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Simultaneous determination of time-dependent coefficients and heat source

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Abstract
This paper presents a numerical solution to the inverse problems of simultaneous determination of the time-dependent coefficients and the source term in the parabolic heat equation subject to overspecified conditions of integral type. The ill-posed problems are numerically discretised using the finite-difference method and the resulting system of nonlinear equations is solved numerically using the MATLAB toolbox routine *lsqnonlin* applied to minimizing the nonlinear Tikhonov regularization functional subject to simple physical bounds on the variables. Numerical examples are presented to illustrate the accuracy and stability of the solution.

Keywords: Inverse problem; Coefficient identification; Heat equation; Finite-difference method; Tikhonov regularization; Nonlinear minimization.

1 Introduction

Determination of a single unknown time-dependent property such as the capacity, conductivity or diffusivity from additional local or non-local measurements of the main dependent variable at the boundary or inside the space domain represents a classical example of a coefficient identification problem, as described for example in Chapter 13 of the excellent book of Cannon [4] on the one-dimensional heat equation. For more recent studies on the same inverse problems, see e.g. [9, 13] and the references therein.

The inverse formulation can be further extended to allow for an unknown free boundary to be determined as well, see e.g. [12]. Moreover, multiple time-dependent coefficient identifications have also been considered theoretically in the past, see e.g. [3, 11], and recently been solved numerically by the authors, [8]. In these studies, the unknowns were mainly coefficients multiplying the temperature and its partial derivatives, but more recent theoretical studies, [14, 15], allow for one of the time-dependent unknown to be in the free term heat source as well. And it is the purpose of this paper to numerically solve a couple of such related multiple coefficient identification problems.

The structure of the paper is as follows. In Section 2 we formulate the two inverse problems that we consider and state the uniqueness theorems. In Section 3 we briefly describe the finite-difference method used to discretise the direct problem, whilst Section 4 introduces the constrained regularized minimization problem that has to be solved using the MATLAB routine *lsqnonlin*. In Section 5, numerical results are presented and discussed and finally conclusions of the paper are given in Section 6.

2 Mathematical formulation

In this paper, we study a couple of coefficient identification problems related to the second-order parabolic partial differential equation

$$\frac{\partial u}{\partial t}(x,t) = a(x,t)\frac{\partial^2 u}{\partial x^2}(x,t) - b(x,t)\frac{\partial u}{\partial x}(x,t) - d(x,t)u(x,t) + f(t)g(x,t),\ (x,t) \in Q_T. \tag{1}$$

where $Q_T = [-\ell,\ell] \times [0,T]$, with $\ell > 0$ and $T > 0$, represents the solution domain, $a(x,t)$ is a given positive function involving physical quantities of the medium $(-\ell,\ell)$ such as conductivity, capacity, storage, diffusivity, $u(x,t)$ is the unknown dependent variable, e.g. the temperature in heat conduction, the pressure in porous media or the piezometric head in groundwater flow, $f(t)g(x,t)$ with $f(t)$ unknown and $g(x,t)$ given function represents a source (heat or hydraulic), and either one of the coefficients b (representing an advection/convection coefficient) or d (representing a reaction or perfusion coefficient in bio-heat conduction) are unknown (though we shall further assume that, when unknown, the corresponding quantity b or d depends on time only). To be more explicit, let us particularize equation (1) to the following two cases, namely,

$$\frac{\partial u}{\partial t}(x,t) = a(x,t)\frac{\partial^2 u}{\partial x^2}(x,t) - b(t)\frac{\partial u}{\partial x}(x,t) - d(x,t)u(x,t) + f(t)g(x,t),\ (x,t) \in Q_T \tag{2}$$

with unknown triplet $(u(x,t), f(t), b(t))$ and

$$\frac{\partial u}{\partial t}(x,t) = a(x,t)\frac{\partial^2 u}{\partial x^2}(x,t) - b(x,t)\frac{\partial u}{\partial x}(x,t) - d(t)u(x,t) + f(t)g(x,t),\ (x,t) \in Q_T. \tag{3}$$

with unknown triplet $(u(x,t), f(t), d(t))$.

We emphasize that such particularizations are often necessary when seeking to establish the uniqueness of the solution. Together with (2) or (3) we impose the initial condition

$$u(x,0) = \phi(x), \quad x \in [-\ell,\ell], \tag{4}$$

and the homogenous Dirichlet boundary conditions

$$u(\pm\ell,t) = 0, \quad t \in [0,T]. \tag{5}$$

As over-determination conditions we consider, [14],

$$\int_{-\ell}^{\ell} \omega(x)u(x,t)dx = \varphi(t), \quad t \in [0,T], \tag{6}$$

$$\int_{-\ell}^{\ell} \omega(x)u_x(x,t)dx = \psi(t), \quad t \in [0,T], \tag{7}$$

where ω is given weight function. Integral observation such as (6) have been considered before in numerous studies, see e.g. [5, 6, 10] to mention only a few, and physically it represents the mass/energy specification obtained by measuring the temperature $u(x,t)$ with thermocouples/ sources and then averaging over the space domain of the finite slab $[-\ell,\ell]$. This is because sometimes it might be practically impossible to measure the state of an object (or a process) at individual points and instead only the mean value of the state over the entire object can be specified, [1]. Remark also that if ω is differentiable then integration by parts in (7) and using (5) imply

$$\int_{-\ell}^{\ell} \omega'(x)u(x,t)dx = -\psi(t), \quad t \in [0,T], \tag{8}$$

so (7) may be thought to have the same physical meaning as (6) previously described.

About the input data we assume that they satisfy the following conditions:

(A) $0 < a_0 \leq a(x,t) \leq a_1$, $|a_x(x,t)| \leq K_a^*$, $|a_{xx}(x,t)| \leq K_a^{**}$, $(x,t) \in Q_T$.

(B) $|g(x,t)| \leq K_g$, $(x,t) \in Q_T$.

(C) $\omega \in W_\infty^3([-\ell,\ell])$, $\omega(\pm\ell) = \omega'(\pm\ell) = 0$, $|\omega''(x)| \leq K_\omega^{**}$, $x \in [-\ell,\ell]$, $\int_{-\ell}^{\ell}\omega(x)\phi(x)dx = \varphi(0)$, $\int_{-\ell}^{\ell}\omega(x)\phi'(x)dx = \psi(0)$.

(D) $\phi \in \overset{\circ}{W}{}_2^1([-\ell,\ell])$, $|\phi(x)| \leq M_0$, $x \in [-\ell,\ell]$.

(E) $\varphi(t)$, $\psi(t) \in W_\infty^1([0,T])$.

For the notation of the spaces of functions involved, see [16]. Then we have the following theorems of uniqueness of the solution for the inverse problems considered.

Theorem 1 (see [14])**.** *Assume conditions (A)–(E) on the input data hold. Assume also that* $0 < \psi_0 \leq |\psi(t)|$, $t \in [0,T]$, $|d(x,t)| \leq d_1$, $(x,t) \in Q_T$, *and that*

$$\left| \int_{-\ell}^{\ell} \omega'(x)g(x,t)dx \right| \geq G_0 > 0, \quad t \in [0,T]. \tag{9}$$

In addition, let the inequality

$$2\ell|G_1(t)|K_\omega^{**}(M_0 + K_g T R_0)e^{d_1 T} \leq \frac{1}{2}G_0\psi_0, \quad t \in [0,T], \tag{10}$$

hold for some $R_0 > 0$, *where*

$$G_1(t) = \int_{-\ell}^{\ell} \omega(x)g(x,t)dx, \quad t \in [0,T]. \tag{11}$$

Then there exists at most one solution

$$(u(x,t), f(t), b(t)) \in \left(W_2^{1,2}(Q_T) \cap C^{0,\alpha}(Q_T)\right) \times L_\infty([0,T]) \times L_\infty([0,T]), \tag{12}$$

for some $\alpha \in (0,1)$, *of the inverse problem (2), (4)–(7) such that*

$$\|f\|_{L_\infty([0,T])} \leq R_0. \tag{13}$$

In particular, if it happens that $G_1(t) \equiv 0$ *on* $[0,T]$ *then (10) holds for any* $R_0 > 0$ *and thus the uniqueness of solution holds without the restriction (13).*

Theorem 2 (see [15])**.** *Assume conditions (A)–(E) on the input data hold. Assume also that* $|b(x,t)| \leq K_b$, $|b_x(x,t)| \leq K_b^*$, $(x,t) \in Q_T$, *and that*

$$\Delta_1(t) := \psi(t)\int_{-\ell}^{\ell} \omega(x)g(x,t)dx + \varphi(t)\int_{-\ell}^{\ell} \omega'(x)g(x,t)dx \geq \delta_1 > 0, \quad t \in [0,T]. \tag{14}$$

Then there exists at most one solution

$$(u(x,t), f(t), d(t)) \in \left(W_2^{1,2}(Q_T) \cap C^{0,\alpha}(Q_T)\right) \times L_\infty([0,T]) \times L_\infty^+([0,T]), \tag{15}$$

of the inverse problem (3)–(7).

3 Numerical Solution of the Direct Problem

In this section, we consider the direct (forward) initial value problem given by equations (1), (4) and (5) when the coefficients $b(x,t)$, $d(x,t)$ and $f(t)$ are given and the dependent variable $u(x,t)$ is the solution to be determined. We use the finite-difference method (FDM) with Crank-Nicolson scheme, [18], which is unconditionally stable and second order accurate in space and time.

The discrete form of the direct problem is as follows. Taking the positive integer numbers M and N, the solution domain $Q_T = [-\ell, \ell] \times [0,T]$ is divided by a $M \times N$ mesh with spatial step size $\Delta x = 2\ell/M$ in x-direction and the time step size $\Delta t = T/N$. The solution at the node (i,j) is denoted by $u_{i,j} := u(x_i, t_j)$, where $x_i = -\ell + i\Delta x$, $t_j = j\Delta t$, $a_{i,j} := a(x_i,t_j)$, $b_{i,j} := b(x_i,t_j)$, $f_j := f(t_j) =$, $d_{i,j} := d(x_i,t_j)$ and $g_{i,j} := g(x_i,t_j)$ for $i = \overline{0,M}$ and $j = \overline{0,N}$.

Considering the general form of partial differential equation

$$u_t = G(x,t,u,u_x,u_{xx}), \tag{16}$$

equation (16) can be approximated as

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{1}{2}\left(G_{i,j} + G_{i,j+1}\right), \quad i = \overline{1,M},\ j = \overline{0,(N-1)}, \tag{17}$$

$$u_{i,0} = \phi(x_i), \quad i = \overline{0,M}, \tag{18}$$

$$u_{0,j} = 0, \quad u_{M,j} = 0, \quad j = \overline{0,N}, \tag{19}$$

where

$$G_{i,j} = G\left(x_i, t_j, \frac{u_{i+1,j} - u_{i-1,j}}{2(\Delta x)}, \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}\right), \ i = \overline{1,(M-1)},\ j = \overline{0,N}. \tag{20}$$

For our problem, equation (1) can be discretised in the form of (17) as

$$\begin{aligned} &- A_{i,j+1}u_{i-1,j+1} + (1 + B_{i,j+1})u_{i,j+1} - C_{i,j+1}u_{i+1,j+1} = \\ &\qquad A_{i,j}u_{i-1,j} + (1 - B_{i,j})u_{i,j} + C_{i,j}u_{i+1,j} + \frac{\Delta t}{2}\left(f_j g_{i,j} + f_{j+1}g_{i,j+1}\right), \end{aligned} \tag{21}$$

for $i = \overline{1,(M-1)}$, $j = \overline{0,(N-1)}$, where

$$A_{i,j} = \frac{(\Delta t)a_{i,j}}{2(\Delta x)^2} + \frac{b_{i,j}(\Delta t)}{4(\Delta x)}, \quad B_{i,j} = \frac{(\Delta t)a_{i,j}}{(\Delta x)^2} + \frac{\Delta t}{2}d_{i,j}, \quad C_{i,j} = \frac{(\Delta t)a_{i,j}}{2(\Delta x)^2} - \frac{b_{i,j}(\Delta t)}{4(\Delta x)}.$$

At each time step t_{j+1}, for $j = \overline{0,(N-1)}$, using the homogenous Dirichlet boundary conditions (19), the above difference equation can be reformulated as a $(M-1)\times(M-1)$ system of linear equations of the form,

$$D\mathbf{u}_{j+1} = \mathrm{E}\mathbf{u}_j + \mathbf{b}, \tag{22}$$

where

$$\mathbf{u}_{j+1} = (u_{1,j+1}, u_{2,j+1}, ..., u_{M-1,j+1})^{\mathrm{T}},$$

$$
D = \begin{pmatrix}
1+B_{1,j+1} & -C_{1,j+1} & 0 & \cdots & 0 & 0 & 0 \\
-A_{2,j+1} & 1+B_{2,j+1} & -C_{2,j+1} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -A_{M-2,j+1} & 1+B_{M-2,j+1} & -C_{M-2,j+1} \\
0 & 0 & 0 & \cdots & 0 & -A_{M-1,j+1} & 1+B_{M-1,j+1}
\end{pmatrix},
$$

$$
E = \begin{pmatrix}
1-B_{1,j} & C_{1,j} & 0 & \cdots & 0 & 0 & 0 \\
A_{2,j} & 1-B_{2,j} & C_{2,j} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & A_{M-2,j} & 1-B_{M-2,j} & C_{M-2,j} \\
0 & 0 & 0 & \cdots & 0 & A_{M-1,j} & 1-B_{M-1,j}
\end{pmatrix},
$$

and

$$
\mathbf{b} = \begin{pmatrix}
\frac{\Delta t}{2}(f_j g_{1,j} + f_{j+1} g_{1,j+1}) \\
\frac{\Delta t}{2}(f_j g_{2,j} + f_{j+1} g_{2,j+1}) \\
\vdots \\
\frac{\Delta t}{2}(f_j g_{M-2,j} + f_{j+1} g_{M-2,j+1}) \\
\frac{\Delta t}{2}(f_j g_{M-1,j} + f_{j+1} g_{M-1,j+1})
\end{pmatrix}.
$$

The numerical solutions for $\varphi(t)$ and $\psi(t)$ are calculated using the trapezoidal rule for integrals in (6) and (7), namely,

$$
\varphi(t_j) = \int_{-\ell}^{\ell} \omega(x) u(x, t_j) dx = \Delta x \left(\sum_{i=1}^{M-1} u_{i,j} \omega_i \right), \quad j = \overline{0, N}, \tag{23}
$$

$$
\psi(t_j) = \int_{-\ell}^{\ell} \omega(x) u_x(x, t_j) dx = \frac{\Delta x}{2} \left(u_{x0,j} \omega_0 + u_{xM,j} \omega_M + 2 \sum_{i=1}^{M-1} u_{xi,j} \omega_i \right), \quad j = \overline{0, N}, \tag{24}
$$

where $\omega_i := \omega(x_i)$ for $i = \overline{0, M}$, and

$$
\begin{aligned}
u_{x0,j} &= \frac{4u_{1,j} - u_{2,j} - 3u_{0,j}}{2(\Delta x)}, \quad u_{xM,j} = -\frac{4u_{M-1,j} - u_{M-2,j} - 3u_{M,j}}{2(\Delta x)}, \\
u_{xi,j} &= \frac{u_{i+1,j} - u_{i-1,j}}{2(\Delta x)}, \quad i = \overline{1, (M-1)}, \quad j = \overline{0, N}.
\end{aligned}
$$

4 Numerical Solutions of the Inverse Problems

In this section, we aim to obtain accurate and stable simultaneous identifications for the temperature $u(x, t)$, source $f(t)$ and the coefficients $b(t)$ or $d(t)$ for the inverse problems (2), (4)–(7) or (3)–(7), respectively. In the former case we minimize the nonlinear Tikhonov functional

$$
\begin{aligned}
F_1(b, f) := &\left\| \int_{-\ell}^{\ell} \omega(x) u(x, t) dx - \varphi(t) \right\|^2 + \left\| \int_{-\ell}^{\ell} \omega(x) u_x(x, t) dx - \psi(t) \right\|^2 \\
&+ \beta_1 \left\| b(t) \right\|^2 + \beta_2 \left\| f(t) \right\|^2,
\end{aligned} \tag{25}
$$

whilst in the latter case we minimize

$$F_2(d,f):=\Big\|\int_{-\ell}^{\ell}\omega(x)u(x,t)dx-\varphi(t)\Big\|^2+\Big\|\int_{-\ell}^{\ell}\omega(x)u_x(x,t)dx-\psi(t)\Big\|^2$$
$$+\beta_3\big\|d(t)\big\|^2+\beta_2\big\|f(t)\big\|^2, \tag{26}$$

where $\beta_i\geq 0$, $i=1,2,3$, are regularization parameters which are introduced in order to stabilise the numerical solution and the norm is the $L^2[0,T]$ norm. The discretizations of (25) and (26) are

$$F_1(\underline{b},\underline{f}):=\sum_{j=1}^{N}\Big[\int_{-\ell}^{\ell}\omega(x)u(x,t_j)dx-\varphi(t_j)\Big]^2+\sum_{j=1}^{N}\Big[\int_{-\ell}^{\ell}\omega(x)u_x(x,t_j)dx-\psi(t_j)\Big]^2$$
$$+\beta_1\sum_{j=1}^{N}b_j^2+\beta_2\sum_{j=1}^{N}f_j^2, \tag{27}$$
$$F_2(\underline{d},\underline{f}):=\sum_{j=1}^{N}\Big[\int_{-\ell}^{\ell}\omega(x)u(x,t_j)dx-\varphi(t_j)\Big]^2+\sum_{j=1}^{N}\Big[\int_{-\ell}^{\ell}\omega(x)u_x(x,t_j)dx-\psi(t_j)\Big]^2$$
$$+\beta_3\sum_{j=1}^{N}d_j^2+\beta_2\sum_{j=1}^{N}f_j^2. \tag{28}$$

respectively.

The unregularized case, i.e., $\beta_i=0$ for $i=1,2,3$, yields the ordinary nonlinear least-squares method which is usually producing unstable solutions when noisy data are inverted.

The noisy data is numerically simulated as

$$\varphi^{\epsilon 1}(t_j)=\varphi(t_j)+\epsilon 1_j,\quad \psi^{\epsilon 2}(t_j)=\psi(t_j)+\epsilon 2_j,\quad j=\overline{1,N}, \tag{29}$$

where $\epsilon 1_j$ and $\epsilon 2_j$ are random variables generated from a Gaussian normal distribution with mean zero and standard deviation $\sigma 1$ and $\sigma 2$, respectively, given by

$$\sigma 1=p\times\max_{t\in[0,T]}|\varphi(t)|,\quad \sigma 2=p\times\max_{t\in[0,T]}|\psi(t)|, \tag{30}$$

where p represents the percentage of noise. We use the MATLAB function *normrnd* to generate the random variables $\underline{\epsilon 1}=(\epsilon 1_j)_{j=\overline{1,N}}$ and $\underline{\epsilon 2}=(\epsilon 2_j)_{j=\overline{1,N}}$ as follows:

$$\underline{\epsilon 1}=normrnd(0,\sigma 1,N),\quad \underline{\epsilon 2}=normrnd(0,\sigma 2,N). \tag{31}$$

In the case of noisy data (6) and (7), we replace $\varphi(t_j)$ and $\psi(t_j)$ by $\varphi^{\epsilon 1}(t_j)$ and $\psi^{\epsilon 2}(t_j)$, respectively, in (27) and (28).

The minimization of F_1 or F_2 subject to simple bounds on the variables is accomplished using the MATLAB optimization toolbox routine *lsqnonlin*, which does not require supplying (by the user) the gradient of the objective function, [17]. This routine attempts to find a minimum of a sum of squares, starting from an initial guess, subject to constraints and this generally is referred to as a constrained nonlinear optimization.

We take bounds for the quantities $b(t)$ and $f(t)$ say, we seek them in the interval $[-10^3,10^3]$, whilst the non-negative quantity $d(t)$ is sought in the interval $[0,10^3]$. We also take the parameters of the routine as follows:

- Maximum number of iterations = $10 \times$ (number of variables).
- Maximum number of objective function evaluations = $10^5 \times$ (number of variables).
- Solution tolerance = 10^{-10}.
- Object function tolerance = 10^{-10}.

5 Numerical Results and Discussion

In this section, we present numerical results for the recovery of the unknowns $f(t)$, $b(t)$ or $d(t)$, in the case of exact and noisy data (29). To measure the accuracy of the numerical solution we employ the root mean square error ($rmse$) defined by:

$$rmse(f) = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\left(f_{numerical}(t_j) - f_{exact}(t_j)\right)^2}, \tag{32}$$

and similar expressions exist for $b(t)$ and $d(t)$.

Remark 1.
During the computation we need the values of $f(0)$ and $b(0)$ or $d(0)$. One can easily derive these values from the governing equations (2) or (3) with the help of the initial and boundary conditions (4) and (5), as follows.

Apply (2) or (3) at $x = \pm\ell$ to obtain

$$u_t(\pm\ell,t) = a(\pm\ell,t)u_{xx}(\pm\ell,t) - b(t)u_x(\pm\ell,t) - d(\pm\ell,t)u(\pm\ell,t) + f(t)g(\pm\ell,t), \tag{33}$$

or

$$u_t(\pm\ell,t) = a(\pm\ell,t)u_{xx}(\pm\ell,t) - b(\pm\ell,t)u_x(\pm\ell,t) - d(t)u(\pm\ell,t) + f(t)g(\pm\ell,t), \tag{34}$$

respectively. Then apply (33) and (34) at $t = 0$, and use the compatibility conditions for the initial data (4) and the boundary conditions (5) to result in

$$0 = a(\pm\ell,0)\phi''(\pm\ell) - b(0)\phi'(\pm\ell) + f(0)g(\pm\ell,0), \tag{35}$$

or

$$0 = a(\pm\ell,0)\phi''(\pm\ell) - b(\pm\ell,0)\phi'(\pm\ell) + f(0)g(\pm\ell,0), \tag{36}$$

respectively. Solving the (2×2) linear system of equations (35) for $b(0)$ and $f(0)$ we obtain

$$b(0) = \frac{-g(-\ell,0)a(\ell,0)\phi''(\ell) + g(\ell,0)a(-\ell,0)\phi''(-\ell)}{-\phi'(-\ell)g(\ell,0) + \phi'(\ell)g(-\ell,0)}, \tag{37}$$

$$f(0) = \frac{\phi'(-\ell)a(\ell,0)\phi''(\ell) + \phi'(\ell)a(-\ell,0)\phi''(-\ell)}{-\phi'(-\ell)g(\ell,0) + \phi'(\ell)g(-\ell,0)}, \tag{38}$$

provided that the denominator $-\phi'(-\ell)g(\ell,0) + \phi'(\ell)g(-\ell,0) \neq 0$. Also, from equation (36) an expression for $f(0)$ can be obtained as

$$f(0) = \frac{-a(\pm\ell,0)\phi''(\pm\ell) + b(\pm\ell,0)\phi'(\pm\ell)}{g(\pm\ell,0)}, \tag{39}$$

provided that the denominator $g(\pm\ell, 0) \neq 0$. For $d(0)$ we use a different method which uses the overdermination conditions (6) or (7), as follows. Multiplying equation (3) by $\omega(x)$ and integrating with respect to x, using (6), we obtain

$$\varphi'(t) = \int_{-\ell}^{\ell} \omega(x)(a(x,t)u_{xx}(x,t) - b(x,t)u_x(x,t))dx - d(t)\varphi(t)$$
$$+ f(t) \int_{-\ell}^{\ell} \omega(x)g(x,t)dx. \tag{40}$$

Setting $t = 0$ in (40) we obtain

$$d(0) = \frac{-\varphi'(0) + \int_{-\ell}^{\ell} \omega(x)\left(a(x,0)\phi''(x) - b(x,0)\phi'(x)\right)dx + f(0)\int_{-\ell}^{\ell} \omega(x)g(x,0)dx}{\varphi(0)}, \tag{41}$$

provided that $\varphi(0) \neq 0$, where $f(0)$ is computed by expression (39). Alternatively, differentiating equation (3) with respect to x and multiplying it by $\omega(x)$ and then integrating it with respect to x, and using (7), we obtain

$$\psi'(t) = \int_{-\ell}^{\ell} \omega(x)[(a(x,t)u_{xx}(x,t))_x - (b(x,t)u_x(x,t))_x]dx - d(t)\psi(t)$$
$$+ f(t) \int_{-\ell}^{\ell} \omega(x)g_x(x,t)dx. \tag{42}$$

Setting $t = 0$ in (42) we obtain

$$d(0) = \frac{-\psi'(0) + \int_{-\ell}^{\ell} \omega(x)\left(a(x,0)\phi''(x) - b(x,0)\phi'(x)\right)' dx + f(0)\int_{-\ell}^{\ell} \omega(x)g_x(x,0)dx}{\psi(0)}, \tag{43}$$

provided that $\psi(0) \neq 0$, where $f(0)$ is computed by expression (39).

5.1 Example 1

Consider first the inverse problem (2), (4)–(7), with unknown coefficients $f(t)$ and $b(t)$, and the following input data:

$$a(x,t) = 1, \quad d(x,t) = 0, \quad g(x,t) = -x^3, \quad (x,t) \in Q_T, \tag{44}$$
$$\phi(x) = x(\ell^2 - x^2), \quad \omega(x) = (x^2 - \ell^2)^2, \quad x \in [-\ell, \ell], \tag{45}$$
$$\varphi(t) = \int_{-\ell}^{\ell} \omega(x)u(x,t)dx = 0, \quad t \in [0,T], \tag{46}$$
$$\psi(t) = \int_{-\ell}^{\ell} \omega(x)u_x(x,t)dx = \frac{64\ell^7 e^{-6t}}{105}, \quad t \in [0,T]. \tag{47}$$

One can easily observe that the conditions of Theorem 1 are satisfied by the above input data (in particular note that $G_1(t) = \int_{-\ell}^{\ell} \omega(x)g(x,t)dx = -\int_{-\ell}^{\ell} x^3(x^2 - \ell^2)dx = 0$) and hence the inverse problem has at most one solution in the class of functions (12). In fact, it can easily be checked by direct substitution that the analytical solution is given by

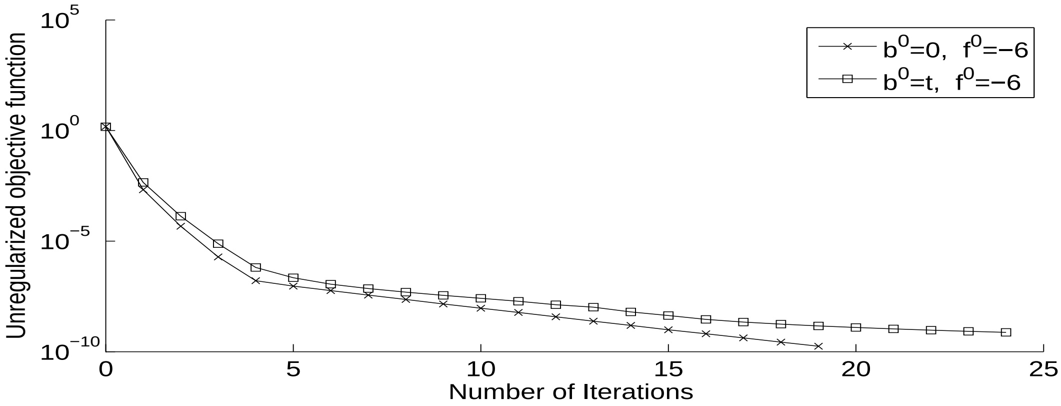
$$b(t) = 0, \quad f(t) = -\frac{6e^{\frac{-6t}{\ell^2}}}{\ell^2}, \quad t \in [0, T], \tag{48}$$

$$u(x,t) = e^{\frac{-6t}{\ell^2}} x(\ell^2 - x^2), \quad (x,t) \in Q_T. \tag{49}$$

We take for simplicity, $\ell = T = 1$ and employ the FDM described in Section 3 with M=N=40 at each iteration of minimization procedure described in Section 4. Remark that from (37) and (38) we obtain $b(0) = 0$ and $f(0) = -6$ and therefore, appropriate candidates for the initial guesses of b and f are $b^0 = 0$ and $f^0 = -6$. However, because the exact solution for $b(t)$ is actually the trivial zero function we also investigate another initial guess for b given by $b^0(t) = t$.

For exact data, i.e., $p = 0$ in (30), numerical results of the inversion with and without regularization in (27) and various initial guesses are presented in Figures 1–3 and Table 1. From Figure 1 and Table 1 it can be seen that, as expected, the farther the initial guess is, the more iterations and computational time are required to achieve convergence. However, for both initial guesses considered, the objective function (27) converges to the same minimum value which is of $O(10^{-10})$. Furthermore, from Figure 1(a) and Table 1 it can be seen that, in case of no regularization being employed, better results are obtained for the closer initial guess for $b(t)$. However, the results for $b(t)$ obtained for the farther initial guess in Figure 2(a) oscillate for the last 7-8 time steps near the final time showing that instability starts to manifest. In order to alleviate these oscillations some little regularization is recommended and these improvements over Figure 2 are clearly illustrated in Figure 3, see also the corresponding rows in Table 1 for further comparison. Observe in particular from Table 1 that including regularization also reduces the number of iterations and computational time in addition to achieving the stability of solution.

(a)



(b)

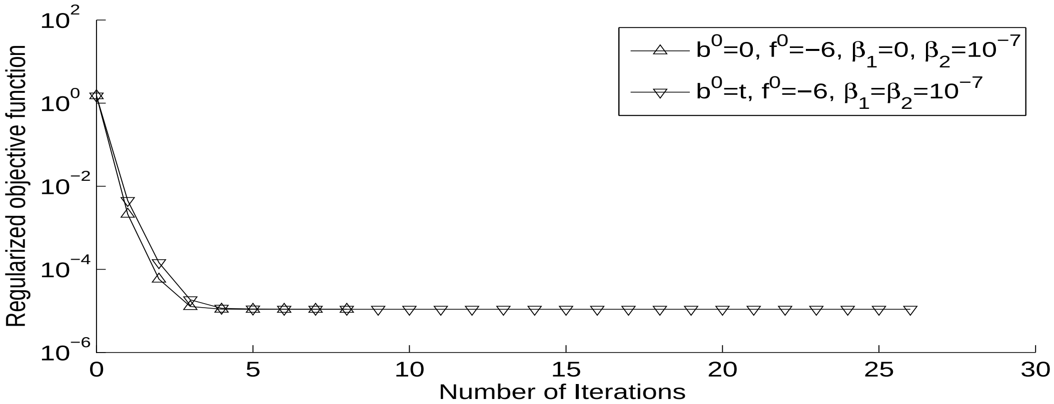
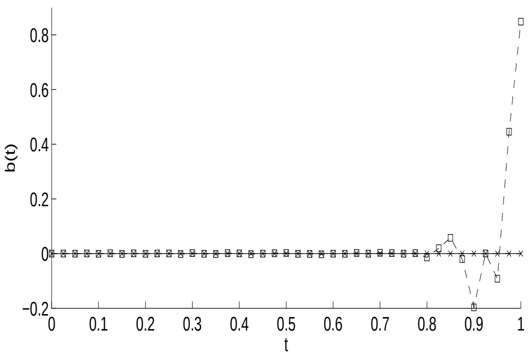


Figure 1: The objective function (27), (a) without and (b) with regularization, and various initial guesses, for Example 1 with exact data.

(a)



(b)

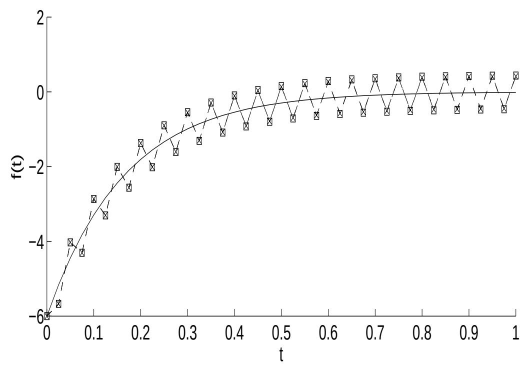


Figure 2: The exact (—) and numerical solutions without regularization, and various initial guesses $b^0 = 0$ (- $\times$ -) and $b^0 = t$ (- $\square$ -) for: (a) $b(t)$ and (b) $f(t)$, for Example 1 with exact data.

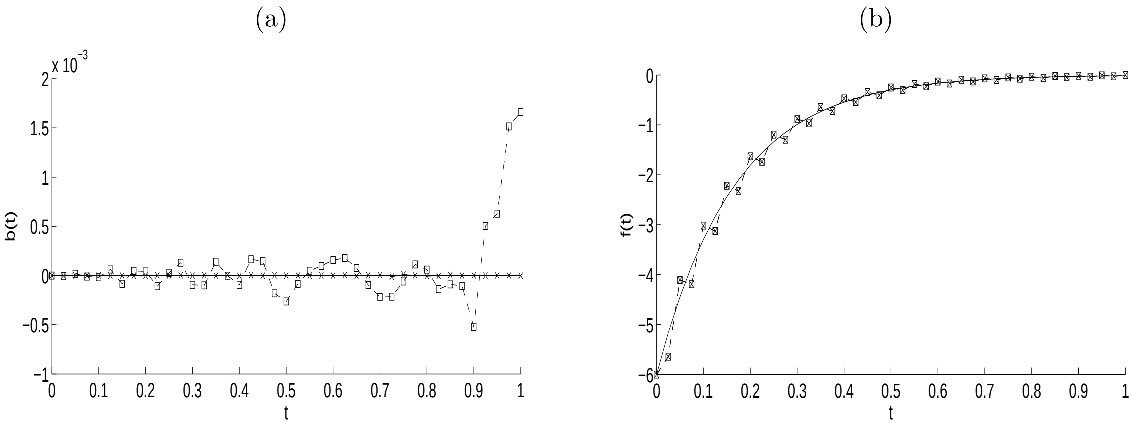


Figure 3: The exact (—) and numerical solutions with regularization and various initial guesses $b^0 = 0$, $\beta_1 = 0$, $\beta_2 = 10^{-7}$ (- $\times$ -) and $b^0 = t$, $\beta_1 = \beta_2 = 10^{-7}$ (- $\square$ -) for: (a) $b(t)$ and (b) $f(t)$, for Example 1 with exact data.

In the remaining of this subsection, for brevity, we only illustrate the results obtained with the initial guess $b^0 = t$ and $f^0 = -6$.

Table 1: Number of iterations, number of function evaluations, value of the objective function (27) at final iteration, the *rmse* values and the computational time with and without regularization and various initial guesses for Example 1 with exact data.

$\beta_1 = \beta_2 = 0$	$b^0 = 0,\ f^0 = -6$	$b^0 = t,\ f^0 = -6$
No. of iterations	19	24
No. of function evaluations	1660	2075
Value of objective function (27) at final iteration	1.7E-10	7.4E-10
$rmse(b)$	6.1E-6	0.1557
$rmse(f)$	0.4379	0.4536
Computational time	20 mins	24 mins
$\beta_2 = 10^{-7}$	$b^0 = 0,\ f^0 = -6,\ \beta_1 = 0$	$b^0 = t,\ f^0 = -6,\ \beta_1 = 10^{-7}$
No. of iterations	8	9
No. of function evaluations	747	830
Value of objective function (27) at final iteration	1.0E-5	1.0E-5
$rmse(b)$	3.5E-6	4.0E-4
$rmse(f)$	0.1514	0.1516
Computational time	9 mins	10 mins

In order to investigate the stability of the solution we add $p = 1\%$ noise to the input data (6) and (7), as in (29). The objective function (27), as a function of the number of iterations, is plotted in Figure 4. From this figure it can be seen that in the absence of regularization a slow and smooth convergence is recorded and, in fact, the process of minimization of the routine *lsqnonlin* is stopped when the prescribed tolerance of solution $= 10^{-10}$ is reached. The corresponding numerical results for the unknown coefficients are presented in Figure 5. From this figure it can be seen that unstable results are obtained for both coefficients $b(t)$ and $f(t)$ (compare with the results for exact data in Figure 2). This is expected since the problem under investigation is ill-posed. Consequently, regularization should be applied to restore the stability of the solution in the components $b(t)$ and $f(t)$.

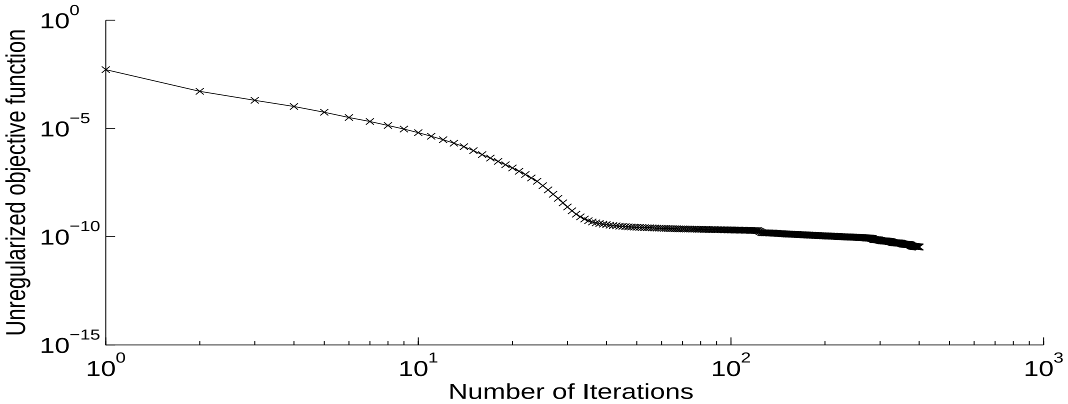


Figure 4: The objective function (27) without regularization for Example 1 with $p = 1\%$ noise data.

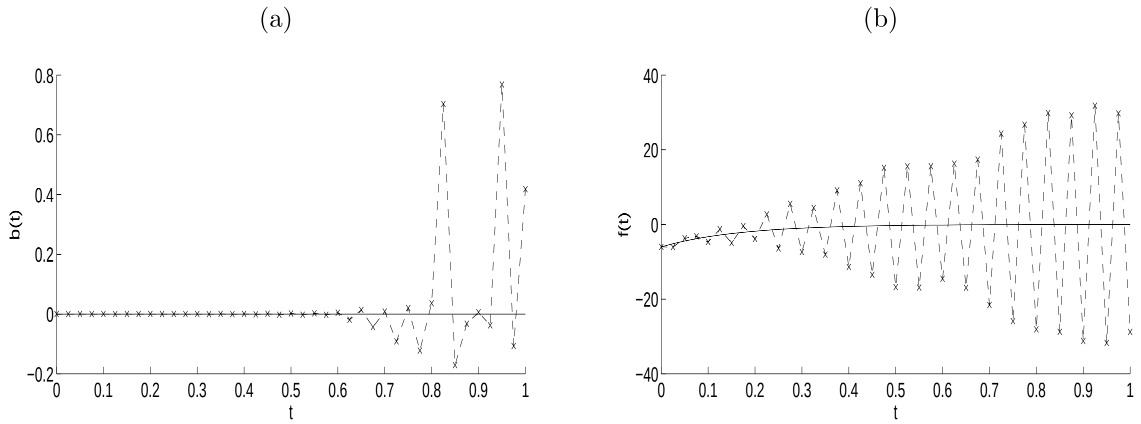


Figure 5: The exact (—) and numerical (- $\times$ -) solutions without regularization for: (a) $b(t)$ and (b) $f(t)$, for Example 1 with $p = 1\%$ noisy data.

Regularization parameters have been chosen by trial and error and numerical results obtained from some typical choices are given in Table 2 and Figures 6 and 7. Justifying more rigorously the choice of the regularization parameters β_1 and β_2 possibly using the L-surface method, [2], is nevertheless very important and will be the subject of future work. From Figure 6 it can be noticed that convergence in less than 8 iterations is achieved for each selection of regularization parameters. The corresponding numerical reconstructions for $b(t)$ and $f(t)$ are presented in Figure 7. By comparing Figure 5 with Figure 7 one can immediately notice the dramatic improvement in stability and accuracy which is achieved through the inclusion of regularization in the objective function (27).

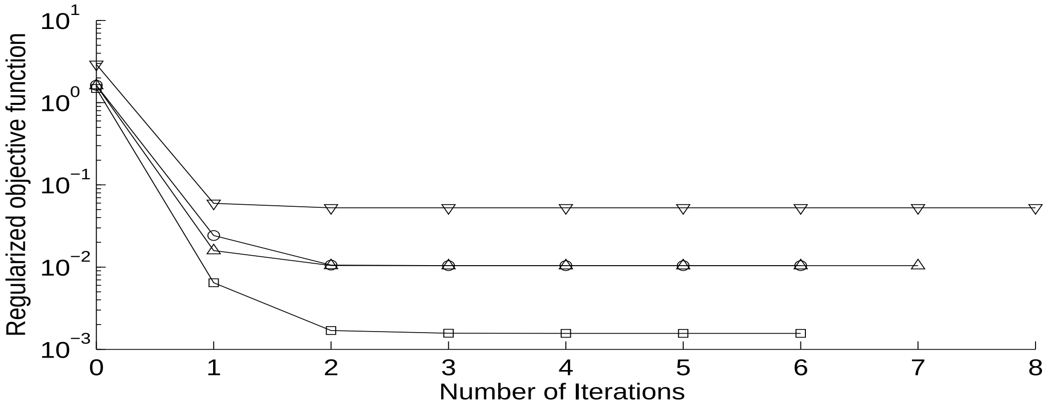


Figure 6: The objective function (27) with regularization parameters $\beta_1 = \beta_2 = 10^{-5}$ (-□-), $\beta_1 = \beta_2 = 10^{-4}$ (-△-), $\beta_1 = \beta_2 = 10^{-3}$ (-▽-) and $\beta_1 = 10^{-3}$, $\beta_2 = 10^{-4}$ (-○-), for Example 1 with $p = 1\%$ noisy data.

(a) (b)

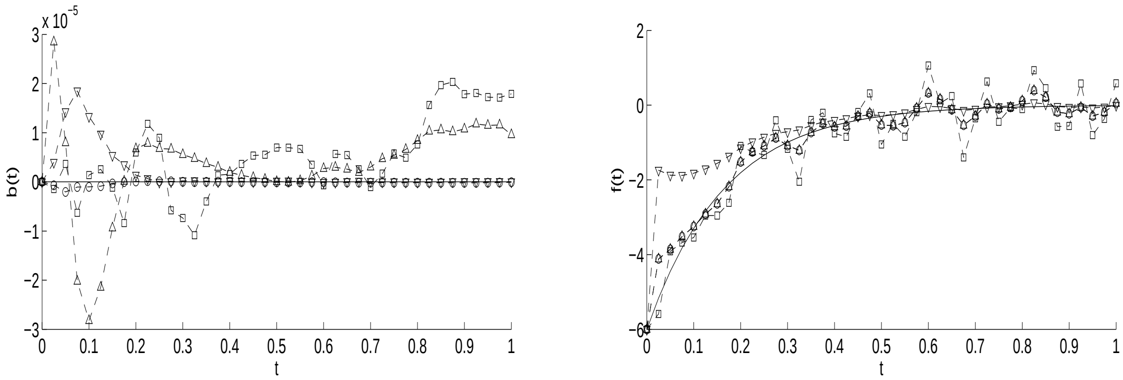


Figure 7: The exact (—) and numerical solutions with regularization parameters $\beta_1 = \beta_2 = 10^{-5}$ (-□-), $\beta_1 = \beta_2 = 10^{-4}$ (-△-), $\beta_1 = \beta_2 = 10^{-3}$ (-▽-) and $\beta_1 = 10^{-3}$, $\beta_2 = 10^{-4}$ (-○-) for: (a) $b(t)$ and (b) $f(t)$, for Example 1 with $p = 1\%$ noisy data.

Table 2: Number of iterations, number of function evaluations, value of the objective function (27) at final iteration, the $rmse$ values and the computational time, with regularization for Example 1 with $p = 1\%$ noisy data.

$p = 1\%$	β_1=β_2=10^{-5}	β_1=β_2=10^{-4}	β_1=β_2=10^{-3}	β_1=10^{-3}, β_2=10^{-4}
No. of iterations	6	7	8	6
No. of function evaluations	581	664	747	581
Value of objective function (27) at final iteration	0.0015	0.0104	0.0526	0.0104
$rmse(b)$	9.5E-6	1.0E-5	4.6E-6	4.5E-7
$rmse(f)$	0.5698	0.2884	0.8412	0.2884
Computational time	7 mins	8 mins	9 mins	7 mins

5.2 Example 2

In this example, we consider solving the second inverse problem given by equations (3)–(7) with unknown coefficients $f(t)$ and $d(t) \geq 0$, and the following input data:

$$b(x,t) = 1, \quad g(x,t) = \frac{(5-t)x^3}{\ell^2} - 3x^2 + (1+t)x + \ell^2, \quad (x,t) \in Q_T, \tag{50}$$

and a, ϕ, ω, φ, and ψ given by equations (45)–(47).

One can easily check the the conditions of Theorem 2 are satisfied; in particular

$$\begin{aligned}\Delta_1(t) &= \int_{-\ell}^{\ell} g(x,t)\,(\omega(x)\psi(t) + \omega'(x)\varphi(t))\,dx \\ &= \frac{4096e^{-6t/\ell^2}\ell^{14}}{11025} \geq \frac{4096e^{-6T/\ell^2}\ell^{14}}{11025} =: \delta_1 > 0, \quad t \in [0,T],\end{aligned}$$

and therefore the inverse problem has at most one solution in the class of functions (15). In fact, it can easily be checked by direct substitution that the analytical solution is given by

$$d(t) = \frac{1+t}{\ell^2}, \quad f(t) = e^{-\frac{6t}{\ell^2}}, \quad t \in [0,T], \tag{51}$$

and $u(x,t)$ is given by (49).

As in Example 5.1, we take $\ell = T = 1$ and employ the FDM with M=N=40. Remark that from (39) and (43) we obtain that $f(0)$=1 and $d(0)$=1. So, we take the initial guesses d^0=f^0=1 in the minimization of the functional (28).

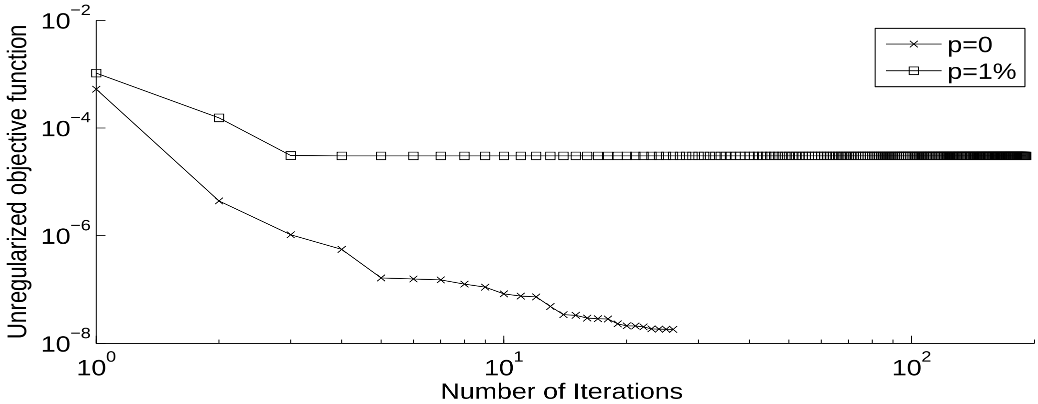


Figure 8: The objective function (28) without regularization, for Example 2 with exact data and $p = 1\%$ noisy data.

Figures 8 and 9 illustrate the convergence of the unregularized objective function (28) with $\beta_2 = \beta_3 = 0$ and the corresponding recovered coefficients $d(t)$ and $f(t)$, respectively, for exact data $p = 0$ and for $p = 1\%$ noisy data. First, from Figure 8 it can be seen that for exact data the unregularized objective function decreases rapidly in about 26 iterations to a low threshold of $O(10^{-8})$. However, for $p = 1\%$ noisy data, the number of iterations necessary to achieve the required degree of convergence with respect to the tolerance chosen increases to 191, see also the second column of Table 3 where, in particular, one can observe the long computational time recorded to be in excess of 4 hours. In Figure 9, reasonable good retrievals for the unknown coefficients can be observed for exact data, but the instability clearly manifests for noisy data. In order to stabilise the solution for noisy data, as in Example 5.1, regularization needs to be included in the functional (28) which is minimized.

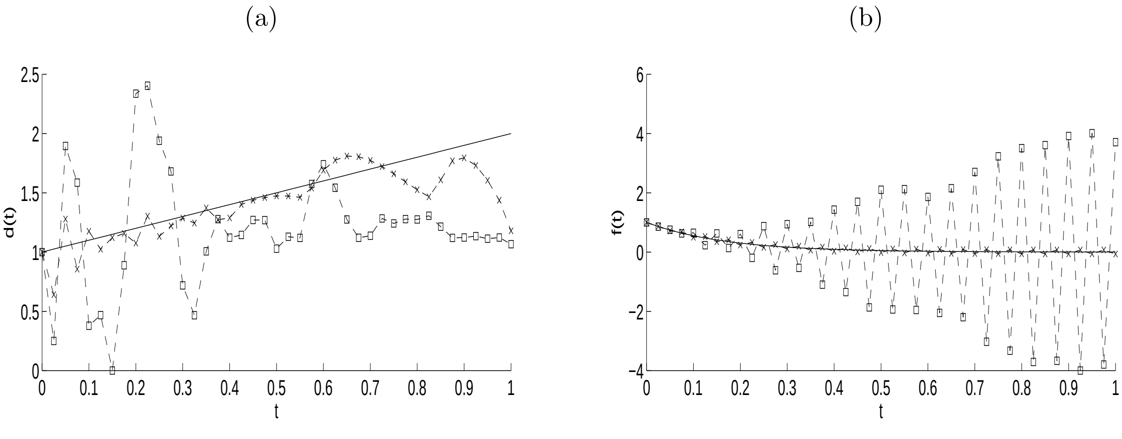


Figure 9: The exact (—) and numerical solutions without regularization for: (a) $d(t)$ and (b) $f(t)$, for Example 2 with exact data (-×-) and with $p = 1\%$ noisy data (-□-).

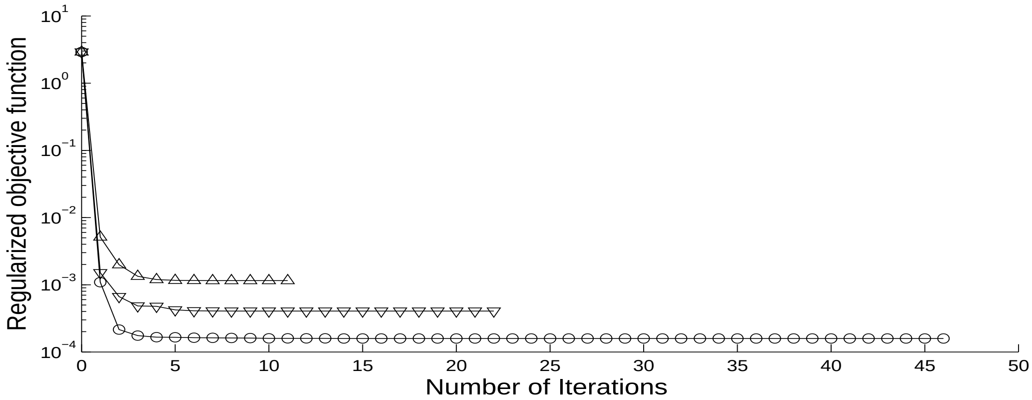


Figure 10: The objective function (28) with regularization parameters $\beta_2 = \beta_3 = 10^{-4}$ (-△-), $\beta_2 = \beta_3 = 10^{-5}$ (-▽-) and $\beta_2 = \beta_3 = 10^{-6}$ (-○-), for Example 2 with $p = 1\%$ noisy data.

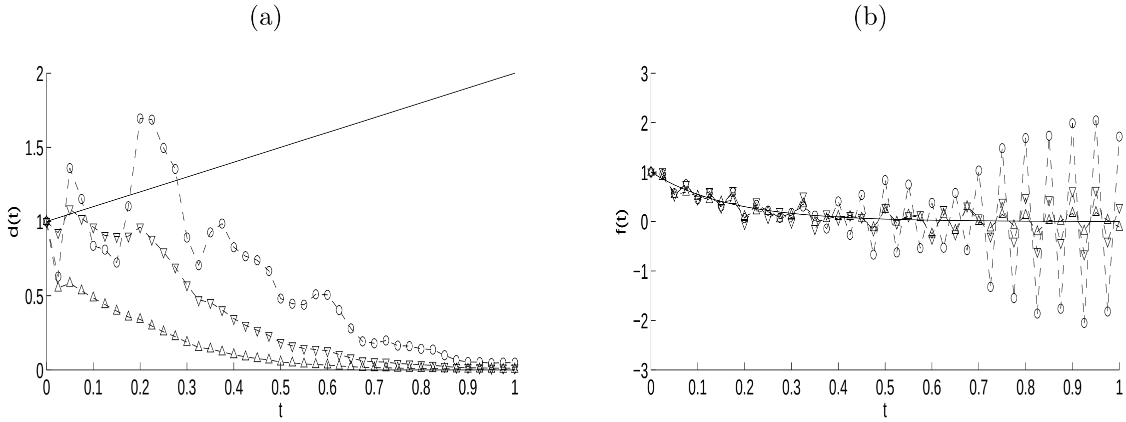


Figure 11: The exact (—) and numerical solutions with regularization parameters $\beta_2 = \beta_3 = 10^{-4}$ (-△-), $\beta_2 = \beta_3 = 10^{-5}$ (-▽-) and $\beta_2 = \beta_3 = 10^{-6}$ (-○-) for: (a) $d(t)$ and (b) $f(t)$, for Example 2 with $p = 1\%$ noisy data.

Table 3: Number of iterations, number of function evaluations, value of the objective function (28) at final iteration, *rmse* values and the computational time, for various regularization parameters, for Example 2 with $p = 1\%$ noisy data.

$p = 1\%$	$\beta_2=\beta_3=0$	$\beta_2=\beta_3=10^{-6}$	$\beta_2=\beta_3=10^{-5}$	$\beta_2=\beta_3=10^{-4}$
No. of iterations	191	46	22	11
No. of function evaluations	15936	3901	1909	996
Value of objective function (28) at final iteration	3E-5	0.0001	0.0004	0.0011
$rmse(d)$	0.6283	1.1731	1.3207	1.4409
$rmse(f)$	2.3165	1.0330	0.3127	0.1325
Computational time	4 hours	57 mins	28 mins	15 mins

Figure 10 shows the objective function (28), as a function of the number of the iterations, for various selections of regularization parameters β_2=$\beta_3 \in \{10^{-6}, 10^{-5}, 10^{-4}\}$, when the input data (6) and (7) is contaminated with $p = 1\%$ noise. From this figure it can be remarked that a rapid convergent is achieved for each selection of regularization parameters. The corresponding exact and numerical solutions for $d(t)$ and $f(t)$ are presented in Figure 11 and other numerical features of the solutions are summarised in Table 3. First, by comparing Figures 9 and 11 clearly the stabilisation benefit of employing regularization can be appreciated. It is also interesting to remark from Table 3 that retrieving accurately and simultaneously both the coefficients $d(t)$ and $f(t)$ requires an appropriate choice of the regularization parameters β_2 and β_3, e.g. for $\beta_2 = \beta_3 = 0$ the recovery of $d(t)$ is accurate in the detriment of that of $f(t)$, whilst for $\beta_2 = \beta_3 = 10^{-4}$ the accuracy of the simultaneous recovery is viceversa. This situation has also been observed previously in cases where simultaneous identification of multiple coefficients has been attempted, [7, 9]. Therefore, a compromising but balancing choice would be to pick $\beta_2 = \beta_3$ in between, say between 10^{-5} and 10^{-4} as is common with ill-posed problems in which acceptable candidate solutions are those in the region where the accuracy and stability portions meet/ intersect.

Finally, for completeness, the exact and numerical reconstructions for the temperature $u(x,t)$ are presented in Figure 12 and the absolute error between them is also included. From this figure it can be observed that a stable and accurate reconstruction is obtained.

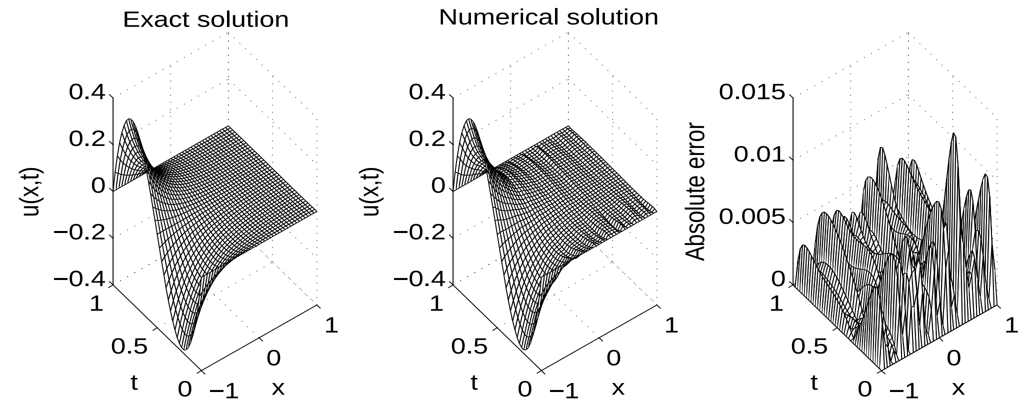


Figure 12: The exact (49) and numerical reconstructions for the temperature $u(x,t)$ with regularization parameters $\beta_1 = \beta_2 = 10^{-5}$, for Example 2 with $p = 1\%$ noisy data.

6 Conclusions

A couple of inverse problems consisting of finding the time-dependent coefficients and the time-dependent heat source term in the parabolic heat equation with integral overdetermination conditions have been numerically investigated. The MATLAB routine *lsqnonlin* has been employed effectively to solve the resulting nonlinear constraint optimization problems subject to both exact or noisy input data. Regularization has been imposed when the noisy data has been inverted. Numerical results presented and discussed for a couple test examples show that reasonably accurate and stable numerical solutions have been achieved.

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