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Huntul, MJ and Lesnic, D (2017) An inverse problem of finding the time-dependent thermal conductivity from boundary data. International Communications in Heat and Mass Transfer, 85. pp. 147-154. ISSN 0735-1933

https://doi.org/10.1016/j.icheatmasstransfer.2017.05.009

An inverse problem of finding the time-dependent thermal conductivity from boundary data

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Abstract

We consider the inverse problem of determining the time-dependent thermal conductivity and the transient temperature satisfying the heat equation with initial data, Dirichlet boundary conditions, and the heat flux as overdetermination condition. This formulation ensures that the inverse problem has a unique solution. However, the problem is still ill-posed since small errors in the input data cause large errors in the output solution. The finite difference method is employed as a direct solver for the inverse problem. The inverse problem is recast as a nonlinear least-squares minimization subject to physical positivity bound on the unknown thermal conductivity. Numerically, this is effectivey solved using the *lsqnonlin* routine from the MATLAB toolbox. We investigate the accuracy and stablity of results on a few test numerical examples.

Keywords: Inverse problem; thermal conductivity; heat equation; nonlinear optimization.

1 Introduction

In inverse problems, the unknown densities or distributed source, or the coefficients involved in the governing partial differential equation or in the boundary conditions for a mathematical model under investigation are sought from additional information on the main dependent variable solution of the original direct initial boundary value problem, [11]. In particular, the inverse problem of identifying the thermal diffusivity/ conductivity from boundary data (temperature and partial heat flux) has been investigated widely by many researchers in the past, see [1–3, 5–8, 12] to mention only a few. In this paper, the novelty consists in the development of a convergent numerical optimization method for solving this nonlinear but well-posed inverse coefficient problem for the heat equation. Numerically, the implementation is realised using the MATLAB toolbox routine *lsqnonlin*.

The paper is organized as follows. In Section 2, the mathematical formulation of the inverse problem is presented. In Section 3, the numerical solution of the direct problem is based on the finite difference method with the Crank-Nicolson scheme. In Section 4, the minimization algorithm to solve the inverse problem is presented. The numerical results are discussed in Section 5. Finally, conclusions are highlighted in Section 6.

2 Mathematical formulation

In the domain $Q_T = \{(x,t)|0 < t < T, 0 < x < L\}$, we consider the inverse problem given by the parabolic heat equation

$$\frac{\partial u}{\partial t}(x,t) = a(t)\frac{\partial^2 u}{\partial x^2}(x,t) + f(x,t), \qquad (x,t) \in Q_T, \tag{1}$$

with known heat source $f(x,t)$, unknown temperature $u(x,t)$ and unknown thermal conductivity $a(t) > 0$, $t \in (0,T]$, subject to the initial condition

$$u(x,0) = \phi(x), \qquad x \in [0,L], \tag{2}$$

the Dirichlet temperature boundary conditions

$$u(0,t) = \mu_1(t), \quad u(L,t) = \mu_2(t), \qquad t \in [0,T], \tag{3}$$

and the Neumann heat flux overdetermination condition

$$a(t)u_x(0,t) = \mu_3(t), \qquad t \in [0,T]. \tag{4}$$

The uniqueness of solution of the inverse problem (1)–(4) has been established in [6] and reads as follows.

Theorem 1. (Uniqueness). *If* $0 < \mu_3 \in C[0,T]$, *then a solution* $(a(t), u(x,t)) \in H^{1+\alpha/2}[0,T] \times H^{2+\alpha,1+\alpha/2}(\overline{Q_T})$, *for some* $\alpha \in (0,1), a(t) > 0$ *for* $t \in [0,T]$, *to the problem (1)–(4) is unique.*

In this theorem, $H^{1+\alpha/2}[0,T]$ denotes the space of Hölder continuously differentiable functions on $[0,T]$ with exponent $\alpha/2$. Also, $H^{2+\alpha,1+\alpha/2}(\overline{Q_T})$ denotes the space of continuous functions u along with their partial derivatives u_x, u_{xx}, u_t in $\overline{Q_T}$, with u_{xx} being Hölder continuous with exponent α in $x \in [0,L]$ uniformly with respect to $t \in [0,T]$, and with u_t being Hölder continuous with exponent $\alpha/2$ in $t \in [0,T]$ uniformly with respect to $x \in [0,L]$. Lower-order terms $b(x,t)\frac{\partial u}{\partial x}(x,t) + c(x,t)u(x,t)$, with b and c known functions, can also be added to the right-hand side of equation (1), with no qualitative change in both analytical and numerical analyses, [6].

3 Numerical solution of direct problem

In this section, we consider the direct initial boundary value problem given by equations (1)–(3). We use the finite-difference method (FDM) with a Crank-Nicholson scheme, [10], which is unconditionally stable and second-order accurate in space and time. The discrete form of the direct problem is as follows. We denote $u(x_i,t_j) = u_{i,j}, a(t_j) = a_j$, and $f(x_i,t_j) = f_{i,j}$, where $x_i = i\Delta x, t_j = j\Delta t$ for $i = \overline{0,M}, j = \overline{0,N}$, and $\Delta x = \frac{L}{M}, \Delta t = \frac{T}{N}$. Then the problem (1)–(3) can be discretised as

$$\begin{aligned} &-A_{j+1}u_{i-1,j+1} + (1+B_{j+1})u_{i,j+1} - A_{j+1}u_{i+1,j+1} \\ &= A_j u_{i-1,j} + (1-B_j)u_{i,j} + A_j u_{i+1,j} + \frac{\Delta t}{2}(f_{i,j} + f_{i,j+1}), \ i = \overline{1,(M-1)}, \ j = \overline{0,N}, \end{aligned} \tag{5}$$

$$u_{i,0} = \phi(x_i), \quad i = \overline{0,M}, \tag{6}$$

$$u_{0,j} = \mu_1(t_j), \quad u_{M,j} = \mu_2(t_j), \quad j = \overline{0, N}, \tag{7}$$

where

$$A_j = \frac{(\Delta t)a_j}{2(\Delta x)^2}, \qquad B_j = \frac{(\Delta t)a_j}{(\Delta x)^2}.$$

At each time step t_{j+1}, for $j = \overline{0, (N-1)}$, using the Dirichlet boundary conditions (7), the above difference equation can be reformulated as a $(M-1) \times (M-1)$ system of linear equations of the form,

$$D\mathbf{u_{j+1}} = E\mathbf{u_j} + \mathbf{b^j}, \tag{8}$$

where

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

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

$$E = \begin{pmatrix} 1-B_j & A_j & 0 & ... & 0 & 0 & 0 \\ A_j & 1-B_j & A_j & ... & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & ... & A_j & 1-B_j & A_j \\ 0 & 0 & 0 & ... & 0 & A_j & 1-B_j \end{pmatrix},$$

and

$$\mathbf{b^j} = \begin{pmatrix} \frac{\Delta t}{2}(f_{1,j} + f_{1,j+1}) + A_j\mu_1(t_j) + A_{j+1}\mu_1(t_{j+1}) \\ \frac{\Delta t}{2}(f_{2,j} + f_{2,j+1}) \\ \vdots \\ \frac{\Delta t}{2}(f_{M-2,j} + f_{M-2,j+1}) \\ \frac{\Delta t}{2}(f_{M-1,j} + f_{M-1,j+1}) + A_j\mu_2(t_j) + A_{j+1}\mu_2(t_{j+1}) \end{pmatrix}.$$

The numerical solution for heat flux in equation (4) on the interval $t \in [0, T]$ is given by

$$\mu_3(t_j) = a(t_j)u_x(0, t_j) = \frac{(4u_{1,j} - u_{2,j} - 3\mu_1(t_j))a_j}{2\Delta x}, \quad j = \overline{0, N}. \tag{9}$$

4 Numerical approach to solve the inverse problem

The nonlinear inverse problem (1)–(4) can be formulated as a nonlinear minimization of the least-squares objective function

$$F(a) := \|a(t)u_x(0, t) - \mu_3(t)\|^2, \tag{10}$$

the discretizations of which is

$$F(\mathbf{a}) = \sum_{j=1}^{N} \Big[a_j u_x(0, t_j) - \mu_3(t_j) \Big]^2, \tag{11}$$

where $\mathbf{a} = (a_j)_{j=\overline{1,N}} \in \mathbb{R}_+^N$.

The minimization of (11) is performed using the MATLAB toolbox routine *lsqnonlin*, which does not require supplying by the user the gradient of the objective function, [9]. This routine attempts to find the minimum of a sum of squares by starting from the arbitrary initial guesses $\mathbf{a}^{(0)}$ for $\mathbf{a}$. We have compiled this routine with the following specifications :

- Algorithm is the Trust Region Reflective (TRR) minimization, see [4].
- Number of variables $M = N$.
- Maximum number of iterations, (MaxIter)= 400.
- Maximum number of objective function evaluations, (MaxFunEvals)= $10^2\times$(number of variables.)
- Termination tolerance on the function value, (TolFun) = 10^{-20}.
- x Tolerance, (xTol)=10^{-20}.

5 Numerical results and discussion

In this section, we present a few test examples in order to test the accuracy and stability of the numerical method introduced in Section 4. The root mean square error (rmse) is used to evaluate the accuracy of the numerical results as follows:

$$rmse(a(t)) = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \Big(a^{numerical}(t_j) - a^{exact}(t_j) \Big)^2}. \tag{12}$$

The inverse problem (1)–(4) is solved subject to both exact and noisy heat flux measurements (4). The noisy data are numerically simulated as

$$\mu_3^{\epsilon}(t_j) = \mu_3(t_j) + \epsilon_j, \quad j = \overline{1, N}, \tag{13}$$

where ϵ_j are random variables generated from a Gaussian normal distribution with mean zero and standard deviation σ given by

$$\sigma = p \times \max_{t\in[0,T]} |\mu_3(t)|, \tag{14}$$

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

$$\boldsymbol{\epsilon} = normrnd(0, \sigma, N). \tag{15}$$

The total amount of noise ϵ is given by

$$\epsilon = |\boldsymbol{\epsilon}| = \sqrt{\sum_{j=1}^{N} (\mu_3^{\epsilon}(t_j) - \mu_3(t_j))^2}. \tag{16}$$

In all the numerical results presented below we take $L = T = 1$. We also take the initial guess for the unknown thermal diffusivity $a(t)$ equal to the constant $a(0)$, which from the compatibility of the conditions (2) and (4) at $t = 0$ is known and given by $a(0) = \mu_3(0)/\phi'(0)$.

5.1 Example 1

In this example, we consider the inverse problem given by (1)–(4) and the input data

$$\phi(x) = u(x, 0) = 2x - x^2\Big(x + \frac{1}{2}\Big)^2, \tag{17}$$

$$\mu_1(t) = u(0, t) = 2t - \frac{t^2}{4}, \quad \mu_2(t) = u(1, t) = 2 + 2t - \frac{9}{4}(1 + t)^2, \tag{18}$$

$$f(x, t) = 2 - 2\Big(x + \frac{1}{2}\Big)^2(x + t) - (1 + t)\Big(-2\Big(x + \frac{1}{2}\Big)^2 - 8\Big(x + \frac{1}{2}\Big)(x + t) - 2(x + t)^2\Big), \tag{19}$$

$$\mu_3(t) = a(t)u_x(0, t) = (1 + t)\Big(2 - \frac{1}{2}t - t^2\Big). \tag{20}$$

It can be easily checked by direct substitution that the analytical solution of the inverse problem (1)–(4) with the input data (17)–(20) is given by

$$u(x, t) = 2t + 2x - \Big(x + \frac{1}{2}\Big)^2(x + t)^2, \tag{21}$$

and

$$a(t) = 1 + t. \tag{22}$$

First, we assess the convergence and accuracy of the FDM solver of Section 3 for solving the direct problem (1)–(3). Figure 1 shows the numerical heat flux in equation (4) in comparison with the exact solution (20) obtained by solving the direct problem (1)–(3) with the input data (17)–(19) and (22) using the FDM, described in Section 3, with $M = N \in \{10, 20, 40\}$. Form this figure it can be seen that the good agreement between the exact solution (20) and the numerical one is obtained and its order is $O((\Delta x)^2)$, as the mesh size decreases.

We now fix $M = N = 40$ and try to recover the unknown thermal conductivity $a(t)$ and the temperature $u(x, t)$ for exact input data, i.e. $p = 0$, as well as for $p \in \{5\%, 10\%\}$ noisy data. The objective function (11) is plotted, as a function of the number of iterations, in Figure 2. From this figure, it can be seen that a very fast convergence is achieved in about 8 to 21 iterations to reach to a very low value of $O(10^{-26})$. The related numerical results for $a(t)$ and $u(x, t)$ are presented in Figures 3 and 4, respectively. From these figures it can be seen clearly that there is good agreement between the numerical results and the analytical solutions for exact data, i.e. $p = 0$, and is proportionate with the errors in the input data for $p > 0$. The numerical solutions for $a(t)$ and $u(x, t)$ converge to their corresponding exact solutions in equations (21) and (22), as the percentage of noise p

decreases from 10% to 5% and then to zero.

For completeness, other the details about number of iterations, the number of function evaluations, the value of the objective function (11) at final iteration, the *rmse* in (12) and the computational time are given in Table 1. From this table it can be seen that accurate and stable numerical results are rapidly achieved by the iterative MATLAB toolbox routine *lsqnonlin*.

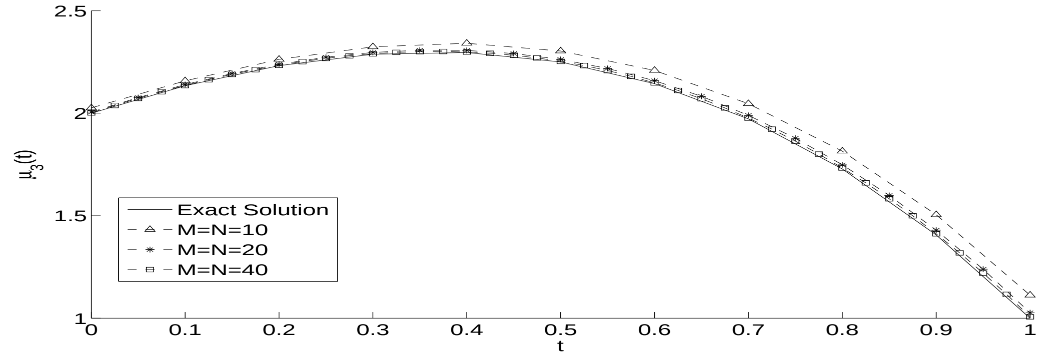

Figure 1: The exact (equation (20)) and numerical solutions for the heat flux (4), for Example 1 with $M = N \in \{10, 20, 40\}$, for the direct problem.

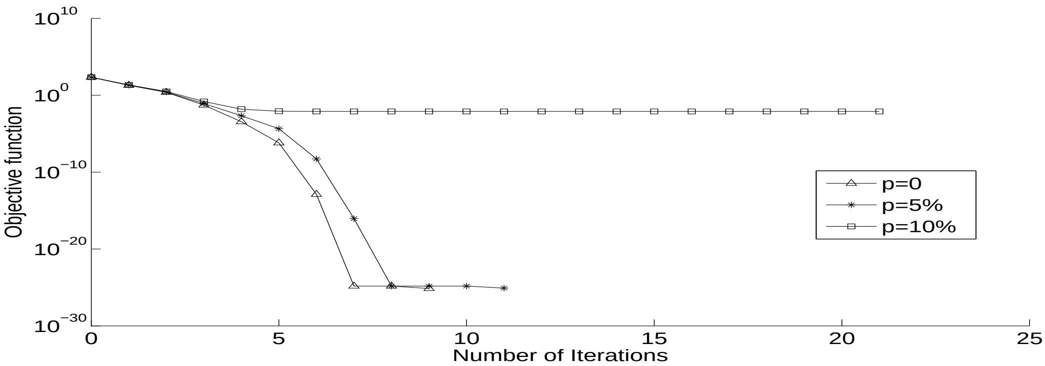

Figure 2: Objective function (11), for Example 1 with $p \in \{0, 5\%, 10\%\}$ noise.

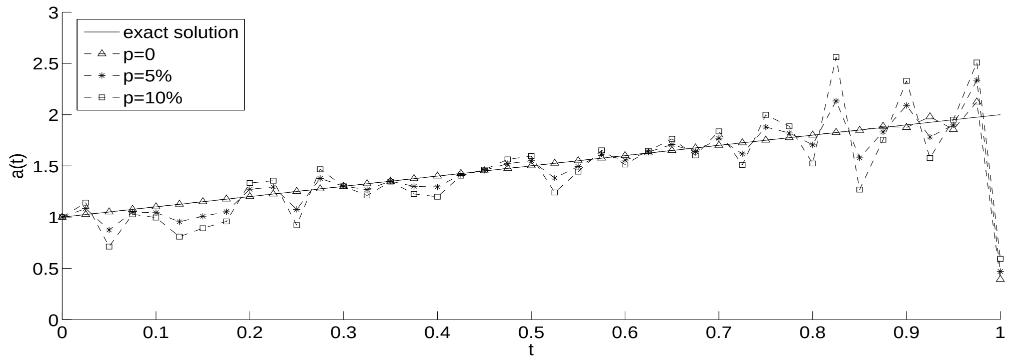

Figure 3: The exact (equation (22)) and numerical solutions for the thermal conductivity $a(t)$, for Example 1 with $p \in \{0, 5\%, 10\%\}$ noise.

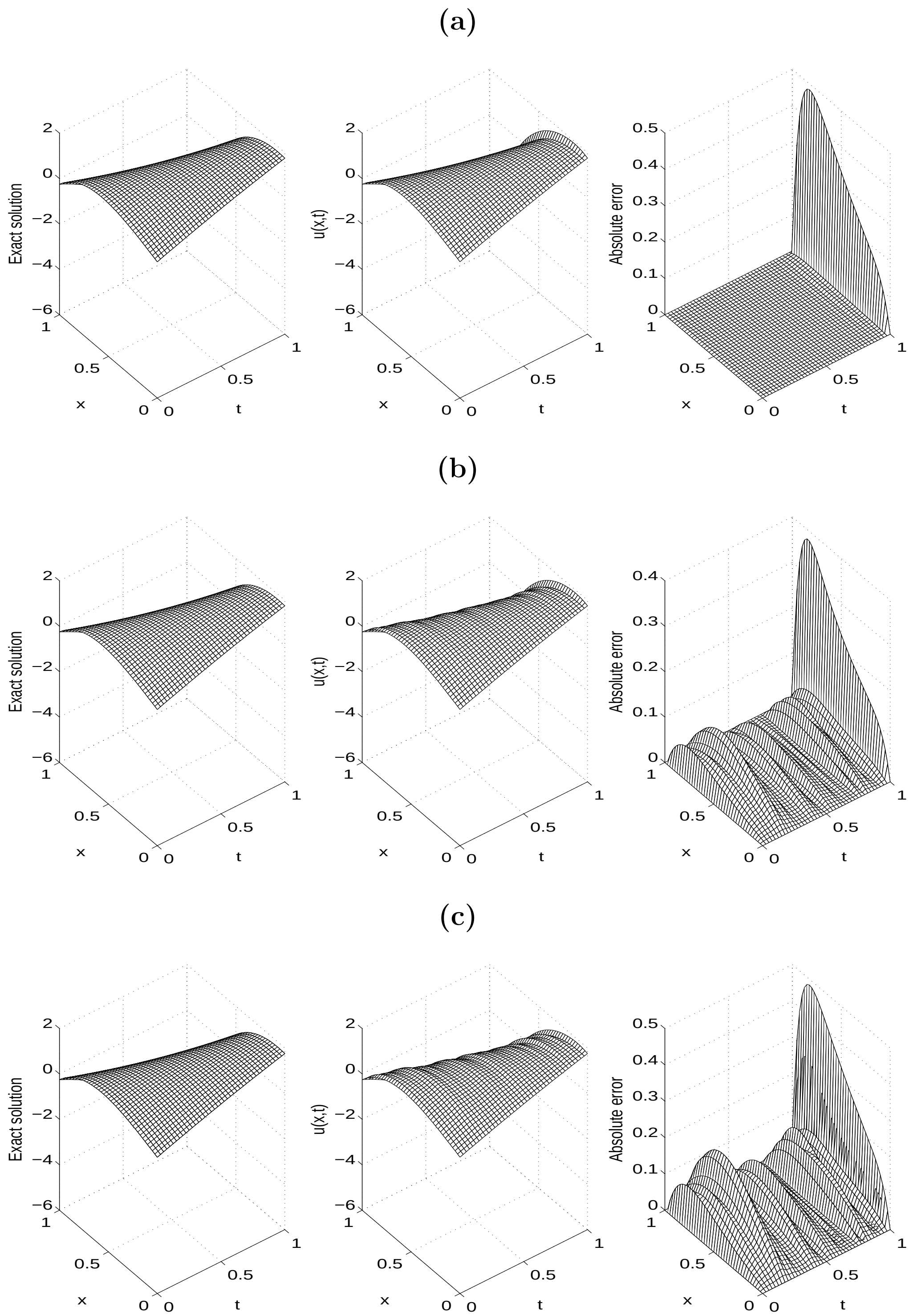

Figure 4: The exact (equation (21)) and numerical solutions for the temperature $u(x, t)$, for Example 1, with (a) no noise, (b) $p = 5\%$ noise, and (c) $p = 10\%$ noise. The absolute error between them is also included.

Table 1: Number of iterations, number of function evaluations, value of the objective function (11) at final iteration, $rmse(a)$ and computational time, for Example 1.

Numerical outputs	$p = 0$	$p = 5\%$	$p = 10\%$
Number of iterations	9	12	21
Number of function evaluations	420	504	924
Value of objective function (11) at final iteration	7.2E-26	8.2E-26	7.8E-3
$rmse(a)$	1.6384	1.8420	2.3598
Computational time	6 mins	7 mins	13 mins

5.2 Example 2

We now consider recovering a non-smooth thermal conductivity, as given by equation (25) below. We take input data given by (17), (18),

$$f(x,t) = 2-2\left(x+\frac{1}{2}\right)^2(x+t)-\left(\left|t-\frac{1}{2}\right|+\frac{1}{2}\right)\left(-2\left(x+\frac{1}{2}\right)^2-8\left(x+\frac{1}{2}\right)(x+t)-2(x+t)^2\right), \quad (23)$$

and

$$\mu_3(t) = a(t)u_x(0,t) = \left(2-\frac{1}{2}t-t^2\right)\left(\left|t-\frac{1}{2}\right|+\frac{1}{2}\right). \quad (24)$$

Then the analytical solution of the inverse problem (1)–(4) with this input data is given by (21) for the temperature $u(x,t)$ and

$$a(t) = \left|t-\frac{1}{2}\right|+\frac{1}{2} \quad (25)$$

for the thermal conductivity.

Figure 5 shows the numerical heat flux in equation (4) in comparison with the exact solution (24) obtained by solving the direct problem (1)–(3) with the input data (17), (18), (22) and (23) using the FDM, described in Section 3, with $M = N \in \{10, 20, 40\}$. From this figure it can be seen that the good agreement between the exact solution (24) and the numerical one is obtained and its order is $O((\Delta x)^2)$, as the mesh size decreases.

We now fix $M = N = 40$ and try to recover the thermal conductivity $a(t)$ and the temperature $u(x,t)$ for exact input data, i.e. $p = 0$, as well as for $p \in \{1\%, 3\%\}$ noisy data. The objective function (11) is plotted, as a function of the number of iterations, in Figure 6. From this figure, it can be seen that a very fast convergence is achieved in about 7 to 11 iterations to reach to a very low value of $O(10^{-27})$. The related numerical results for $a(t)$ and $u(x,t)$ are presented in Figures 7 and 8, respectively. From these figures it can be seen clearly that there is good agreement between the numerical results and the analytical solutions for exact data, i.e. $p = 0$, and is proportionate with the errors in the input data for $p > 0$. The numerical solutions for $a(t)$ and $u(x,t)$ converge to their corresponding exact solutions in equations (25) and (21), as the percentage of noise p decreases from 3% to 1% and then to zero.

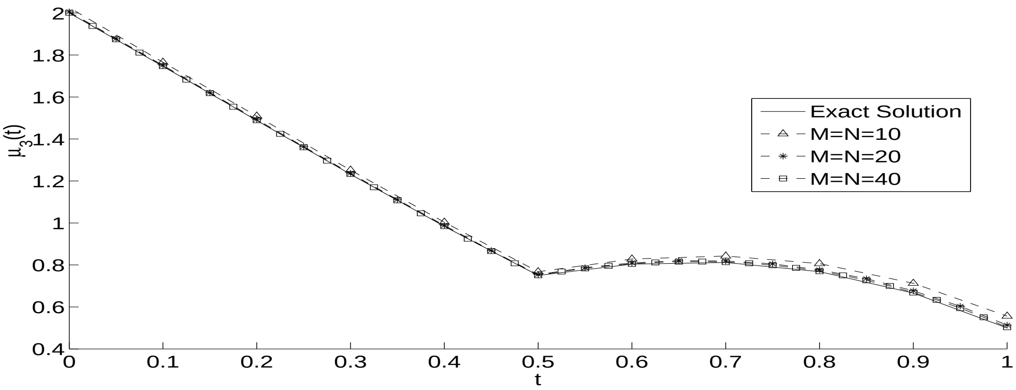

Figure 5: The exact (equation (24)) and numerical solutions for the heat flux (4), for Example 2 with $M = N \in \{10, 20, 40\}$, for the direct problem.

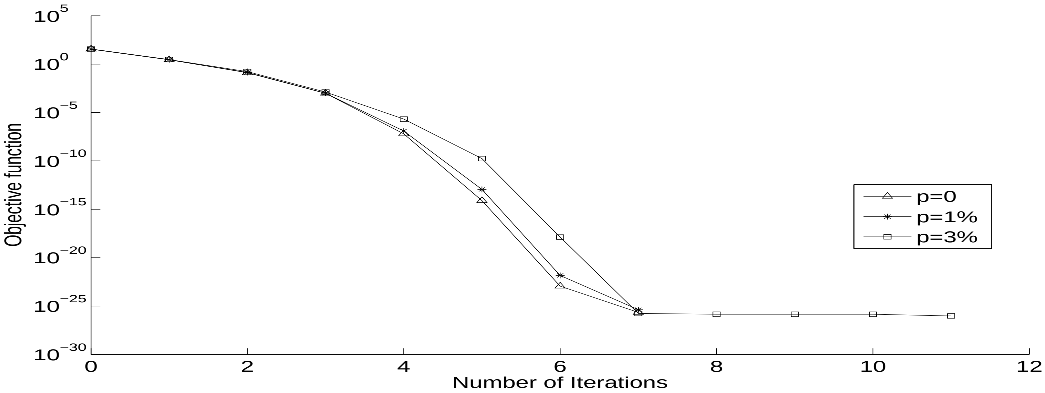

Figure 6: Objective function (11), for Example 2 with $p \in \{0, 1\%, 3\%\}$ noise.

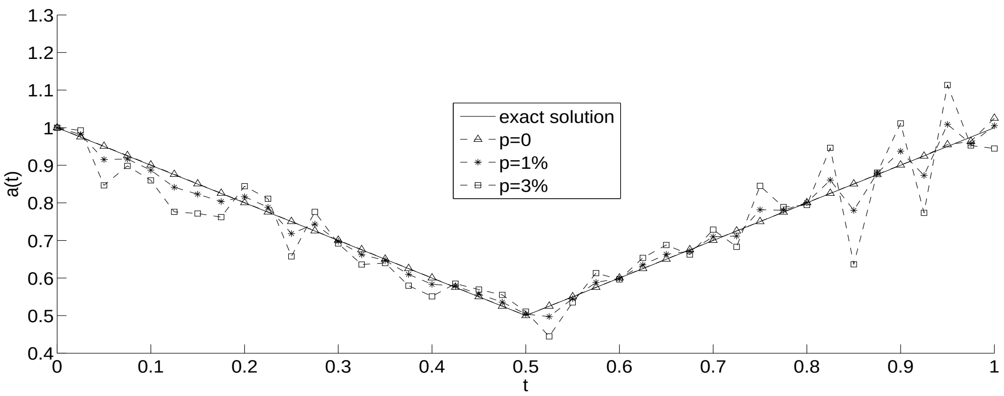

Figure 7: The exact (equation (25)) and numerical solutions for the thermal conductivity $a(t)$, for Example 2 with $p \in \{0, 1\%, 3\%\}$ noise.

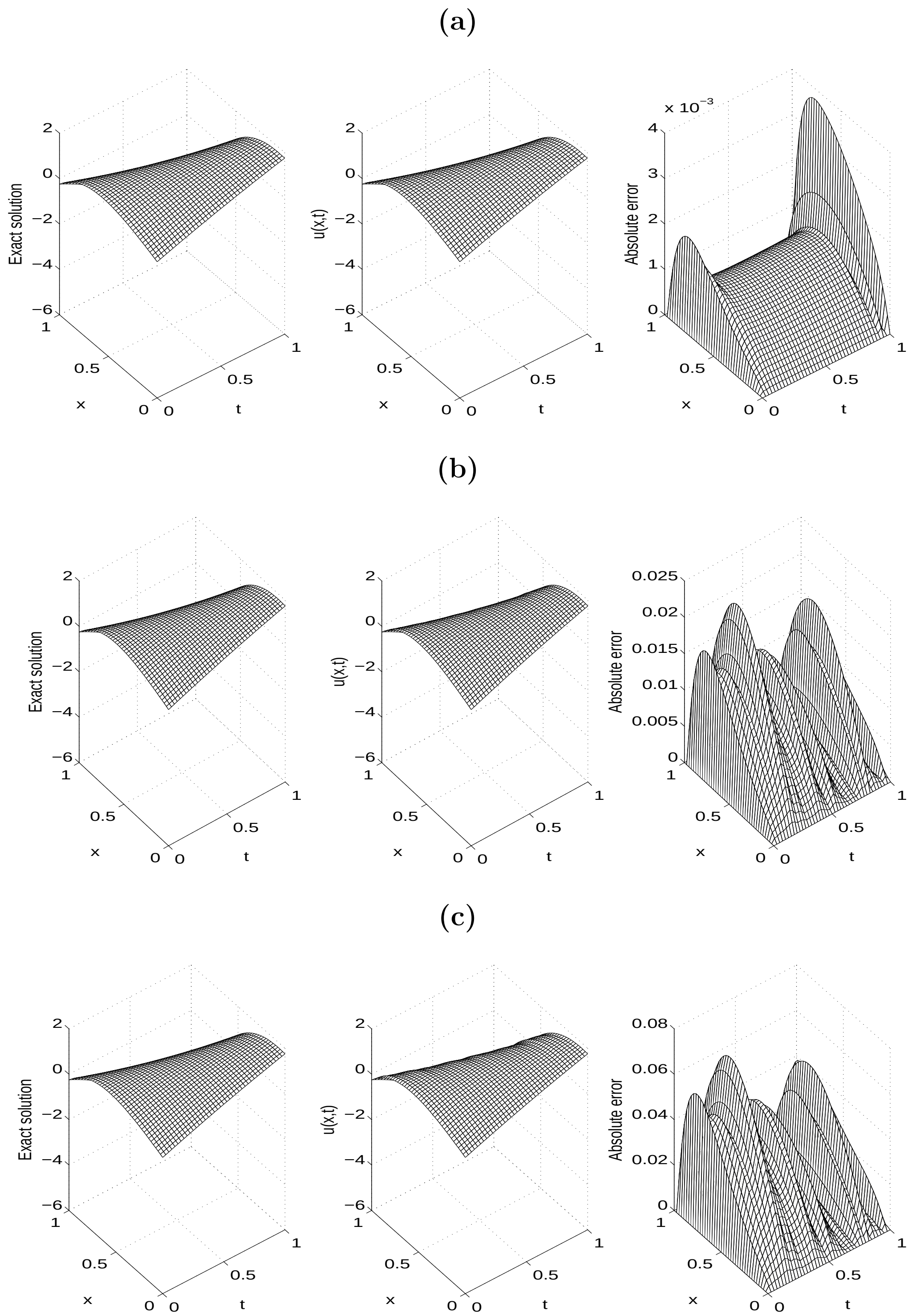

Figure 8: The exact (equation (21)) and numerical solutions for the temperature $u(x,t)$, for Example 2, with (a) no noise, (b) $p = 1\%$ noise, and (c) $p = 3\%$ noise. The absolute error between them is also included.

Other details about number of iterations, the number of function evaluations, the value of the objective function (11) at final iteration, the *rmse* in (12) and the computational time are given in Table 2. From this table it can be seen that accurate and stable numerical results are rapidly achieved by the iterative MATLAB toolbox routine *lsqnonlin*.

Table 2: Number of iterations, number of function evaluations, value of the objective function (11) at final iteration, $rmse(a)$ and the computational time, for Example 2.

Numerical outputs	$p = 0$	$p = 1\%$	$p = 3\%$
Number of iterations	7	7	11
Number of function evaluations	336	336	504
Value of objective function (11) at final iteration	2.2E-26	4.2E-26	9.4E-27
$rmse(a)$	0.0325	0.2123	0.6643
Computational time	4 mins	4 mins	6 mins

5.3 Example 3

Consider the inverse problem (1)–(4) with the input data

$$\phi(x) = u(x, 0) = \sin(\pi x), \quad \mu_1(t) = \mu_2(t) = 0, \quad f(x, t) = 0, \tag{26}$$

$$\mu_3(t) = a(t)u_x(0, t) = \pi(1.01 + \sin(3\pi t)) \exp\Big[- \pi^2\Big(1.01t + \frac{1 - \cos(3\pi t)}{3\pi}\Big)\Big]. \tag{27}$$

The exact solution for the temperature $u(x, t)$ is

$$u(x, t) = \sin(\pi x) \exp\Big[- \pi^2\Big(1.01t + \frac{1 - \cos(3\pi t)}{3\pi}\Big)\Big], \tag{28}$$

and for the thermal conductivity $a(t)$ is

$$a(t) = 1.01 + \sin(3\pi t). \tag{29}$$

This example was considered in [12] and we generate the noisy heat flux measurement (4) for this example as in [12] as multiplicative (rather than additive as in (13)), namely,

$$\mu_3^\epsilon(t_j) = \mu_3(t_j)(1 + p\epsilon_j), \quad j = \overline{1, N}, \tag{30}$$

where p represents the percentage of noise and $\underline{\epsilon} = (\epsilon_j)_{j=\overline{1,N}}$, is a random real number between $[-1, 1]$ generated from uniform distribution using MATLAB function *rand* as

$$\underline{\epsilon} = 2 \times rand(1, N) - 1. \tag{31}$$

The objective function (11), as a function of the number of iterations is shown in Figure 9 with no noise and with various mesh sizes. From this figure it can be seen that very low converging values of the monotonically decreasing objective function F in (11) are achieved. The corresponding numerical results for $a(t)$ are compared with the analytical solution (29) in Figure 10, with the numerical details included in Table 3. From this figure and table it can be seen that the numerical solution for $a(t)$ converges to exact solution (29), as the mesh size decreases.

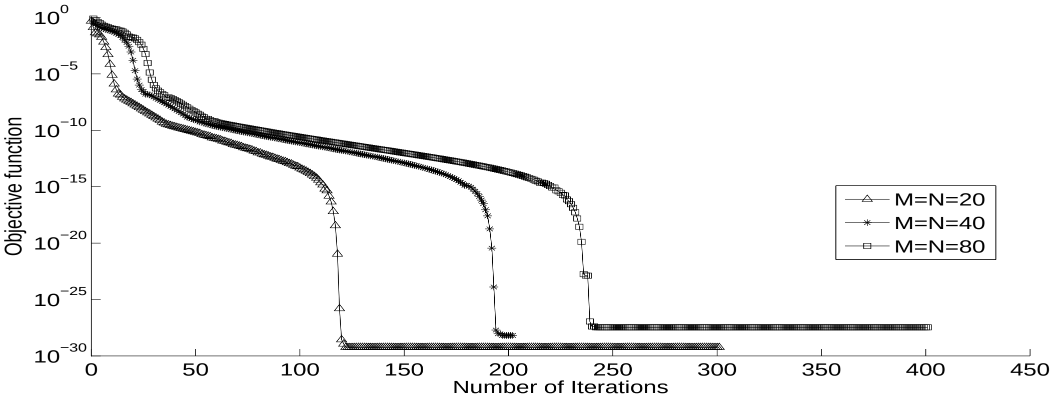

Figure 9: Objective function (11), for Example 3 with no noise and with $M = N \in \{20, 40, 80\}$.

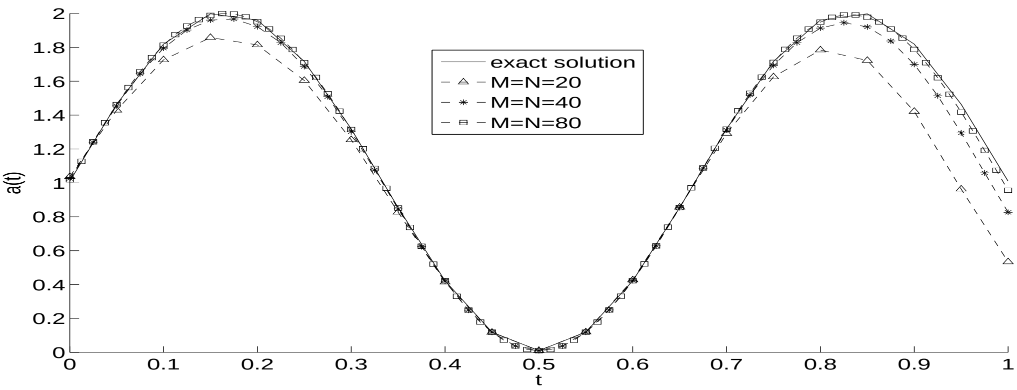

Figure 10: The exact (equation (29)) and numerical solutions for the thermal conductivity $a(t)$, for Example 3 with no noise and with various mesh size $M = N \in \{20, 40, 80\}$.

Table 3: Number of iterations, number of function evaluations, value of the objective function (11) at final iteration, $rmse(a)$ and the computational time, for Example 3 with various mesh size $M = N \in \{20, 40, 80\}$ and with no noise.

Numerical outputs	$M = N = 20$	$M = N = 40$	$M = N = 80$
Number of iterations	301	201	401
Number of function evaluations	6644	16884	32964
Value of objective function (11) at final iteration	5.7E-30	6.4E-29	3.4E-28
$rmse(a)$	0.1977	0.0634	0.0170
Computational time	6 mins	478 mins	10 hours

When we include various levels of noise $p \in \{1, 3, 5\}\%$ as in (30) to the heat flux measurement (4) we obtain stable results for the $a(t)$ as thermal conductivity shown in Figure 11. Furthermore, the results become more accurate as the amount of noise p decreases. Numerical results are also comparable in terms of stability and accuracy with those in [12] obtained using a totally different method.

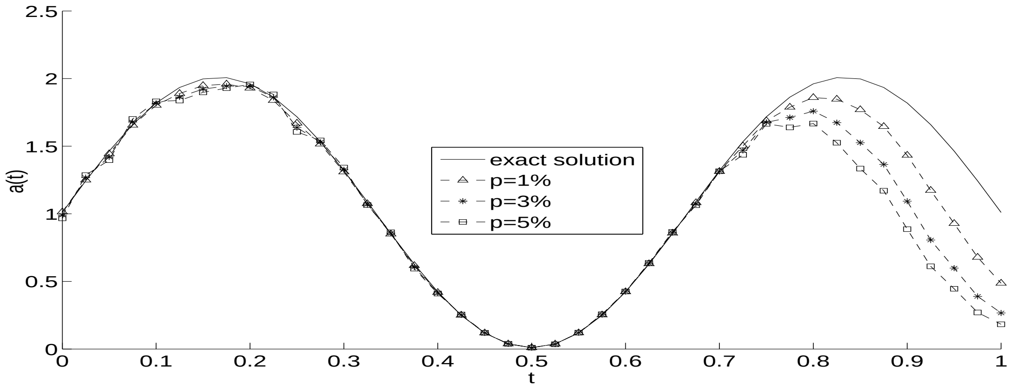

Figure 11: The exact (equation (29)) and numerical solutions for the thermal conductivity $a(t)$, for Example 3 with $p \in \{1\%, 3\%, 5\%\}$ noise and no regularization with $M = N = 40$.

6 Conclusions

This paper has presented the determination of the time-dependent thermal conductivity from heat flux measurements in the one-dimensional parabolic heat equation. The resulting inverse problem has been reformulated as a nonlinear least-squares optimization problem, which has been solved using the MATLAB toolbox routine *lsqnonlin*. The numerical results are shown to be stable and accurate. The inverse problem seems stable, and hence, no regularization was found necessary to be employed.

Acknowledgments

M.J. Huntul would like to thank Jazan University in Saudi Arabia and United Kingdom Saudi Arabian Cultural Bureau (UKSACB) in London for pursuing his PhD at the University of Leeds.

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