr}\, A^T W R W A \tag{2.7}$$

by virtue of (2.6), then the problem'is reduced to

$$\begin{cases} \min\limits_{W>0} \text{tr}\, (A^T W R W A), \\ A^T W A = I. \end{cases} \tag{2.8}$$

This problem has a solution given by the Lyapunov equation :

$$W A A^T R^{-1} + R^{-1} A A^T W = 2\, R^{-1} A (A^T R^{-1} A)^{-1} A^T R^{-1}. \tag{2.9}$$

Unfortunately in most examples, we do not have any information on the noise, then various choices can be envisaged.

- The first one is to take $R = I$ in (2.8)(2.9), but the resulting problem involves the solution of a Lyapunov equation.
- The second one consists in obtaining the uniqueness of W satisfying (2.6) by minimizing a given norm of W.

This can be done by considering the problem

$$\begin{cases} \min\limits_{W>0} \|W\|_F^2, \\ A^T W A = I, \end{cases} \tag{2.10}$$

(where $\|W\|_F^2 = \text{tr}\, W^T W$ is the Frobenius norm of W) which has the solution

$$W = A\ (A^T A)^{-2} A^T. \tag{2.11}$$

Then a step of the gradient algorithm applied to the weighted function $J_W(\theta) = \frac{1}{2} \| A\,\theta - b \|_W^2$ is exactly a step of the Newton algorithm applied to the original function $J(\theta) = \frac{1}{2} \| A\,\theta - b \|^2$.

This is evidently has no interest to solve the least-square problem, which can be done by an orthogonalisation procedure. In fact in the sequel we will adapt these ideas to a less trivial situation.

Remark

One can notice that W defined by (2.11) satisfies (2.9) with R = I. Furthermore the estimator is the same as the original one : $\theta_W = \theta$.

3. LINEAR LEAST-SQUARE PROBLEMS INVOLVING TIME

3.1 The least-squares estimator

Now we consider the problem where the observation depends on time. Let S be the family of matrices :

$$t \mapsto S(t) : [0,T] \to \mathcal{M}_{p,q}$$

Therefore the quadratic least-square error is given by

$$J(\theta) = \frac{1}{2} \int_0^T \| S(t)\theta - z(t) \|_{R^p}^2 dt, \tag{3.1}$$

where $z(t) \in R^p$, is the vector of measurements of the form

$$z(t) = S(t)\bar{\theta} + v(t) \tag{3.2}$$

where v(t) is a noise.

The estimator $\hat{\theta}$ which minimizes (3.1) is given by the condition

$$\left[\int_0^T S^T(t)\, S(t)\, dt \right] (\hat{\theta} - \bar{\theta}) = \int_0^T S^T(t)\, v(t)\, dt \tag{3.3}$$

which, in the case where

$$H = \int_0^T S^T(t)\, S(t)\, dt \;\in \mathcal{S}_q \text{ is invertible,} \tag{3.4}$$

leads to

$$\hat{\theta} = H^{-1} \int_0^T S^T(t)\, z(t)\, dt \,; \quad (\hat{\theta} - \bar{\theta}) = H^{-1} \int_0^T S^T(t)\, v(t)\, dt . \qquad \blacksquare \tag{3.5}$$

3.2. Presentation of two possible time-dependent weightings

Our goal is to adapt the previous ideas by introducing now a family of weighting matrices

$$t \mapsto W(t) : [0,T] \to \mathcal{S}_p$$

and to replace the least square function (3.1) by

$$J_W(\theta) = \frac{1}{2} \int_0^T (S(t)\theta - z(t))^T W(t) (S(t)\theta - z(t))dt. \tag{3.6}$$

The problem of finding a weighting function orthonormalizing the sensitivity functions can be then formulated as

$$\begin{cases} \text{Does there exist a family of symmetric matrices} \\ \qquad t \mapsto W(t) \in \mathscr{S}_p \text{ such that} \\ \int_0^T S^T(t)\, W(t)\, S(t)\, dt = I \end{cases} \tag{3.7}$$

If this problem has a solution (this will be studied below), there is no reason that it should be unique. If we follow the same lines as in the previous section two main choices can be made.

<u>*A First choice for W(.)*</u>

The error on the estimator $\hat\theta_W$ is given by :

$$\left[\int_0^T S^T(t)\, W(t)\, S(t)\, dt\right] (\hat\theta_W - \bar\theta) = \int_0^T S^T(t)\, W(t)\, v(t)\, dt$$

which by (3.7) is simply

$$\hat\theta_W - \bar\theta = \int_0^T S^T(t)\, W(t)\, v(t)\, dt\,. \tag{3.8}$$

As we have the majoration

$$|\hat\theta_W - \bar\theta|^2 \leq \left(\int_0^T |S^T(t)\, W(t)|^2\, dt\right) |v|^2_{L^2(0,T;\mathbb{R}^p)}\,, \tag{3.9}$$

it seems quite natural to look for a family of matrices W (t) such as

$$\min_{W(.)\in \mathscr{S}_p} \int_0^T |S^T(t)\, W(t)|^2\, dt \tag{3.10}$$

$$\int_0^T S^T(t)\, W(t)\, S(t)\, dt = I. \tag{3.7}$$

It remains to choose a *norm* in (3.9). For a practical standpoint it is convenient to take an euclidian norm on $\mathscr{S}_p$, one possible choice (which is similar to (2.8)) being then the ***Frobenius norm*** $|\,.\,|_F$ associated to the scalar product $< A,B >_F$ defined by

$$< A,B >_F = \mathrm{tr}\,(AB^T). \tag{3.11}$$

<u>Formal solution</u>

One way to solve this problem is to introduce the following lagrangian

$$\left\{\begin{aligned} L(W,\Lambda) &= \frac{1}{2}\int_0^T |S^T(t)\,W(t)|^2\,dt + \frac{1}{2}\int_0^T |W(t)\,S(t)\,|^2\,dt \\ &\quad + \langle \Lambda, I - \int_0^T S^T(t)\,W(t)\,S(t)\,dt\ \rangle_F. \end{aligned}\right. \tag{3.12}$$

The condition giving the stationnarity of L with respect to W leads to

$$S(t)S^T(t)\,W(t) + W(t)\,S(t)S(t)^T = S(t)\Lambda S(t)^T, \tag{3.13}$$

which is a Lyapunov equation which does not necessarily have a unique solution (the natural condition being $S(t)S(t)^T > 0$ which is clearly too strong). This choice will not be studied any further.

A second possible choice for W(.).

It consists simply to seek a W of minimum norm :

$$\left\{\begin{aligned} &\min_{W(.)} \int_0^T \|W(t)\|_F^2\,dt \quad , \quad W(t)\text{ symmetric}, \\ &\int_0^T S^T(t)W(t)S(t)\,dt = I \qquad (I : \text{identity in } \mathbb{R}^q) \end{aligned}\right. , \tag{3.14}$$

As before we introduce the lagrangian

$$L(W,\Lambda) = \frac{1}{2}\int_0^T \|W(t)\|_F^2\,dt + \langle \Lambda\,, I - \int_0^T S^T(t)W(t)S(t)\,dt \rangle_F, \tag{3.15}$$

the stationnarity of L with respect to W gives the following condition

$$\int_0^T \langle W(t), \delta W(t) \rangle_F\,dt - \int_0^T \langle S(t)\Lambda S^T(t), \delta W(t) \rangle_F\,dt = 0 \ ,$$

which yields

$$W(t) = S(t)\Lambda S^T(t). \tag{3.16}$$

If we impose that W satisfies the constraint in (3.7), this leads to

$$\int_0^T S^T(t)S(t)\Lambda S^T(t)S(t)\,dt = I, \tag{3.17}$$

which is a linear equation with respect to Λ and which can be explicited via

$$Q.\,\Lambda = I \tag{3.18}$$

where Q is given via a KRONECKER product [1] by :

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(1) The KRONECKER product T of A and B, $T = A \otimes B$, is a *tensor* defined by $T_{ijk\ell} = a_{ij}\,b_{k\ell}$ then if C is a matrix the product T.C is a matrix D defined by $d_{ik} = \sum_{j,\ell} T_{ijk\ell}\; c_{j\ell}$.

$$Q = \int_0^T [S^T(t)S(t)] \otimes [S^T(t)S(t)]\, dt\,.$$

Remark 3.1

It is not clear whether the equation (3.18) admits a solution, this point will be made more precise later. If Λ is a solution of (3.17) then Λ^T is also a solution and, as a consequence, if the solution Λ is unique it is symmetric.

Proposition 3.1

The solution $\overline{W}$ of problem (3.14), if it does exist, is given by the set of two equations :

$$\begin{cases} Q.\Lambda = I \\ \overline{W}(t) = S(t)\Lambda S^T(t) \end{cases}, \tag{3.19}$$

where Λ and $\overline{W}$ are symmetric.

Proof. Equations (3.19) represent the set of necessary conditions of problem (3.14).

4. ANALYSIS OF THE METHOD

4.1. The strong identifiability hypothesis

Let $S : [O;T] \to \mathcal{M}_{p,q}$ be a continuous function ; we want to solve

$$\min_{\theta \in \mathbb{R}^q} \frac{1}{2} \int_0^T \| S(t)\theta - z(t) \|^2_{\mathbb{R}^p}\, dt. \tag{4.1}$$

Definition 4.1

The parameters θ are *identifiable* if the mapping

$$\theta \mapsto S(t)\theta \ :\ \mathbb{R}^q \to L^2(0,T;\mathbb{R}^p) \tag{4.2}$$

is injective.

A necessary and sufficient condition of identifiability is that the identifiability grammian

$$\mathcal{J} = \int_0^T \| S(t)^T S(t) \|\, dt$$

has full rank.

In the sequel we will make an hypothesis which is stronger than (4.2).

Strong identifiability hypothesis.

$$\begin{cases} \text{The mapping } \mathscr{C} \in \mathcal{L}(L^2(0;T;\mathscr{S}_p);\mathscr{S}_q) \text{ defined by} \\ \qquad \mathscr{C}Z = \int_0^T S^T(t)\, Z(t)\, S(t)\, dt \\ \text{is onto.} \end{cases} \tag{4.3}$$

Proposition 4.1

Assumption (4.3) implies identifiability.

Proof. Assume that

$$S(t)\theta \equiv 0, \tag{4.4}$$

then if we define $R = \theta\,\theta^T \in \mathcal{S}_q$, (4.4) implies that

$$\mathcal{C}^*R = S(t)RS^T(t) = S(t)\theta\theta^T S^T(t) = |S(t)\theta|^2 = 0,$$

where $\mathcal{C}^*$ is the adjoint of $\mathcal{C}$ but, from (4.3) $\mathcal{C}^*$ is injective, this implies $R = \theta\theta^T = 0$ which implies $\theta = 0$.

Theorem 4.1

Under assumption (4.3) the problem (3.14) admits a unique solution $\overline{W}$ given by the set of equations

$$\begin{cases} \int_0^T S^T(t)S(t)\Lambda S^T(t)S(t)\,dt = I; \\ \overline{W}(t) = S(t)\Lambda S^T(t). \end{cases} \tag{4.5}$$

Proof.

The first equation of (4.5) may be written as

$$\mathcal{C}\mathcal{C}^*\Lambda = I \tag{4.6}$$

and, as $\mathcal{C}$ is onto this equation admits a unique solution Λ. Then there exists a $\overline{W}$ which satisfies the set of optimality conditions for (3.13). As in that case the function to be minimized is strictly convex and the constraints are linear, the necessary optimality conditions are sufficient, then $\overline{W}$ is the solution of (3.14).

It is possible to show that the weighting W thus computed has the following property : the error on θ_W due to the lack of exact convergence of the minimization algorithm is minimized and equidistributed on the components of $\hat{\theta}_W$.

4.2. Regularization

As we have mentionned previously the sole assumption of identifiability does not imply (4.3). Furthemore, even if (4.3) is satisfied, equation (4.5) may be ill-conditionned.

To overcome this difficulty, we propose a regularization.

Regularization of (3.18)

One can replace equation (3.18) by

$$(Q + \varepsilon I).\,\Lambda = I \qquad \text{where } \varepsilon > 0 \text{ is given}, \tag{3.18$_\varepsilon$}$$

this can be done directly by penalizing the constraint in (3.14) :

$$\begin{cases} \min\limits_{W(.);K} \int_0^T \|W(t)\|_F^2\,dt + \frac{1}{\varepsilon}\| K - I \|_F^2 \\ \int_0^T S^T(t)W(t)S(t)\,dt = K \quad ; \; K \in \mathcal{S}_q \end{cases} \tag{4.7}$$

The corresponding lagrangian is

$$L_\varepsilon(W,K,\Lambda) = \frac{1}{2}\int_0^T \|W(t)\|_F^2\, dt + \frac{1}{2\varepsilon}\| K - I \|_F^2 - < \Lambda , K - \int_0^T S^T(t)W(t)S(t)\, dt >_F. \tag{4.8}$$

Stationnarity of this lagrangian with respect to W and K leads respectively to

$$W_\varepsilon(t) = S(t)\Lambda_\varepsilon S^T(t) ,$$
$$K_\varepsilon = I - \varepsilon\Lambda .$$

Plugging these relations in the second relation of (4.7) one gets

$$\begin{cases} (Q+ \varepsilon I).\ \Lambda_\varepsilon = I \\ W_\varepsilon(t) = S(t)\Lambda_\varepsilon S^T(t) \end{cases} \tag{4.9}$$

4.3. The time discretized problem

Let us consider the time discretization of problem (3.1). Let $\{t_i\}_{i=1}^N$ be the discretization times : $t_i = i\frac{T}{N}$, $S_i = S(t_i)$.

Problem (3.1) becomes the minimization of :

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{N} \| S_i\, \theta - z_i \|^2. \tag{4.10}$$

This problem is of the form (2.1) for the matrix $A \in \mathcal{M}_{p,Nq}$ having S_i's as block rows :

$$A = \begin{bmatrix} S_1 \\ \vdots \\ S_i \\ \vdots \\ S_N \end{bmatrix}$$

So, given a fully discretized problem, it is natural to consider various row splitting of the matrix A.

Let us assume that $N = \ell N'$ and consider the sub-splitting of A :

$$A = \begin{bmatrix} \Sigma_1 \\ \Sigma_2 \\ \vdots \\ \Sigma_{N'} \end{bmatrix} \qquad \Sigma_k \in \mathcal{M}_{\ell p,q} \tag{4.11}$$

$$\Sigma_k = \begin{bmatrix} S_{\ell(k-1)+1} \\ \cdot \\ \cdot \\ \cdot \\ S_{\ell k} \end{bmatrix} \qquad k : 1, \ldots, N'$$

As an analogous of (4.3), we may define the strong identifiability hypothesis for the time discretized problem :

The mapping $\mathscr{C} \in \mathscr{L}((\mathscr{S}_p)^N ; \mathscr{S}_q)$ defined by :

$$\mathscr{C} Z = \sum_{i=1}^{N} S_i^T Z_i S_i \tag{4.12}$$

is onto.

The following result shows how this property depends on the splitting of A.

Theorem 4..2

If the strong identifiability hypothesis (4. 12) is satisfied for the row of splitting A by S_i's, it is also satisfied for the sub splitting by Σ_k's. Furthermore, if A has full rank, the property is true for A itself without splitting.

Proof : By assumption the mapping $\mathscr{C}^*$:

$$\Lambda \in \mathscr{S}_q \rightarrow \{S_i \Lambda S_i^T\}_{i=1}^{N} \text{ is injective.}$$

Assume that there exists a $\Lambda \in \mathscr{S}_q$ such that :

$$\mathscr{C}_\Sigma^* \Lambda = \{\Sigma_k \Lambda \Sigma_k^T\}_{k=1}^{N'} = 0$$

But for each k, the ℓ diagonal blocks of $\Sigma_k \Lambda \Sigma_k^T$ are :

$$S_{\ell(k-1)+j} \Lambda S_{\ell(k-1)+j}^T \quad j = 1, \ldots, \ell$$

and they are null. By the injectiveness of $\mathscr{C}^*$, Λ is null and this proves that $\mathscr{C}_\Sigma^*$ is also injective.

To prove the strong identifiability without row-splitting, we have to prove that :

$$\Lambda \in \mathscr{S}_q \rightarrow A \Lambda A^T \text{ is injective.}$$

As A has full rank :

$$\mathrm{rk}(A \Lambda A^T) = \mathrm{rk}\, \Lambda,$$

and so

$$A \Lambda A^T = 0 \Rightarrow \Lambda = 0. \qquad \blacksquare$$

The practical interest of the preceding result is due to the fact that in order to minimize the volume of computation of J_W and ∇J_W one has to use a row splitting of A as fine as possible. This result suggests to test successive refinements till (4. 12) is no more satisfied. Anyhow to satisfy (4.12) it is necessary that :

$$\frac{N}{\ell} \; \frac{\ell p(\ell p+1)}{2} \geqslant \frac{q(q+1)}{2}.$$

5. THE IDENTIFICATION METHOD

5.1. The weighted identification algorithm

Starting from the example of §1.2, after discretization, the problem is reduced to :

$$\begin{cases} \dfrac{dy}{dt} + A(\theta)\, y = b(t) \quad y(t) \in \mathbb{R}^n \\ y(0) = y_0 \end{cases}, \tag{5.1}$$

where $\theta \in \mathbb{R}^q$, $A(\theta) \in \mathcal{M}_{n,n}$ and $b(t) \in \mathbb{R}^n$. The least square criterion is now

$$J(\theta) = \frac{1}{2} \int_0^T |Cy(t;\theta) - z(t)|^2_{\mathbb{R}^p} dt, \tag{5.2}$$

where $C \in \mathcal{M}_{p,n}$ is the observation operator and $z(t) \in \mathbb{R}^p$ represents the measurements.

The linearized problem around a state $\bar{y}(t) = y(t;\bar{\theta})$ is defined by

$$\begin{cases} \dfrac{d(\delta y)}{dt} + A(\bar{\theta})\, \delta y = B(t;\bar{y}(t))\, \delta\theta \text{ on } (0;T) \\ \delta y(0) = 0 \end{cases}, \tag{5.3}$$

with $B(t;\bar{y}(t))\, \delta\theta \triangleq -[\frac{dA}{d\theta}(\bar{\theta})\, \delta\theta]\, \bar{y}(t)$.

In order to have a closed representation of (5.3) let us introduce the family of operators

$$t \mapsto S(t) : [0,T] \to \mathcal{M}_{p,q}$$

defined by

$$S(t)\, \delta\theta = C\, \delta y(t) \qquad (\delta y \text{ being defined by } (5.3)). \tag{5.4}$$

Therefore the quadratic least-square error (corresponding to the linearized problem) is given by

$$\tilde{J}(\delta\theta) = \frac{1}{2} \int_0^T |S(t)\, \delta\theta - \bar{z}(t)|^2_{\mathbb{R}^p} dt, \tag{5.5}$$

with $\bar{z}(t) = z(t) - C\bar{y}(t)$.

A possible algorithm is defined by the following sequence of calculations :

<u>Step 1</u>. For a given value of $\bar{\theta}$ calculate the solution $\overline{W}$ of (3.19) whith S given by (5.4).
<u>Step 2</u>. Update the value of θ *either* by solving the optimization problem

$$\min_{\theta} \int_0^T [y(t;\theta) - z(t)]^T\, \overline{W}(t)\, [y(t;\theta) - z(t)]\, dt, \tag{5.6}$$

or by performing a finite number of steps of an optimization method for (5.6).

Remark 5.1

We have, for any $\delta y = S\,\delta\theta$ given by (5.3), the relation

$$\int_0^T \delta y^T(t)\ \overline{W}(t)\ \delta y(t)\,dt = \|\delta\theta\|^2, \tag{5.6)'}$$

which gives for the linearized problem a hessian equal to identity. But we can observe in most situations that the terms neglected in the linearization result in a problem which is highly non convex and the behaviour of the problem (5.6)' is very different from (5.6). Futhermore it is clear that, in general, the operator $\overline{W}(t)$ is not *positive definite* (see appendix) and, as a consequence, the problem may be not well posed, thus it is usually necessary to regularize this problem.

5.2. An example of parameter estimation in a parabolic problem satisfying the strong identifiability condition

There are very few results on the identifiability of parabolic equations (Kitamura - Nakagiri [3], Nakagiri [5], Courdesses - Amouroux [2]). The strong identifiability presented in (4.3) on the discretized linearized problem is still more difficult to check. We present here a very simple situation studied in [2] where identifiability and strong identifiability turn out to be equivalent.

Consider the one-dimensionnal problem :

$$\frac{\partial u}{\partial t} - a\frac{\partial^2 u}{\partial x^2} - bu = 0 \qquad \begin{array}{l} x \in \Omega =]0,1[\\ t \in]0,T[\end{array} \tag{5.8}$$

with boundary conditions :

$$u(0,t) = u(1,t) = 0$$

and initial conditions :

$$u(0,x) = \alpha_1 \sqrt{2}\ \sin \pi x + \alpha_2 \sqrt{2}\ \sin 2\pi x.$$

The parameters to estimate are the constants a and b :

$$\theta = (a \quad b)^T \qquad\qquad 0 < a_1 \leqslant a \leqslant a_2$$

The system is observed at point x_0 : $Cu = u(x_0,t)$.

It is shown in [2] that the identifiability of θ is equivalent to :

$$\alpha_1\,\alpha_2 \sin \pi x_0\ \sin 2\pi x_0 \neq 0 \tag{5.9}$$

Let us consider the linearization of the state around $u(\overline{\theta})$ corresponding to a given value $\overline{\theta}$ of the parameter. We obtain :

$$S(t) = \begin{bmatrix} \frac{\partial u}{\partial a}(x_0,t) \\ \frac{\partial u}{\partial b}(x_0,t) \end{bmatrix} = \sqrt{2}\,t\,\alpha_1 \sin \pi x_0\, e^{(b-\pi^2 a)t} \begin{bmatrix} -\pi^2 \\ 1 \end{bmatrix} + \sqrt{2}\,t\,\alpha_2 \sin 2\pi x_0\, e^{(b-4\pi^2 a)t} \begin{bmatrix} -4\pi^2 \\ 1 \end{bmatrix}$$

Using (5.9) and the linear independance of time functions in the fomula, it is easy to show that if :

$$S^T(t)\,\Lambda\,S(t) = 0 \quad \forall\, t \in]0,T[\quad \Lambda \in \mathcal{S}_2$$

then the entries of Λ :

$$\Lambda = \begin{bmatrix} \lambda_1 & \lambda_{12} \\ \lambda_{12} & \lambda_2 \end{bmatrix}$$

must satisfy :

$$\begin{bmatrix} \pi^4 & -2\pi^2 & 1 \\ 4\pi^4 & -5\pi^2 & 1 \\ 16p^4 & -8\pi^2 & 1 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_{12} \\ \lambda_2 \end{bmatrix} = 0$$

which implies $\Lambda = 0$ as this matrix is nonsingular.

6. NUMERICAL EXPERIMENTS

Numerical experimentations are based on the example (1.1) in one dimension :

$$\begin{cases} \frac{\partial u}{\partial t}(x;t) - \frac{\partial}{\partial x}[\tau(x)\frac{\partial u}{\partial x}(x;t)] = f(x;t) \text{ in }]0,1[\times]0,T[\\ u(0,t) = \alpha_0 \\ u(1,t) = \alpha_1, u(x,0) = u_0(x) \end{cases} \tag{6.1}$$

with a "true" value of τ being :

$$\tau(x) = 1 + 5x . \tag{6.2}$$

A classical RITZ-GALERKINE approximation with piecewise linear functions is used to reduce problem (6.1) to a finite dimensional system. In the following numerical results the number of spatial nodes is 7, hence there are 6 parameters to estimate. Observation is distributed or punctual at one or several nodes.

On the various figures the convergence is illustrated by considering the evolution of the mean square error on the coefficients with respect to the number of iterations. It must be mentionned that the curves are piecewise straight lines which join the points where the error is actually calculated, thus the curves do not give information on the local rates of convergence.

Figures 1 and 2 :

- curves (a) coresponds to a minimizaton of the original functional by a BFGS algorithm after 2000 iterations in order to show the error on parameters.

- curves (b) represents the results obtained by the following algorithm : for a given value of ε one computes W_ε by (4.9) and a complete minimization of the weighted functional is performed this gives a new value for θ, then ε is divided by a given factor (for instance 100) and the procedure is repeated.

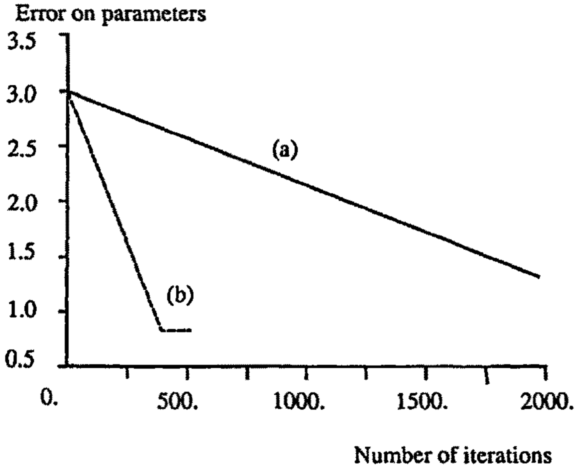

Figure 1

There is only one observation and the identifiability is very poor. The results show simply that the weighted functional gives a better result on the error even if this error does not vanish.

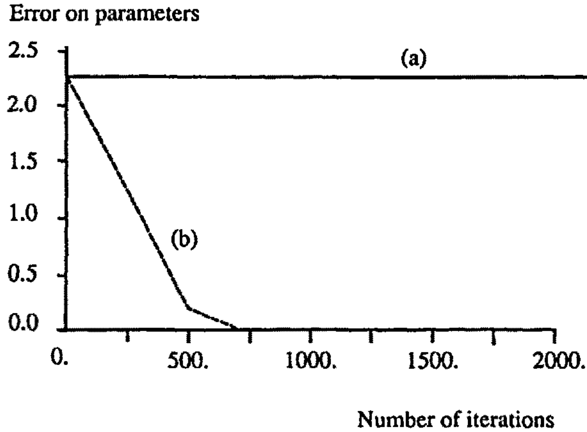

Figure 2

Observation at nodes 1;2,3. The initial guess on θ is (5,...,5). The figure shows the poor convergence of the non weighted functional (a) compared to the weighted one (b).

CONCLUSION

The proposed method improves the convexity of the criterion. It is clear that the computational effort required by this method may be rewarding only in the case of ill conditionned problems. For that reason the efficiency of the method is particularly illustrated by examples where the classical approach fails. A lot of questions still remain pending in partiçular the study of the "strong identifiability hypothesis" and the interpretation of the new estimate θ_w.

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Appendix

A drawback of the method is that the matrix Λ is not nessarily positive definite nor W(t). The next simple example shows the difficulty. The state of the system satisfies

$$\begin{cases} \dot{x}_1(t) = a_1 x_1(t) + \theta_1 e^{a_1 t}, x_1(0) = 0 \\ \dot{x}_2(t) = a_2 x_2(t) + \theta_2 e^{a_2 t}, x_2(0) = 0 \end{cases}$$

and is given by

$$\begin{cases} x_1(t) = t\ \theta_1 e^{a_1 t}, \\ x_2(t) = t\ \theta_2 e^{a_2 t}. \end{cases}$$

The observation is given by

$$y(t) = x_1(t)+x_2(t)$$

and the least square functionnal is given by

$$J(\theta_1,\theta_2) = \int_0^\infty |y(t)-z(t)|^2\,dt\,.$$

Under these conditions we have

$$S(t) \overset{\text{déf}}{=} [s_1(t)\,, s_2(t)\,] = [\ t\ \ e^{a_1 t}, t\ \ e^{a_2 t}]\ .$$

The sytem of equation giving the symmetric matrix $\Lambda = \begin{pmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{12} & \Lambda_{22} \end{pmatrix}$, is

$$\begin{pmatrix} a & 2b & c \\ b & 2c & d \\ c & 2d & e \end{pmatrix} \begin{pmatrix} \Lambda_{11} \\ \Lambda_{12} \\ \Lambda_{22} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

where

$$a = \int_0^\infty s_1^4(t)\,dt\ ,\quad b = \int_0^\infty s_1^3(t)\,s_2(t)\,dt\ ,\ c = \int_0^\infty s_1^2(t)\,s_2^2(t)\,dt\ ,\ d = \int_0^\infty s_1(t)\,s_2^3(t)\,dt\ ,\ e = \int_0^\infty s_2^4(t)\,dt\ .$$

After some calculations it is easy to show that the solution Λ is not definite, and furthermore that the function $W(t)$ is not necessarily positive.