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Numerical Determination of Thermal Conductivity in Heat Equation under Nonlocal Boundary Conditions and Integral as Over specified Condition

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Abstract

In this article, an inverse problem of finding timewise-dependent thermal conductivity has been investigated numerically. Numerical solution of forward (direct) problem has been solved by finite-difference method (FDM). Whilst, the inverse (indirect) problem solved iteratively using Lsqnonlin routine from MATLAB. Initial guess for unknown coefficient expressed by explicit relation based on nonlocal overdetermination conditions and intial input data .The obtained numrical results are presented and discussed in several figures and tables. These results are accurate and stable even in the presense of noisy data.

Keywords: heat equation, inverse problem , nonlocal boundary condition , integral overdetermination condion.

التحديد العددي للموصلية الحرارية في معادلة الحرارة تحت شروط حدودية غير محلية و التكامل كشرط إضافي

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الخلاصة

في هذه المقالة ، تم بحث مسألة عكسية لإيجاد الموصلية الحرارية المعتمدة على الوقت عدديًا. الحل العددي للمسألة الأمامية (المباشرة) تم حلها بطريقة الفروقات المنتهية (FDM). بينما تم حل المسألة العكسية (غير المباشرة) بشكل تكراري باستخدام روتين Lsqnonlin من MATLAB. التخمين الأولي للمعامل الغير معروف معبراً عنه بعلاقة صريحة مبنية على شروط اضافيةغير محلية والشروط الابتدائية. النتائج العددية التي تم الحصول عليها تمت مناقشتها في عدة أشكال وجداول. هذه النتائج دقيقة ومستقرة حتى في وجود البيانات مشوشة.

1. Introduction

This work concerns with the study of an inverse problem not only for a parabolic equation resulting from physical models, but also models from medicine, combustion, ecology, etc. These models are represented by partial differential equations parabolic with periodic coefficients. The identifying of parameters in a parabolic differential equation using

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information of integral overdetermination situation is essential in physics and engineering [1–7]. In our problem, this integral condition is also known as heat moments of order zero [5].

In [5,8], authors studied the chemical diffusion applications in heat conduction processes ,while population dynamics, thermoelasticity, medical science, electrochemistry, engineering, broad scope, chemical engineering , and control theory all necessitate the examination of parabolic partial differential equations with nonlocal boundary conditions are investigated in [9-20].

Various approaches exist for numerically approximating inverse problems. The author of [12] investigated three distinct implicit finite-difference approaches for solving parabolic inverse problem with temperature overspecification data. These approaches are created to identify the controller parameters at specific moment, achieves a specified temperature solution at a particular position in the domain. The quantitative approaches addressed are followed by the second order backward time focused (BTCS) implicit formulation, the second-order Crank–Nicolson implicit scheme . Another method is the boundary element method (BEM) [21]. It is systematic method for obtaining approximate solution and showing numerical results. However, it is effective method for linear problems only. The homotopy perturbation method is used to solve an inverse problem that we transform it into a direct nonlinear problem [22]. We will solve this equation by using Crank-Nicolson finite difference as a direct solver then the inverse problem will be solved in the form of optimization.

The organization of our paper is as follows, mathematical formulation in section 2, numerical solution for the direct heat equation in section 3. Whilst, solution of the inverse problem via minimisation of objective functional in section 4. Numerical outputs are discussed in section 5 . Finally, the conclusions are highlited in section 6.

2. Mathematical formulation

Suppose that the problem of determining simultaneously is the temperature distribution $u(x,t)$ and time- dependent thermal conductivity coefficient *a(t)* satisfying the heat equation of the form

$$u_t = a(t)u_{xx} + f(x,t), \qquad (x,t) \in Q_T \tag{1}$$

with initial condition

$$u(x,0) = \varphi(x), \qquad 0 \le x \le 1 \tag{2}$$

and the boundary conditions of nonlocal type

$$u(0,t) = 0,\ u_x(0,t) = u_x(1,t) + \alpha u(1,t),\ 0 \le t \le T, \tag{3}$$

and the energy condition as overspecified data

$$\int_0^1 u(x,t)dx = E(t), \qquad 0 \le t \le T, \tag{4}$$

where Q_T is the domain of the problem and which is defined by $Q_T = \{(x,t):\ 0 < x < 1,\ 0 < t \le T\}$, the parameter α is an arbitrary real number and $f(x,t), \varphi(x), E(t)$ are given functions. The nonlocal boundary condition in (3) is the main specific feature of this problem; for $\alpha = 0$, it acquires the form

$$u_x(0,t) = u_x(1,t), \quad u(0,t) = 0, \quad 0 \le t \le T, \tag{5}$$

and was previously investigated in [23], it is well known as the Samarskii – Ionkin conditions, whilst (4) is an integral additional specification of the energy type. The problem of finding a pair $\{a(t), u(x,t)\}$ will be called an inverse problem.

Definition 1: The pair $\{a(t), u(x,t)\}$ from the class $(C[0,T] \times (C^{2,1}(Q_T) \cap C^{1,0}(\bar{Q}_T)))$ for which equations (1) -(4) are satisfied and $a(t) \geq 0$ on the interval $[0,T]$, is called the $classical$ solution of the inverse problem $(1)-(4)$.
The unique solvability for this problem has been established in [24] and no numerical realisation has been carried out, thus the aim of the current paper is to find the stable numerical solution of this inverse problem based on reliable algorithm. The existence and uniqueness theorems are stated below;

2.1 Unique solvability of the inverse problem solution

Theorem 1. If the following assumptions $(A_1)-(A_3)$ on the input data of the problem (1) -(4) are satisfied, then the inverse problem (1)-(4) has a unique classical solution.

$$(A_1): \begin{cases} (A_1)_1: \varphi(x) \in C^2[0,1]; \\ (A_1)_2: \varphi_x(0) = \varphi_x(1) + \alpha\varphi(1), \ \ \varphi(0) = 0; \\ (A_1)_3: \varphi_0 \geq 0, \varphi_{2k-1} \geq 0, k = 1,2,\ldots, \end{cases}$$

$$(A_2): \begin{cases} (A_2)_1: E(t) \in C^1[0,T]; \\ (A_2)_2: E(0) = \int_0^1 \varphi(x)dx; \\ (A_2)_3: E'(t) \leq 0, \end{cases}$$

$$(A_3): \begin{cases} (A_3)_1: f(x,t) \in [\bar{Q}_T], f(\cdot,t) \in C^2[0,1]; \\ (A_3)_2: f_x(0,t) = f_x(1,t) + \alpha f(1,t), f(0,t) = 0, 0 \leq t \leq T; \\ (A_3)_3: F_0(t) \geq 0, \ \ F_{2k-1}(t) \geq 0, \ k = 1,2,\ldots, \end{cases}$$

where, $\varphi_k = \int_0^1 \varphi(x)\, Y_k(x)dx, \qquad F_k\,(x) = \int_0^1 f(x,t)\, Y_k(x)dx, \qquad k = 1,2,\ldots$

$Y_k{}^{(2)}(x) = C_k{}^{(2)} \cos(\beta_k\,(1-2x)), \quad k = 0,1,2,\ldots;$

$Y_k{}^{(1)}(x) = C_k{}^{(1)} \cos\begin{pmatrix} \beta_k(1-2k) \\ +arctan(\frac{\alpha}{2\pi k}) \end{pmatrix}, \quad k = 0,1,2,\ldots;$

$where$,

$$C_k{}^{(1)} = -2\left(sin\left(arctan\left(\frac{\alpha}{2\pi k}\right)\right)\right)^{-1}, \quad k = 0,1,2,\ldots$$

$$C_k{}^{(2)} = 2\left((sin\beta_k)|\left(1 + \frac{sin(2\beta_k)}{2\beta_k}\right)\right)^{-1}, \qquad k = 0,1,2,\ldots$$

$$Y_0(x) = Y_0{}^{(2)}(x)(2\beta_0)$$

$$Y_{2k}(x) = \left(Y_k{}^{(2)}(x) + Y_k{}^{(1)}(x)\right), \qquad k = 1,2,\ldots$$

$$Y_{2k-1}(x) = \left(2(\beta_k - \pi k)\right)Y_k{}^{(2)}(x), \qquad k = 1,2,\ldots$$

3. Numerical solution for direct heat equation

In this section, we consider the forward boundary value problem (1) -(3). Where the functions $f\,(x,t)$, $\varphi(x)$ and $a(t)$ are known and the solution $u(x,t)$ is to be evaluated. In addition , the condition (4) is a desired output . In order to solve the problem, we invoke the Crank-Nicolson (FDM) scheme which is unconditionally stable and second order accurate in time and space[25].

The discretization of the direct problem (1)-(3) is as follows. Fix two positive integers M and

N and assume $\Delta x = \frac{1}{M}$ and $\Delta t = \frac{T}{N}$ be the step lengths in space and time direction, respectively. We subdivide the domain Q_T into $M \times N$ subregions of equally step lengths. At the node (i, j), we denote

$u_{i,j} := u(x_i, t_j)$, $a(t_j) := a_j$, and $f(x_i, t_j) := f_{i,j}$ where $x_i = i\Delta x$, $t_j = j\Delta t$, for $i = \overline{0, M}$, $j = \overline{0, N}$.

Applying Crank-Nicolson Scheme to equation (1) , we obtain:

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{1}{2}\left[a_{j+1} \left(\frac{u_{i+1,j+1} - u_{i,j+1} + u_{i-1,j+1}}{(\Delta x)^2}\right) + f_{i,j+1} + a_j \left(\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}\right) + f_{i,j}\right] \tag{6}$$

for $i = \overline{1, M}$, $j = \overline{0, N}$

$$u(x_i, 0) = \varphi(x_i), \qquad i = \overline{0, M}, \tag{7}$$

$$u(0, t_j) = 0, \qquad \frac{4u_{1,j} - u_{2,j} - 3u_{0,j}}{2(\Delta x)} = \frac{u_{M+1,j} - u_{M,j}}{2(\Delta x)} + \alpha u_{M,j}, \qquad j = \overline{0, N}, \tag{8}$$

The difference equation for (6)-(8) will be in the form

$$-A_{j+1}u_{i-1,j+1} + [1 + B_{j+1}]u_{i,j+1} - A_{j+1}u_{i+1,j+1} = A_j\, u_{i-1,j} + [1 - B_j]u_{i,j} + A_j u_{i+1,j} + \frac{\Delta t}{2}(f_{i,j} + f_{i,j+1}) \tag{9}$$

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

$$A_j = \frac{\Delta t(a_j)}{2(\Delta x)^2}, \quad B_j = \frac{\Delta t(a_j)}{\Delta (x)^2}, \tag{10}$$

At each time step t_{j+1} for $j = \overline{0, N-1}$ we use the boundary conditions (2)-(3) , then we obtain an *(*$M \times M$) linear system of linear take the form

$$\boldsymbol{A}U_{j+1} = \boldsymbol{E}U_j + \boldsymbol{d} \tag{11}$$

where,

$U_{j+1} = (u_{1,j+1}, u_{2,j+1}, \ldots, u_{M-1,,j+1}, u_{M,j+1})$ and $U_j = (u_{1,j}, u_{2,j}, \ldots, u_{M-1,j}, u_{M,j})$, **A** and **E** are $(M \times M)$ matrices of the form;

$$\mathbf{A} = \begin{bmatrix} 1+\tilde{b} & -\tilde{a} & 0 & 0 & \cdots & 0 & 0 & 0 \\ -\tilde{a} & 1+\tilde{b} & -\tilde{a} & 0 & \cdots & 0 & 0 & 0 \\ 0 & -\tilde{a} & 1+\tilde{b} & -\tilde{a} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \cdots & -\tilde{a} & 1+\tilde{b} & -\tilde{a} \\ -\tilde{a} & 0 & 0 & 0 & \cdots & 0 & -\tilde{a} & 1+\tilde{b}-\tilde{a}+\alpha(\Delta x)\tilde{a} \end{bmatrix}$$

$$\mathbf{E} = \begin{bmatrix} 1-e_1 & e_2 & 0 & 0 & \cdots & 0 & 0 & 0 \\ e_2 & 1-e_1 & e_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & e_2 & 1-e_1 & e_2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \cdots & e_2 & 1-e_1 & e_2 \\ e_2 & 0 & 0 & 0 & \cdots & 0 & e_2 & 1-e_1+e_2-\alpha(\Delta x)e_2 \end{bmatrix}$$

$$\mathbf{d} = \begin{bmatrix} -A_{j+1}u_{0,j+1} + A_0 u_{0,j} + \frac{\Delta t}{2}(f_{1,j} + f_{1,j+1}) \\ \frac{\Delta t}{2}(f_{2,j} + f_{2,j+1}) \\ \vdots \\ \frac{\Delta t}{2}(f_{M-1,j} + f_{M-1,j+1}) \\ \frac{\Delta t}{2}(f_{M,j} + f_{M,j+1}) \end{bmatrix}$$

where, $\tilde{b} = B_{j+1}$, $\tilde{a} = A_{j+1}$, $e_1 = B_j$, $e_2 = A_j$.

3.1 Example for direct problem

Let the problem (1)-(3) with T=1 and the following input data are taken

$a(t)=e^{-t}$, $\varphi(x)=\frac{x^2}{2}$, $\qquad (x,t)\in Q_T$

$f(x,t)=\frac{\left(-2e^{-t}(2+t^2+e^t t x^2)\right)}{(2+t^2)^2}$, $(x,t)\in Q_T$, and $\quad \alpha=-2$

The desired output is $E(t)=\frac{1}{(6+3t^2)}$ $\qquad t\in[0,T]$ (12)

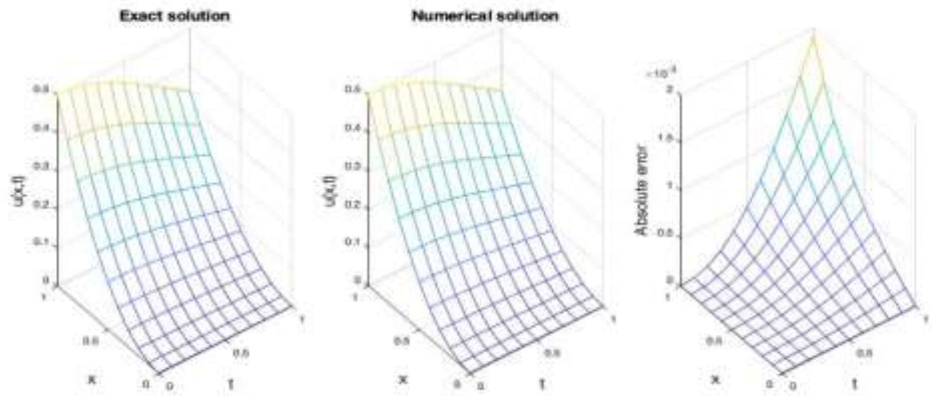
The exact solution for the direct problem (1)-(4) is given by

$$u(x,t)=\frac{x^2}{(2+t^2)} \qquad (x,t)\in Q_T \tag{13}$$

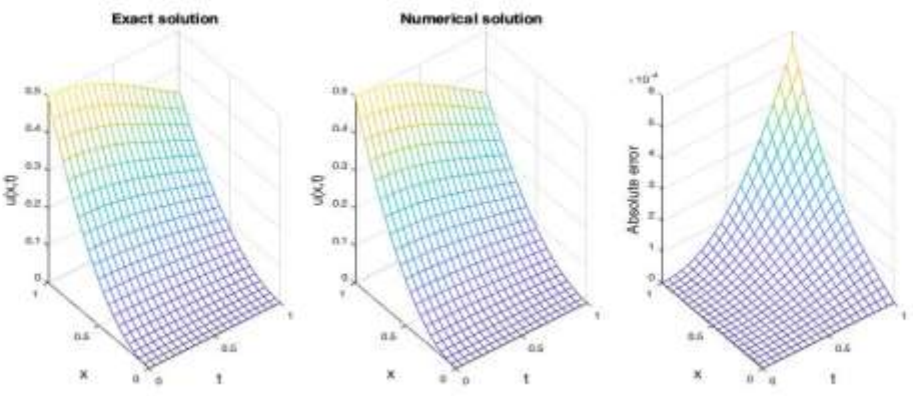
The approximate and exact solutions for the heat solution $u(x,t)$ at various mesh size M=N $\in$ $\{10,20,40\}$ are shown in Figure 1. From this figure one can clearly notice that an accurate and stable solutions are obtained. We can also see that if the number of mesh points are increased,then the more accurate solutions are obtained. This revels that the mesh independent is achieved. It can be clearly noticed in Figure 3 when the mesh size increases, the error level will decrease to very low level of order $O(10^{-6})$. Also, the trapezoidal rule is employed to computed the integral condition in (5) based on the following formula

$$\int_0^1 u(x,t_j)dx=\frac{1}{2M}\left(u(0,t_j)+u(1,t_j)+2\sum_{i=1}^{M-1}u(x_i,t_j)\right), \qquad j=\overline{0,N} \tag{14}$$

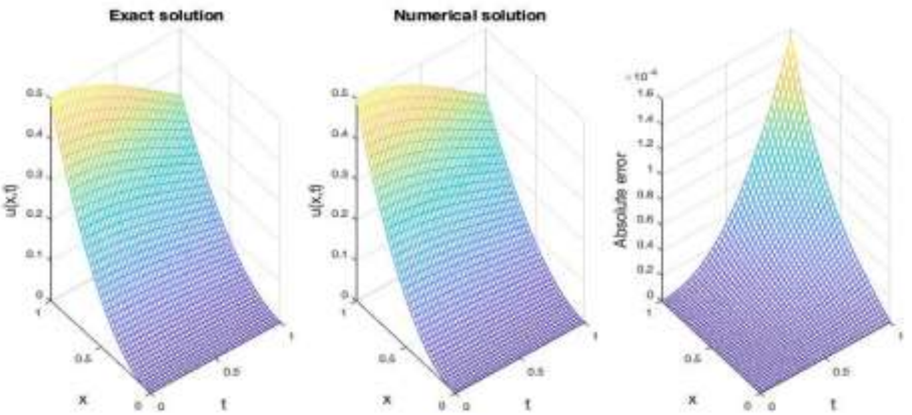
Figure 2, illustrates the desired output in various mesh size and one can observe that as the mesh number increases the more accurate results obtained.



(a)



(b)



(c)

Figure 1: The exact and the numerical solutions for the direct problem (1)-(3), for various mesh size (a)M=N=10 (b) M=N=20 (c) M=N=40 for Example 1. Also, the absolute error graph is included

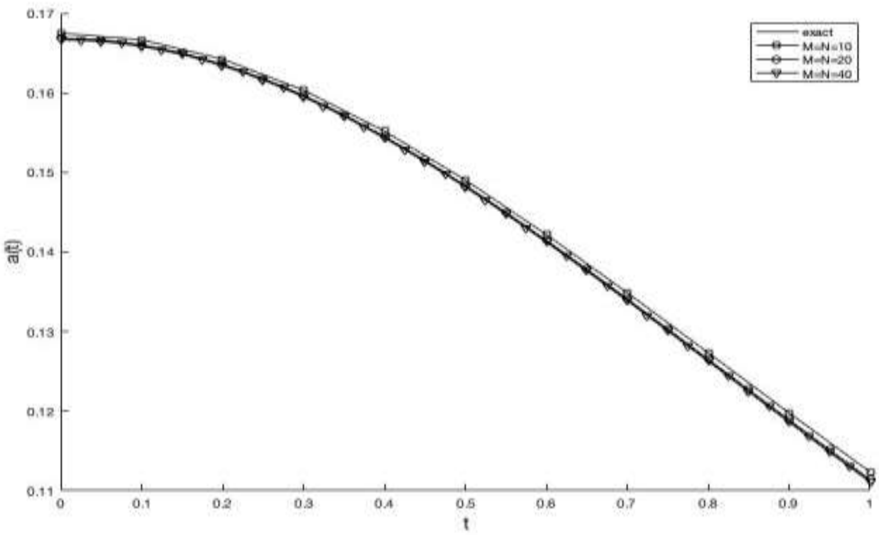


Figure 2: The exact and numerical solution for E(t) in (13) for various mesh size $M = N \in \{10,20,40\}$.

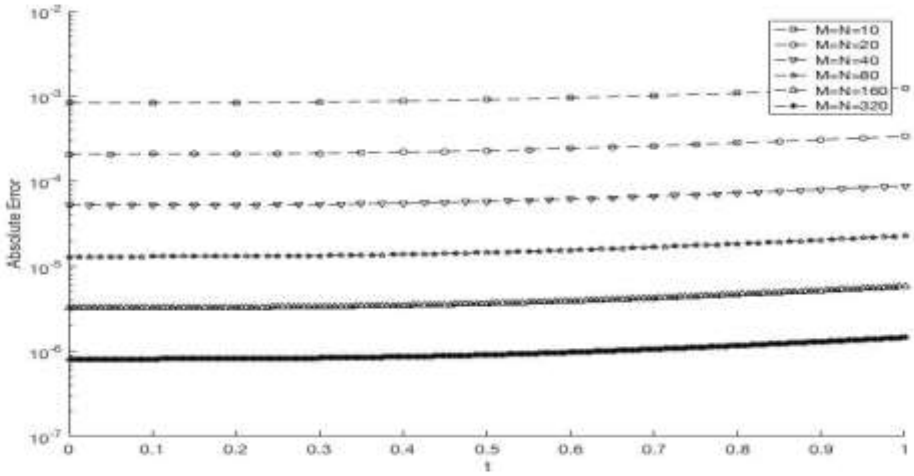


Figure 3: The absolute error for E(t) in (13) for various mesh size $M = N \in \{10,20,40,80,160,320\}$.

4. The inverse problem

The aim is to find stable numerical reconstructions for the problem under consideration which is described in Section 2. We focus our attention on finding the unknown coefficient $a(t)$. At initial time; i.e. at $t = 0$, we can use the input data to get initial values for $a(0)$ which will be described in next subsection. These values are essential and will be considered as initial guess for iterative process of solving the inverse problem. We reformulate the inverse problem as nonlinear least-squares minimization problem. That is, we minimize the gap between the measured data and numerically obtained solution via the objective function of the form;

$$F(a) := \left\| \int_0^1 u(x,t)dx - E(t) \right\|^2 , \tag{15}$$

or, in discredited form,

$$F(\underline{a}) = \sum_{j=1}^{N} \left(\int_0^1 u(x,t_j)dx - E(t_j) \right)^2 , \tag{16}$$

The norm in objective functional is the usual norm in $L^2[0,T]$.

The minimization of the objective functional (16), performed subject to simple physical bound constrain > 0 , since the coefficient can not be zero or negative which is performed by lsqnonline routine, for more details see [26]. During the iterative simulation process, we need some values of parameters of the routine to be set in order to terminate the processes;

- Maximum number of iterations (MaxIter) $= 10^4 \times$ $(number\ of\ variables)$.
- Maximum number of objective function evaluations (MaxEval) $=$ $10^6 \times$ $(number$ of variables).
- Solution tolerance (SolTOL) $=$ 10^{-10}
- Objective function tolerance (FunTOL) $=$ 10^{-10}

For both exact and noisy measurements the inverse problem is solved. The noisy data is simulated numerically by adding random errors as:

$$E^{\epsilon}(t_j) = E(t_j) + \epsilon, \qquad j = \overline{0, N}, \tag{17}$$

where ϵ is Gaussian random vector with mean zero and standard deviation σ which is obtained by

$$\sigma = p \times max_{\,t\in[0,T]}|E(t)|, \tag{18}$$

where p is the percentage of noise. The MATLAB bulletin function *normrnd* used to generate the random variable $\underline{\epsilon} = (\epsilon_j)$, $\quad j = \overline{0, N}$ as follows:

$$\underline{\epsilon} = \ normrnd(0, \sigma, N), \tag{19}$$

4.1 Initial guess for the unknown coefficient a(t)

During iterative minimization process of solving the inverse problem we need initial guess to start with. These values for a (0) can be computed from input data as follows:

Integrating the equation (1) for both side with respect to x from [0,1] as;

$$\int_0^1 u_t(x,t)dx = a(t)\int_0^1 u_{xx}(x,t)dx + \int_0^1 f(x,t)dx \tag{20}$$

applying Leibniz's formula for integral, we obtain

$$\frac{\partial}{\partial t}\left(\int_0^1 u(x,t)dx\right) = a(t)\int_0^1 u_{xx}(x,t)dx + \int_0^1 f(x,t)dx\,,$$

$$E'(t) = a(t)[u_x(1,t) - u_x(0,t)] + \int_0^1 f(x,t)dx,$$

by using boundary condition (3)

$$E'(\mathrm{t}) = a(t)[-\alpha u(1,t)] + \int_0^1 f(x,t)dx,$$

$$a(t)= \frac{E'(t)-\int_0^1 f(x,t)}{-\alpha u(1,t)}, \tag{21}$$

evaluating last equation at initial time, we have

$$a\ (0)= \frac{\int_0^1 f(x,0)-E'(0)}{\alpha\varphi(1)}, \tag{22}$$

provided that $\alpha\varphi(1) \neq 0$.

5. Computational results and discussion

We present numerical solutions for the recovery of timewise coefficient *a(t)* and the temperature $u(x,t)$, in the case of noisy and exact data (4). To assess the accuracy of the numerical results, we utilize the root mean square error (rmse) as:

$$rmse(a)=\left[\frac{T}{N}\sum_{j=1}^{N}(a^{numerical}\,(t_j) - a^{exact}(t_j))^2\right]^{\frac{1}{2}}, \tag{23}$$

In our simulation we fix T=1.

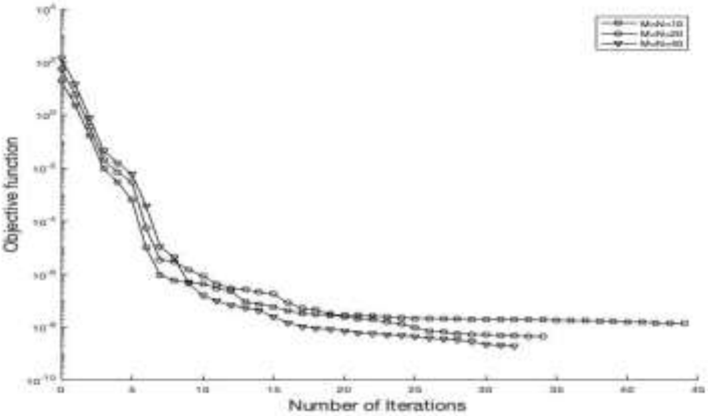
5.1 Example 1: for inverse problem

Assume the inverse problem (1)-(4) with the input data in the example of direct problem except

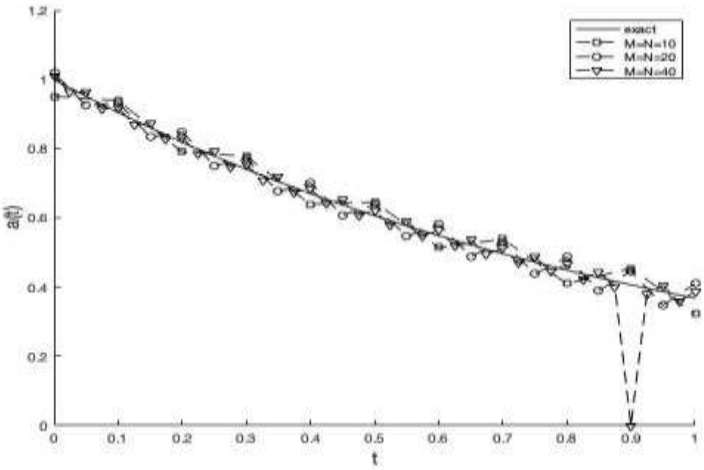
the coefficient a is unknown. One can notice that the conditions of unique solvability of Theorem 1 are satisfied and hence the solution exist and unique. The initial guess for the unknown thermal conductivity *a(t)* equal to vector of constant $\underline{a}(0) = \underline{1}$ which is obtained explicitly via equation (22).

5.1.1 Case 1: No noise and no regularization

We start the computationl investigation with the case of no noise included in the measurement (4), i.e. $p = 0$ in the equation (18).



(a)



(b)

Figure 3: (a) Objective function (16) as a function of the number of iterations (b) Thermal conductivity, with no noise included and for various mesh size $M = N \in \{10,20,40\}$.

In this case, in order to choose an approperate mesh size, we take M=N∈ $\{10,20,40\}$ and find the numerical recontruction at each mesh, as it is plotted in Figure 3(b). From this figure it can be clearly seen that when M=N=20, the best result can be obtained. Hence, in our numerical approximation we fix M=N=20. One can also choose higher mesh sizes such as M=N= 80, 160, 320 to gain more accurate retrievals, however the computational time will be beyond our purpose. Also, it can be observed from the last column in Table 1 when M=N=20 we have the lowest rmse(a).

Table 1: The ture and numerical values for desired output $a(t)$ with $M = N \in \{10,20,40\}$, with no noise.

T	0.1	0.5	0.6	0.8	0.9	1	rmse(a)
M=N=10	0.8887	0.5799	0.5852	0.4925	0.3644	0.4192	0.0342
M=N=20	0.9116	0.5983	0.5390	0.4370	0.3933	0.3544	0.0097
M=N=40	0.9183	0.6383	0.5806	0.4866	0.4483	0.4134	0.0315
Exact	0.9048	0.6065	0.5488	0.4493	0.4066	0.3679	

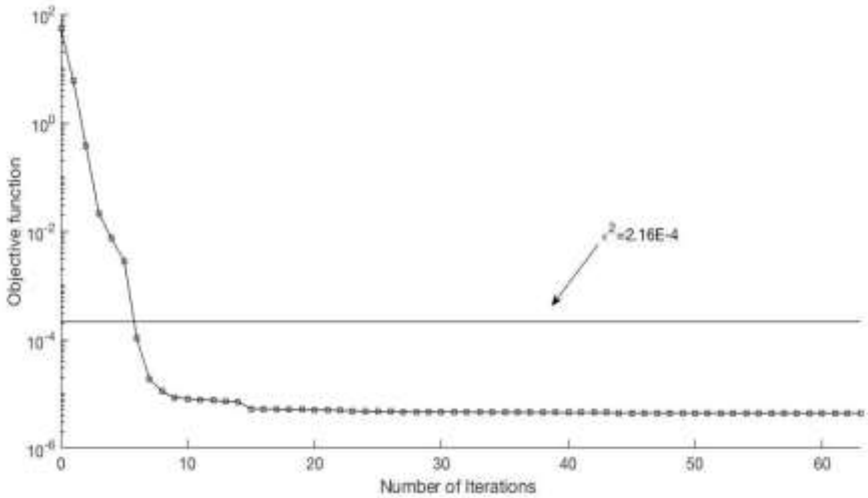
5.1.2 Case 2: with (p=1%) noise

Next, we perturb the measured data equation (4) as in (17) via (18) with 1% noise. Figure 4 (a) illustrates the objective function (16), as a function of the number of iterations together with the horizontal noise threshold ϵ^2=2.16E−4, which evaluated using the formula $\epsilon=\sqrt{\sum_{j=1}^{N}\left(E^{\epsilon}(t_j)-E(t_j)\right)^2}$. This threshold is essential to employ the discrepancy principle in order to terminate the iterative process before the errors in the outputs start to dominate. From Figure 4(a) the criterion yields the iteration number iter(discrepancy)=7. Also Figure 4(a) revel that the objective function (16) minimization has been convergent to small stationary value of order O(10^{-5}) after iter(convergent)=63. The rmse(a) as a function of the number of iterations plotted in Figure 4(b). From this figure it can be notice the best retrieval occurs at iter(optimal)=4. For more detailes, see numerical results in Figure 5 and in Table 2.

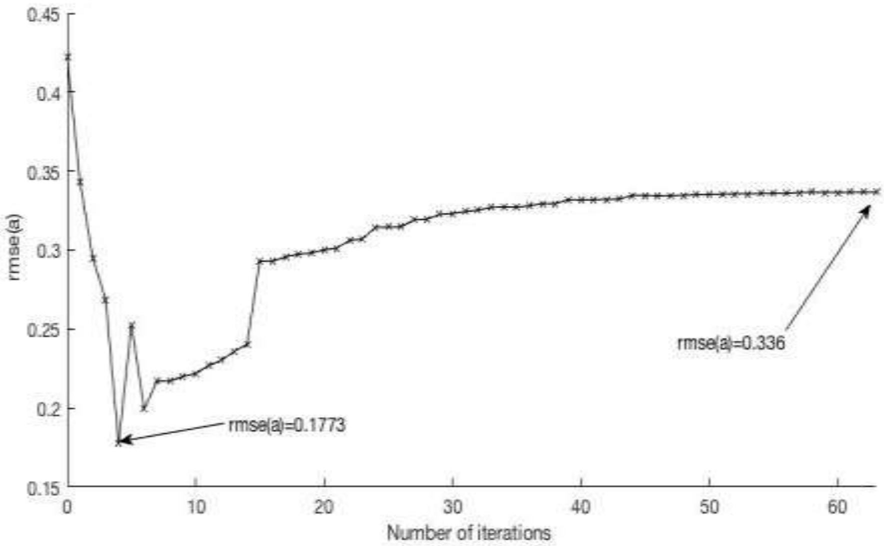
Table 2: The number of iterations, the rmse(a) values (23) based on stopping criteria , for Example 1 with p=1% noise.

Stopping Criterion	No. of iterations	rmse(a)
to achieve convergence	iter.conv.=63	0.3367
to achieve minimum rmse(a)	iter.opt.=4	0.1773
discrepancy principle	iter.discr.= 7	0.1994

Remark: We have also tried to add some regularization penalty term $\beta\|a(t)\|^2_{L^2[0,T]}$ with $\beta > 0$, some regularization parameter to the functional (16), but the stability of the retrieved solution did not improved . Hence, all results related to regularization part which are omitted from discussion.



(a)



(b)

Figure 4: (a) Objective function (16) with horizontal noise threshold =2.16E-4, and (b) the rmse(k) values (23), for Example 1 with $\rho = 1\%$ noise.

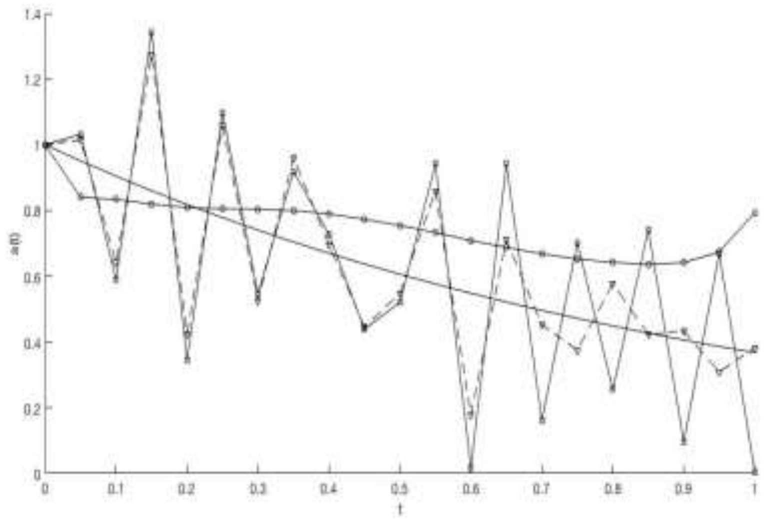


Figure 5: Exact (—) and the numerical solutions for a(t) obtained after $iter_{conv.}=63$ (- □ -), $iter_{opt.}=4$ (-o-), and $iter_{discr.}=7$ (-△-), for Example 1 with $\rho = 1\%$ noise.

6. Conclusions

The problem of finding the timewise-dependent conductivity with nonclassical boundary conditions and nonlocal (energy/mass) overspecified measurement has been numerically investigated. The obtained inverse problem has been reformulated as nonlinear least-squares mimimization problem with simple bound. This problem has been efficiently solved by using Lsqnonlin routine from MATLAB. The numerical results are accurate, and reasonably stable retrieval in term of high oscilation free.

Furthermore, this inverse problem seems rather stable and hence in general, no regularization needs to be applied. Discrepancy principal is also used to terminate the iterative process before the errors start to dominate.

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