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Identification of Parameters in One-Dimensional IHCP

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Abstract—We present a new numerical method based on discrete mollification for identification of parameters in one-dimensional inverse heat conduction problems (IHCP). With the approximate noisy data functions (initial temperature on the boundary $t = 0$, $0 \leq x \leq 1$, temperature and space derivative of temperature on the boundary $x = 0$, $0 \leq t \leq 1$) measured at a discrete set of points, the diffusivity coefficient, the heat flux, and the temperature functions are approximately recovered in the unit square of the (x, t) plane. In contrast to other related results, the method *does not require* any information on the amount and/or characteristics of the noise in the data and the mollification parameters are chosen *automatically*. Another important feature of the algorithm is that it allows for the recovery of much more general diffusivity parameters, including *discontinuous* coefficients. Error bounds and numerical examples are provided.

Keywords—Ill-posed problems, IHCP, Discrete mollification, Automatic filtering.

1. INTRODUCTION

The identification of parameters in one-dimensional inverse heat conduction problems (IHCP) has received considerable attention from many researchers using a variety of different methods. A brief list of investigators who studied the estimation of spatially dependent thermal transmissivity includes Ciampi *et al.* [1], Kravaris and Seinfeld [2], Liu and Chen [3], and Huang and Öziçik [4]. See Chapter 6 in [5] for more details and further references.

The use of space marching schemes along with certain regularization procedures has proven to be an effective way for solving these problems. A finite difference space marching scheme with hyperbolic regularization, which requires exact initial data, was introduced by Ewing and Lin in [6]. By combining the mollification method and hyperbolic regularization, Mejía and Murio [7] modified the scheme in [6] allowing for the presence of noise in both initial and boundary data.

In this paper, we present a numerical space marching scheme based on discrete mollification and automatic iterative filtering by the method of Generalized Cross Validation (GCV) for the identification of parameters in one-dimensional IHCP. In contrast to other related results, the method *does not require* any information on the amount and/or characteristics of the noise in the data and the mollification parameters are chosen *automatically*. Another important feature of the algorithm is that it allows for the recovery of much more general diffusivity parameters, including *discontinuous* coefficients.

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The paper is organized as follows. The results of mollification and discrete mollification are presented in Section 2. The space marching scheme and the error analysis are considered in Section 3. Section 4 includes details on the implementation of the algorithm and numerical results.

2. MOLLIFICATION

The δ-mollification is based on convolution with the kernel

$$\rho_{\delta,p}(t) = \begin{cases} A_p \delta^{-1} \exp\left(-\frac{t^2}{\delta^2}\right), & |t| \le p\delta, \\ 0, & |t| > p\delta, \end{cases}$$

where $p > 0$, $\delta > 0$, and $A_p = (\int_{-p}^{p} \exp(-s^2)\, ds)^{-1}$. For simplicity, in the future, we denote $\rho_{\delta,p}(t)$ by $\rho_\delta(t)$.

Let $I = [0,1]$, $I_\delta = [p\delta, 1 - p\delta]$, $K = \{t_1, t_2, \dots, t_n\}$ $(0 \le t_1 < t_2 < \cdots < t_{n-1} < t_n \le 1)$, and $\Delta t = \max_j |t_{j+1} - t_j|$. If f is integrable on I, we define its δ-mollification by the convolution

$$J_\delta f(t) = \int_0^1 \rho_\delta(t - s) f(s)\, ds, \qquad \text{for } t \in I_\delta.$$

Let $G = \{g_j\}_{j=1}^{n}$ be a discrete function defined on K. We define the discrete δ-mollification of G as follows: for $t \in I_\delta$,

$$g_\delta(t) = \sum_{j=1}^{n} \left(\int_{s_{j-1}}^{s_j} \rho_\delta(t - s)\, ds \right) g_j,$$

where $s_0 = 0$, $s_n = 1$, and $s_j = (1/2)(t_j + t_{j+1})$ $(1 \le j \le n - 1)$.

From now on, C will represent a generic constant independent of the mollification parameter δ, and the grid size Δt. The following theorems were established in [8]. A complete description of the mollification method and several of its applications can be found in [5].

THEOREM 2.1. *Consistency of δ-mollification.*

1. *If f is uniformly Lipschitz on I, then there is a constant C such that*

$$\|J_\delta f - f\|_{\infty, I_\delta} \le C\delta.$$

2. *If f' is uniformly Lipschitz on I, then there exists a constant C such that*

$$\left\|(J_\delta f)' - f'\right\|_{\infty, I_\delta} \le C\delta.$$

3. *If f' is uniformly Lipschitz on I and f^ε is an integrable function on I, satisfying $\sup_I |f - f^\varepsilon| \le \varepsilon$, then there exists a constant C such that*

$$\left\|(J_\delta f^\varepsilon)' - f'\right\|_{\infty, I_\delta} \le C\left(\delta + \frac{\varepsilon}{\delta}\right).$$

Notice that if ε is known, then an "optimal" selection of δ is provided by $\delta = O(\sqrt{\varepsilon})$.

THEOREM 2.2. *If $G = \{g(t_j)\}_{j=1}^{n}$ and $G^\varepsilon = \{g_j^\varepsilon\}_{j=1}^{n}$ is a perturbed version of g satisfying $\|G - G^\varepsilon\|_{\infty, K} \le \varepsilon$, then the following holds.*

1. *If g is integrable, then there exists a constant C such that*

$$\|g_\delta^\varepsilon - J_\delta g\|_{\infty, I_\delta} \le C\,(\varepsilon + \Delta t),$$

where g_δ^ε is the discrete δ-mollification of G^ε.

2. *If g' is uniformly Lipschitz on I, then there exists a constant C such that*

$$\left\|\frac{d}{dt}g_\delta^\varepsilon - \frac{d}{dt}g\right\|_{\infty,I_\delta} \le C\left(\delta + \frac{\varepsilon}{\delta} + \frac{\Delta t}{\delta}\right).$$

3. *If g is uniformly Lipschitz on I, then there exists a constant C such that*

$$\left\|\frac{d}{dt}g_\delta^\varepsilon - \frac{d}{dt}J_\delta g\right\|_{\infty,I_\delta} \le C\left(\frac{\varepsilon}{\delta} + \frac{\Delta t}{\delta}\right).$$

Assuming, from now on, that $|t_{j+1}-t_j| = \Delta t$ for all $j = 1,2,\dots,n-1$, the following proposition holds.

THEOREM 2.3.

1. *If $G = \{g_j\}_{j=1}^n$ is a discrete function defined on K, then*

$$\left\|D_0^\delta(G)\right\|_{\infty,K\cap\widetilde{I_\delta}} \le \frac{2A_p}{\delta}\|G\|_{\infty,K},$$

where $\widetilde{I_\delta} \equiv [p\delta + \Delta t, 1 - p\delta - \Delta t]$, $D_0^\delta(G) = D_0(g_\delta)|_{K\cap\widetilde{I_\delta}}$, and $D_0(g_\delta)$ is the centered difference approximation of the mollified derivative $\frac{d}{dt}g_\delta$.

2. *If g is uniformly Lipschitz on I, $G = \{g(t_j)\}_{j=1}^n$ and $G^\varepsilon = \{g_j^\varepsilon\}_{j=1}^n$ are discrete functions satisfying $\|G - G^\varepsilon\|_{\infty,K} \le \varepsilon$, then there exist a constant C and a constant C_δ, depending on δ, such that*

$$\left\|D_0\left(g_\delta^\varepsilon\right) - \frac{d}{dt}J_\delta g\right\|_{\infty,K\cap\widetilde{I_\delta}} \le C\left(\frac{\varepsilon}{\delta} + \frac{\Delta t}{\delta}\right) + C_\delta(\Delta t)^2.$$

Moreover, if g' is uniformly Lipschitz on I, then we have

$$\left\|D_0\left(g_\delta^\varepsilon\right) - \frac{d}{dt}g\right\|_{\infty,K\cap\widetilde{I_\delta}} \le C\left(\delta + \frac{\varepsilon}{\delta} + \frac{\Delta t}{\delta}\right) + C_\delta(\Delta t)^2.$$

3. THE IDENTIFICATION PROBLEM

3.1. Description of the Problem

Find $a(x)$ in I and u, u_x throughout the domain $[0,1]\times[0,1]$ of the (x,t) plane, from measured approximations of $\alpha(t)$, $\beta(t)$, γ, and $\tau(x)$ (or $\eta(x)$) satisfying

$$\begin{aligned}
u_t &= \left(a(x)u_x\right)_x + f, && 0 < t < 1,\ 0 < x < 1,\\
u(0,t) &= \alpha(t), && 0 \le t \le 1,\\
u_x(0,t) &= \beta(t), && 0 \le t \le 1,\\
a(0) &= \gamma, &&\\
u(x,0) &= \tau(x), \quad (\text{or } u_x(x,0) = \eta(x)), && 0 \le x \le 1.
\end{aligned}$$

Notice that $\alpha(t)$, $\beta(t)$, γ, and $\tau(x)$ (or $\eta(x)$) are not known exactly. The available data α^ε, β^ε, γ^ε, and τ^ε(or η^ε) are measured approximations of $\alpha(t)$, $\beta(t)$, γ, and $\tau(x)$ (or $\eta(x)$), respectively, and they satisfy the estimates $\|\alpha - \alpha^\varepsilon\|_{\infty,I} \le \varepsilon$, $\|\beta - \beta^\varepsilon\|_{\infty,I} \le \varepsilon$, $|\gamma - \gamma^\varepsilon| \le \varepsilon$, and $\|\tau - \tau^\varepsilon\|_{\infty,I} \le \varepsilon$ (or $\|\eta - \eta^\varepsilon\|_{\infty,I} \le \varepsilon$).

We further assume that $a(x) \ge \xi > 0$, $|u_x(x,0)| \ge \zeta > 0$ for $x \in [0,1]$, where ξ and ζ are constants.

3.2. Regularized Problem

First, we stabilize our problem using the mollification method. The stabilized problem is: find v, v_x, and $a(x)$ satisfying

$$\begin{aligned} v_t &= (a(x)v_x)_x + f, && 0 < t < 1,\ 0 < x < 1, \\ v(0,t) &= J_\delta \alpha(t), && 0 \le t \le 1, \\ v_x(0,t) &= J_{\delta^*}\beta(t), && 0 \le t \le 1, \\ a(0) &= \gamma, && \\ v(x,0) &= J_{\delta'}\tau(x), \quad (\text{or } v_x(x,0) = J_{\delta'}\eta(x)), && 0 \le x \le 1, \end{aligned}$$

where all δ-mollifications are taken with respect to t except $J_{\delta'}\tau(x)$ (or $J_{\delta'}\eta(x)$) in which the δ-mollification is taken with respect to x.

Let $h = \Delta x = 1/M$ and $k = \Delta t = 1/N$ be the parameters of the finite difference discretization. We denote by Q_j^n, R_j^n, W_j^n, U_j', U_j'', A_j, and P_j^n the discrete approximations of the mollified heat flux $a(jh)v_x(jh, nk)$, the mollified space derivative of temperature $v_x(jh, nk)$, the mollified time derivative of temperature $v_t(jh, nk)$, the derivative of the initial temperature $v_x(jh, 0)$, the second derivative of the initial temperature $v_{xx}(jh, 0)$, the coefficient $a(jh)$ and the derivative of the coefficient $a'(jh)$, respectively, obtained by the numerical method. We also denote $f(jh, nk)$ by F_j^n.

3.3. The Algorithm

INPUT. Parameter p and grid sizes h and k.

Step 1.

1. Select δ_1, δ_2^0, and δ_3. Extend α^ϵ, β^ϵ, and τ^ϵ(or η^ϵ) and compute $\alpha_{\delta_1}^\epsilon$, $\beta_{\delta_2^0}^\epsilon$, and $\tau_{\delta_3}^\epsilon$(or $\eta_{\delta_3}^\epsilon$) in the interval $[0,1]$. Set $R_0^n = (\beta^\epsilon)_n$, $Q_0^n = \gamma^\epsilon(\beta_{\delta_2^0}^\epsilon)_n$, and $A_0 = \gamma^\epsilon$.
2. Perform mollified differentiation in time of $\alpha_{\delta_1}^\epsilon$, perform mollified differentiation in space of $\tau_{\delta_3}^\epsilon$(or $\eta_{\delta_3}^\epsilon$) to get the approximation of $v_x(x,0)$ (or $v_{xx}(x,0)$). (If the initial condition is $u(x,0) = \tau(x)$, we then select δ_3' and perform mollified differentiation in space of $D_0(\tau_{\delta_3}^\epsilon)$ to get the approximation of $v_{xx}(x,0)$.)
   1. Set $W_0^n = (D_0(\alpha_{\delta_1}^\epsilon))_n$. The mollified derivative is approximated by centered differences.
   2. Set U_j', U_j'' to be the discrete approximations of $v_x(x,0)$ and $v_{xx}(x,0)$ given by $D_0(\tau_{\delta_3}^\epsilon)$ and $D_0^{\delta_3'}(\, D_0(\tau_{\delta_3}^\epsilon))$ (or $\eta_{\delta_3}^\epsilon$ and $D_0(\eta_{\delta_3}^\epsilon)$), respectively.
   3. Set $P_0 = [W_0^0 - A_0 U_0'' - F_0^0]/U_0'$.

   Note: when using centered differences to approximate derivatives, we apply linear extrapolation to get the endpoint values.

Step 2. Initialize $j = 0$. Do while $j < M$.

1. $Q_{j+1}^n = Q_j^n + h(W_j^n - F_j^n)$.
2. $A_{j+1} = A_j + hP_j$.
3. $W_{j+1}^n = W_j^n + hD_0^{\delta_2^j}(R_j^n)$.
4. $R_{j+1}^n = Q_{j+1}^n / A_{j+1}^n$.
5. $P_{j+1} = [W_{j+1}^0 - A_{j+1}U_{j+1}'' - F_{j+1}^0]/U_{j+1}'$.
6. Select δ_2^{j+1}, perform mollified differentiation in time of R_{j+1}^n, use extrapolation to get the endpoint values.
7. $j = j + 1$.

Step 3. Use quadrature formulae to approximate

$$\begin{aligned} &v(jh, 0) \text{ from } U_j', && j = 0, \dots, M, \\ &v(jh, nk) \text{ from } W_j^l, && j = 1, \dots, M,\ n = 1, \dots, N,\ l = 0, \dots, n-1. \end{aligned}$$

3.4. Analysis

In what follows, we denote $|Y_j| = \max_n |Y_j^n|$. We also rewrite Step 2 in the algorithm as follows:

$$A_{j+1} = A_j + \frac{h\left[W_j^0 - A_j U_j'' - F_j^0\right]}{U_j'}, \tag{3.1}$$

$$Q_{j+1}^n = Q_j^n + h\left(W_j^n - F_j^n\right), \tag{3.2}$$

$$W_{j+1}^n = W_j^n + h\frac{1}{A_j} D_0^{\delta_2^j} Q_j^n, \qquad \text{if } j > 0, \tag{3.3}$$

$$W_1^n = W_0^n + hD_0^{\delta_2^0}\beta^\varepsilon. \tag{3.4}$$

Notice that A_j, Q_j^n, and W_j^n are the quantities that we need to compute.

According to the considerations in Section 3.1, the corresponding **assumptions for our numerical data** are $A_j \geq \xi_1 > 0$, $|U_j'| \geq \zeta_1 > 0$ for all $j = 0, 1, \ldots, M$, for some constants ξ_1 and ζ_1.

THEOREM 3.1. *(Stability of the algorithm.) There exist two constants C, C_0 such that*

$$\max\{A_M, |Q_M|, |W_M|\} \leq \left(\exp\left(\frac{C}{\delta_2}\right)\right)(\max\{A_0, |Q_0|, |W_0|\} + C_0),$$

where $\delta_2 = \min_j \delta_2^j$.

PROOF. Let $C_1 = 1/\zeta_1$, $C_2 = \max_j\{|U_j''|\}$, and $C_3 = \max_{[0,1]\times[0,1]} |f(x,t)|$. From the algorithm, we readily see that

$$A_{j+1} \leq A_j + hC_1\left(\left|W_j^0\right| + C_2 A_j + C_3\right),$$
$$\left|Q_{j+1}^n\right| \leq \left|Q_j^n\right| + h\left(|W_j| + C_3\right),$$
$$\left|W_{j+1}^n\right| \leq \left|W_j^n\right| + h\frac{1}{A_j}\left\|D_0^{\delta_2^j}\right\| |Q_j|.$$

Thus,

$$\max\{A_{j+1}, |Q_{j+1}|, |W_{j+1}|\} \leq (1 + hM_\delta)\max\{A_j, |Q_j|, |W_j|\} + hC_1',$$

where $M_\delta = \max\{1, C_1 + C_1C_2, 2A_p/(\delta_2\xi_1)\}$ and $C_1' = \max\{C_3, C_1C_3\}$.

The iteration of the last inequality leads to

$$\max\{A_M, |Q_M|, |W_M|\} \leq (1 + hM_\delta)^M \left(\max\{A_0, |Q_0|, |W_0|\} + \frac{C_1'}{M_\delta}\right),$$

which implies

$$\max\{A_M, |Q_M|, |W_M|\} \leq (\exp M_\delta)\left(\max\{A_0, |Q_0|, |W_0|\} + \frac{C_1'}{M_\delta}\right).$$

To prove convergence, we set δ, δ^*, and δ' in the regularized problem to be δ_1, δ_2^0, and δ_3, which we use in the scheme, respectively. First, we use Taylor series to obtain some useful equations satisfied by the mollified solution v. They are as follows:

$$a((j+1)h) = a(jh) + h\frac{v_t(jh,0) - a(jh)v_{xx}(jh,0) - f(jh,0)}{v_x(jh,0)} + O\left(h^2\right), \tag{3.5}$$

$$q((j+1)h, nk) = q(jh, nk) + h(v_t(jh, nk) - f(jh, nk)) + O\left(h^2\right), \tag{3.6}$$

$$v_t((j+1)h, nk) = v_t(jh, nk) + h\frac{1}{a(jh)}\frac{d}{dt}q(jh, nk) + O\left(h^2\right), \tag{3.7}$$

where $q(x,t) \equiv a(x)v_x(x,t)$.

We now define the discrete error functions

$$\Delta A_j = A_j - a(jh),$$
$$\Delta Q_j^n = Q_j^n - q(jh, nk),$$
$$\Delta W_j^n = W_j^n - v_t(jh, nk).$$

Here we only present the proof for the case when the initial condition is given by $u_x(x,0) = \eta(x)$ ($x \in [0,1]$). Let $\delta_{\min} = \min_{j>0} \delta_2^j$. By comparing (3.1) and (3.5), we have

$$\Delta A_{j+1} = \Delta A_j + h\Phi_1 - h\Phi_2 - f(jh,0)h\Phi_3 + O\left(h^2\right), \tag{3.8}$$

where

$$\Phi_1 = \frac{W_j^0}{U_j'} - \frac{v_t(jh,0)}{v_x(jh,0)},$$
$$\Phi_2 = \frac{A_j U_j''}{U_j'} - \frac{a(jh) v_{xx}(jh,0)}{v_x(jh,0)},$$
$$\Phi_3 = \frac{1}{U_j'} - \frac{1}{v_x(jh,0)}.$$

Notice that

$$\Phi_1 = v_t(jh,0)\Phi_3 + \frac{1}{U_j'}\Delta W_j^0,$$
$$\Phi_2 = a(jh) v_{xx}(jh,0)\Phi_3 + \frac{U_j''}{U_j'}\Delta A_j + \frac{a(jh)}{U_j'}\left(U_j'' - v_{xx}(jh,0)\right).$$

Applying Theorems 2.2 and 2.3 to U_j', we have

$$\left|U_j' - v_x(jh,0)\right| \le C(\varepsilon + h),$$
$$\left|U_j'' - v_{xx}(jh,0)\right| \le \frac{C}{\delta_3}(\varepsilon + h) + C_\delta h^2.$$

Hence (3.8) implies

$$|\Delta A_{j+1}| \le |\Delta A_j| + hC\left(|\Delta W_j| + |\Delta A_j|\right) + \frac{Ch}{\delta_3}(\varepsilon + h) + O\left(h^2\right). \tag{3.9}$$

By subtracting (3.6) from (3.2), we obtain

$$\Delta Q_{j+1}^n = \Delta Q_j^n + h\Delta W_j^n + O\left(h^2\right). \tag{3.10}$$

This implies

$$|\Delta Q_{j+1}| \le |\Delta Q_j| + h|\Delta W_j| + O\left(h^2\right). \tag{3.11}$$

Finally, (3.3) and (3.7) give

$$\Delta W_{j+1}^n = \Delta W_j^n + h(\Psi_1 + \Psi_2) + O\left(h^2\right), \tag{3.12}$$

where

$$\Psi_1 = \frac{1}{A_j}\left(D_0^{\delta_2^j} Q_j^n - q_t(jh,nk)\right),$$
$$\Psi_2 = -\frac{q_t(jh,nk)}{A_j a(jh)}\Delta A_j.$$

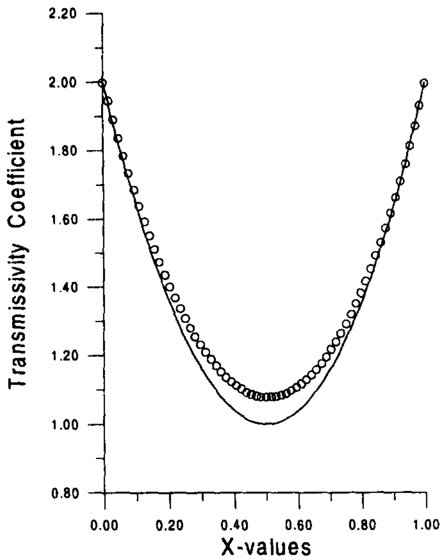

Figure 1. Example 1. Exact (—) and computed (o) coefficient with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

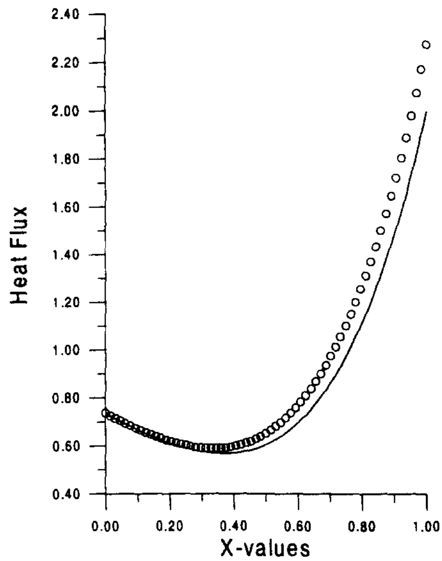

Figure 2. Example 1. Exact (—) and computed (o) heat flux at $t = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

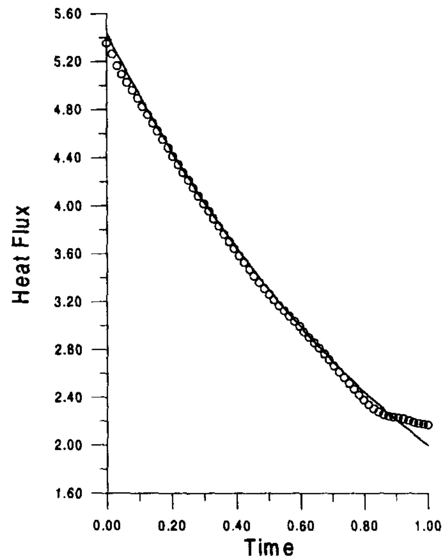

Figure 3. Example 1. Exact (—) and computed (o) heat flux at $x = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

By Theorem 2.3, neglecting the effect of the δ_2^j mollification on the already mollified solution q_t, we have

$$|\Psi_1| \leq \frac{C}{\delta_2^j}\left(|\Delta Q_j| + \Delta t\right) + C_\delta (\Delta t)^2.$$

Consequently, (3.12) implies

$$|\Delta W_{j+1}| \leq |\Delta W_j| + \frac{Ch}{\delta_2^j}|\Delta Q_j| + Ch|\Delta A_j| + C_\delta h\Delta t + O\left(h^2\right). \tag{3.13}$$

Set $\Delta_j = \max\{|\Delta A_j|, |\Delta Q_j|, |\Delta W_j|\}$. By (3.9), (3.11), and (3.13), we have

$$\Delta_{j+1} \leq \left(1 + \frac{Ch}{\delta_{\min}}\right)\Delta_j + Ch\left(\frac{\varepsilon + h}{\delta_3}\right) + C_\delta h\Delta t + O\left(h^2\right),$$

where $\delta_{\min} = \min_j \delta_2^j$.

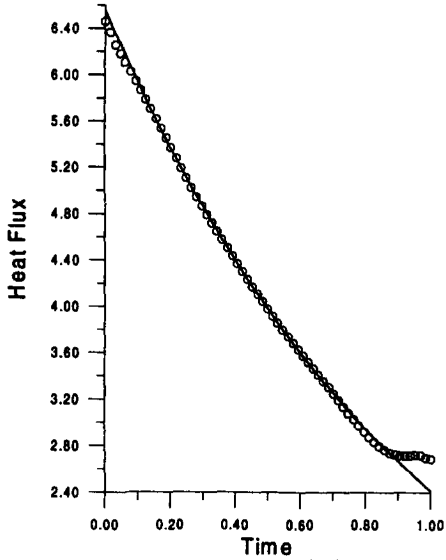

Figure 4. Example 2. Exact (—) and computed (o) heat flux at $x = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

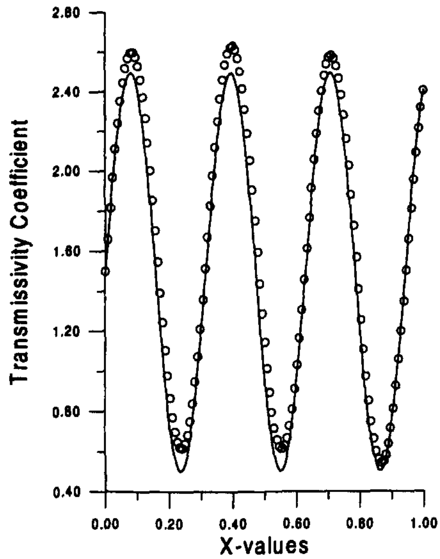

Figure 5. Example 2. Exact (—) and computed (o) coefficient with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

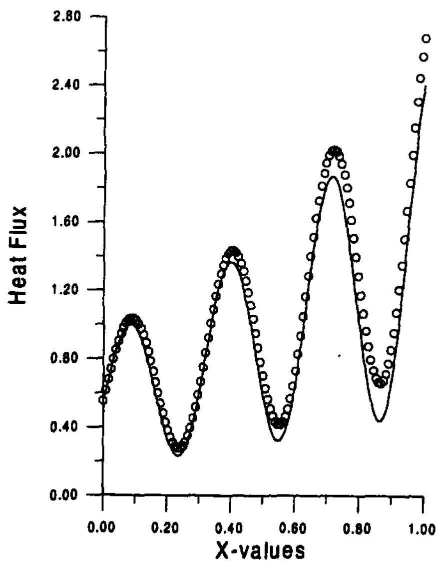

Figure 6. Example 2. Exact (—) and computed (o) heat flux at $t = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

Therefore,

$$\Delta_M \le \exp\left(\frac{C}{\delta_{\min}}\right)(\Delta_0 + C(\varepsilon + h + \Delta t)).$$

Since $\Delta_0 \le (C/\delta_1)(\varepsilon + \Delta t)$ by Theorem 2.2, we have proved the following convergence theorem.

THEOREM 3.2. *If the initial condition is given by* $u_x(x,0) = \eta(x)$ $(0 \le x \le 1)$*, then* $\max\{|\Delta A_M|, |\Delta Q_M|, |\Delta W_M|\}$ *converges to zero as* Δt*,* h*, and* ε *tend to zero.*

If the initial condition is $u(x,0) = \tau(x)$, then the leading term for the error $\|U_j'' - v_{xx}(jh,0)\|_\infty$, according to Theorem 2.2, is given by $C((\varepsilon/\delta_3 + h/\delta_3)/\delta_3') = C(\varepsilon + h)/\delta_3\delta_3'$. In practice, this error might be more difficult to control.

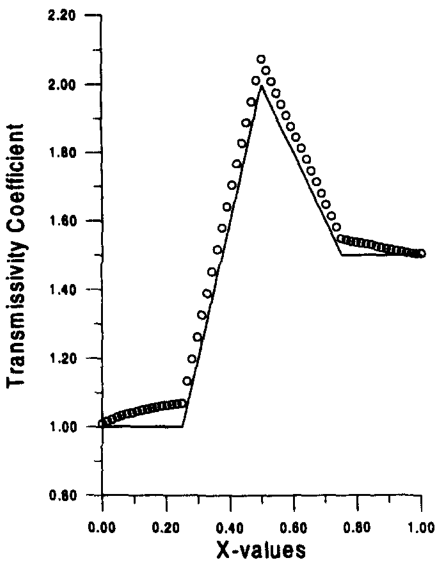

Figure 7. Example 3. Exact (—) and computed (o) coefficient with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

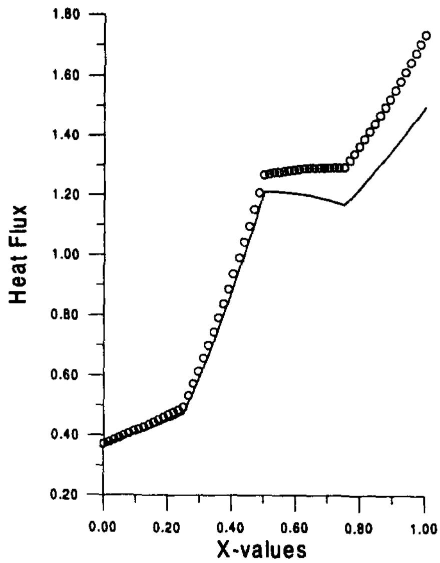

Figure 8. Example 3. Exact (—) and computed (o) heat flux at $t = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

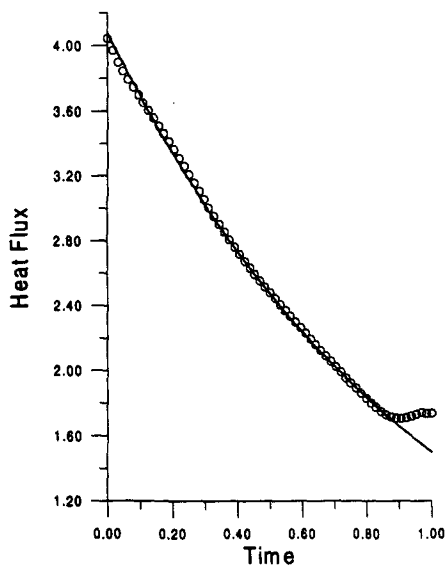

Figure 9. Example 3. Exact (—) and computed (o) heat flux at $x = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

4. IMPLEMENTATION

4.1. Extension of Data

Computation of $J_\delta(g)$ and g_δ throughout $I = [0,1]$, requires the extension of g to a slightly bigger interval $I'_\delta = [-p\delta, 1 + p\delta]$. We seek constant extensions g^* of g to the intervals $[-p\delta, 0]$ and $[1, 1 + p\delta]$, satisfying the conditions

$$\| J_\delta (g^*) - g \|_{L^2[0,p\delta]} \text{ is minimum}$$

and

$$\| J_\delta (g^*) - g \|_{L^2[1-p\delta,1]} \text{ is minimum.}$$

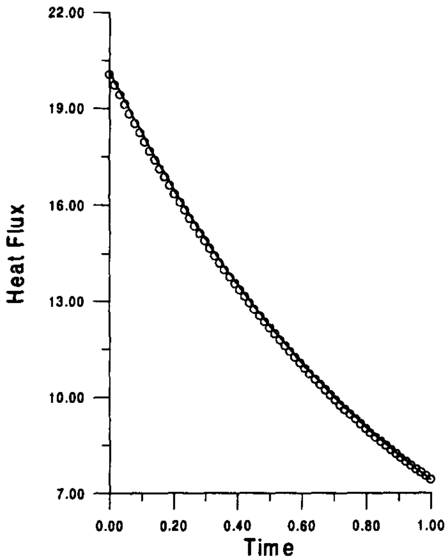

Figure 10. Example 4. Exact (—) and computed (o) heat flux at $x = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

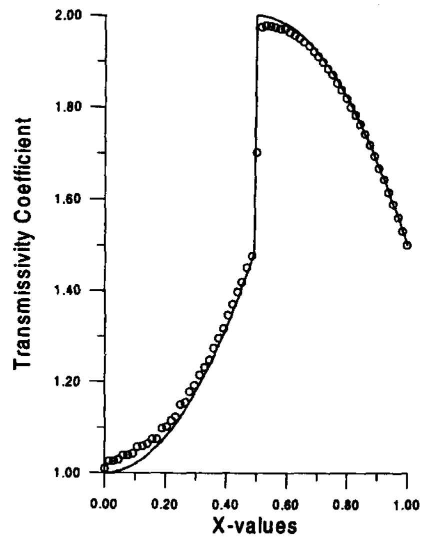

Figure 11. Example 4. Exact (—) and computed (o) coefficient with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

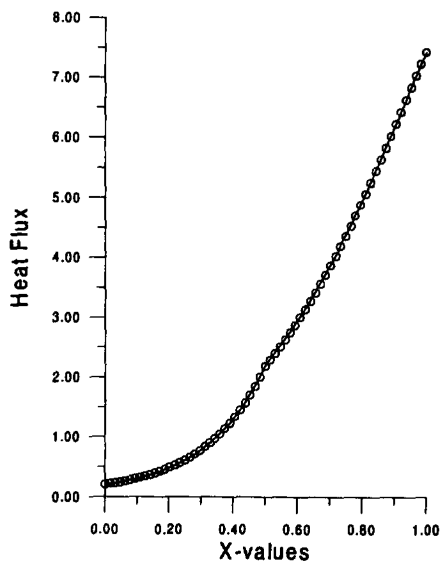

Figure 12. Example 4. Exact (—) and computed (o) heat flux at $t = 1$ with $\varepsilon = 0.01$ and $\Delta x = \Delta t = 128$.

The unique solution to this optimization problem at the boundary $t = 1$ is given by

$$g^* = \frac{\int_{1-p\delta}^{1} \left[g(t) - \int_0^1 \rho_\delta(t-s) g(s)\, ds \right] \left[\int_1^{1+p\delta} \rho_\delta(t-s)\, ds \right] dt}{\int_{1-p\delta}^{1} \left[\int_1^{1+p\delta} \rho_\delta(t-s)\, ds \right]^2 dt}.$$

A similar result holds at the end point $t = 0$. A proof of these statements can be found in [7].

For each $\delta > 0$, the extended function is defined on the interval I'_δ and the corresponding mollified function is computed on $I = [0, 1]$. All the conclusions of the previous sections still hold in the subinterval I_δ.

Table 1. Example 1. Errors of the recovered parameter $a(x)$ and the recovered heat flux au_x at $x = 1$ and $t = 1$.

h	ε	$a(x)$	Heat Flux	Heat Flux
			$x = 1$	$t = 1$
$\frac{1}{64}$	0.00	0.018	0.026	0.022
	0.01	0.038	0.027	0.125
	0.02	0.051	0.022	0.106
$\frac{1}{128}$	0.00	0.009	0.013	0.010
	0.01	0.041	0.019	0.108
	0.02	0.044	0.015	0.094
$\frac{1}{256}$	0.00	0.005	0.006	0.005
	0.01	0.037	0.019	0.121
	0.02	0.034	0.019	0.112

Table 2. Example 2. Errors of the recovered parameter $a(x)$ and the recovered heat flux au_x at $x = 1$ and $t = 1$.

h	ε	$a(x)$	Heat Flux	Heat Flux
			$x = 1$	$t = 1$
$\frac{1}{64}$	0.00	0.088	0.011	0.081
	0.01	0.114	0.015	0.143
	0.02	0.119	0.013	0.117
$\frac{1}{128}$	0.00	0.044	0.005	0.041
	0.01	0.077	0.014	0.118
	0.02	0.076	0.013	0.113
$\frac{1}{256}$	0.00	0.022	0.002	0.021
	0.01	0.052	0.016	0.115
	0.02	0.047	0.015	0.107

4.2. Selection of the Radius of Mollification

Using matrix notation, the computation of the discrete mollified data vector $g_\delta^\epsilon = [(g_\delta^\epsilon)_1, \dots, (g_\delta^\epsilon)_n]^{\mathrm{T}}$ from the noisy data vector $G^\epsilon = [g_1^\epsilon, \dots, g_n^\epsilon]^{\mathrm{T}}$ can be viewed as follows.

Given δ and Δt, the data extension discussed in the previous section requires the addition of $r = \mathrm{INT}\,(p\delta/\Delta t)$ constant values, say $\{\mu_i\}_{i=1}^r$, $\mu_i = \mu$ and $\{\xi_i\}_{i=1}^r$, $\xi_i = \xi$, $i = 1, 2, \dots, r$, to G^ϵ to obtain

$$G_{\mathrm{ext}}^\epsilon = \left[\mu_{-r}, \mu_{-r+1}, \dots, \mu_{-2}, \mu_{-1}, g_1^\epsilon, g_2^\epsilon, \dots, g_{n-1}^\epsilon, g_n^\epsilon, \xi_1, \xi_2, \dots, \xi_{r-1}, \xi_r\right]^{\mathrm{T}}.$$

Now define the $n \times (n + 2r)$ circulant matrix A_δ where the first row is given by

$$(A_\delta)_{1j} = \begin{cases} \int_{s_{j-1}}^{s_j} \rho_\delta(-s)\, ds, & j = 1, 2, \dots, n, \\ 0, & j = n+1, \dots, n+2r. \end{cases}$$

Then

$$A_\delta G_{\mathrm{ext}}^\epsilon = g_\delta^\epsilon.$$

Table 3. Example 3. Errors of the recovered parameter $a(x)$ and the recovered heat flux au_x at $x = 1$ and $t = 1$.

h	ε	$a(x)$	Heat Flux $x = 1$	Heat Flux $t = 1$
$\frac{1}{64}$	0.00	0.001	0.005	0.006
	0.01	0.043	0.018	0.094
	0.02	0.038	0.018	0.081
$\frac{1}{128}$	0.00	0.001	0.002	0.003
	0.01	0.040	0.020	0.097
	0.02	0.044	0.018	0.091
$\frac{1}{256}$	0.00	0.000	0.001	0.001
	0.01	0.039	0.020	0.099
	0.02	0.034	0.018	0.084

Table 4. Example 4. Errors of the recovered parameter $a(x)$ and the recovered heat flux au_x at the boundaries $x = 1$ and $t = 1$.

h	ε	$a(x)$	Heat Flux $x = 1$	Heat Flux $t = 1$
$\frac{1}{64}$	0.00	0.027	0.015	0.022
	0.01	0.025	0.014	0.015
	0.02	0.026	0.015	0.022
$\frac{1}{128}$	0.00	0.020	0.008	0.011
	0.01	0.020	0.007	0.005
	0.02	0.025	0.006	0.004
$\frac{1}{256}$	0.00	0.015	0.004	0.006
	0.01	0.018	0.003	0.002
	0.02	0.020	0.003	0.002

We observe that the mollified data vector requires the computation of n inner products. Since the noise in the data is not known, an appropriate mollification parameter, introducing the correct degree of smoothing, should be selected. Such a parameter is determined by the Principle of Generalized Cross Validation as the value of δ that minimizes the functional

$$\frac{\left(G_{\text{ext}}^{\epsilon}\right)^{\top}\left(I^{\top}-A_{\delta}^{\top}\right)\left(I-A_{\delta}\right)G_{\text{ext}}^{\epsilon}}{\text{Trace}\left[\left(I^{\top}-A_{\delta}^{\top}\right)\left(I-A_{\delta}\right)\right]},$$

where the $n \times (n+2r)$ matrix I has entries

$$I_{ij} = \begin{cases} 1, & i = j, \quad i = 1, 2, \dots n, \\ 0, & \text{otherwise.} \end{cases}$$

The desired δ-minimizer is obtained by a Golden Section Search Procedure. We observe that for fixed Δt, the data extension procedure dynamically updates the δ-depending dimensions of all the vectors involved and also that the denominator of the GCV functional can be evaluated explicitly for each $\delta > 0$. Basic references on the subject are [9,10].

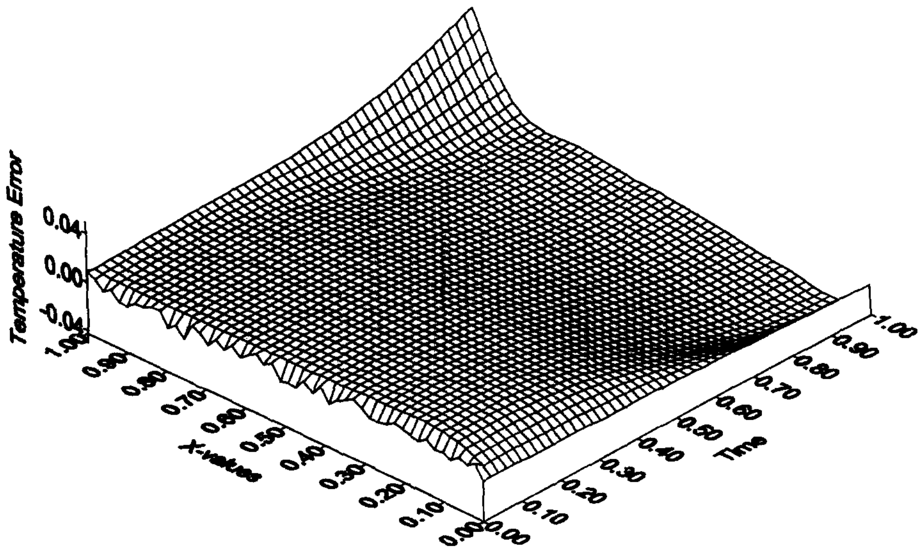

Figure 13. Example 1. Errors of reconstructed temperature in [0, 1] × [0, 1].

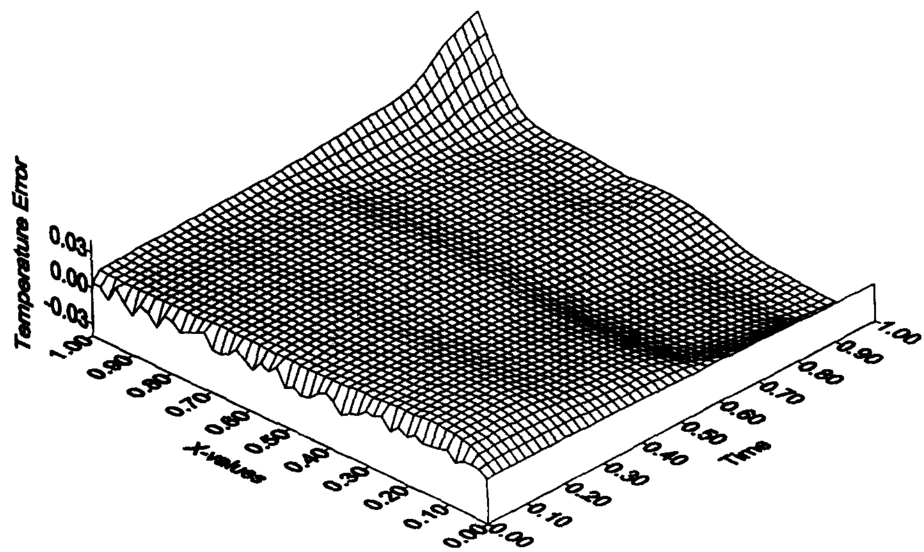

Figure 14. Example 2. Errors of reconstructed temperature in [0, 1] × [0, 1].

4.3. Numerical Examples

The algorithm of the previous section has been thoroughly tested. In this section, we present numerical results from four examples. In all cases, the discretization parameters are as follows: the number of space divisions is M and $\Delta x = h = 1/M$; the number of time divisions is N and $\Delta t = k = 1/N$; the maximum level of noise in the data function is ε; and we set $p = 3$. The value 3 is appropriate because the difference between ρ_δ for $p = 3$ and ρ_δ for $p > 3$ is not significant.

The use of average perturbation values ε is only necessary for the purpose of preparing the simulations. The filtering procedure introduced in Sections 4.1 and 4.2 automatically adapts the regularization parameters to the quality of the data.

Discretized measured approximations of the initial and boundary data are modeled by adding random errors to the exact data functions. Specifically, for a boundary data function $g(t)$, its discrete noisy version is

$$g_n^\varepsilon = g(t_n) + \varepsilon_n, \qquad n = 0, 1, \ldots, N,$$

where the (ε_n)'s are Gaussian random variables with variance $\sigma^2 = \varepsilon^2$.

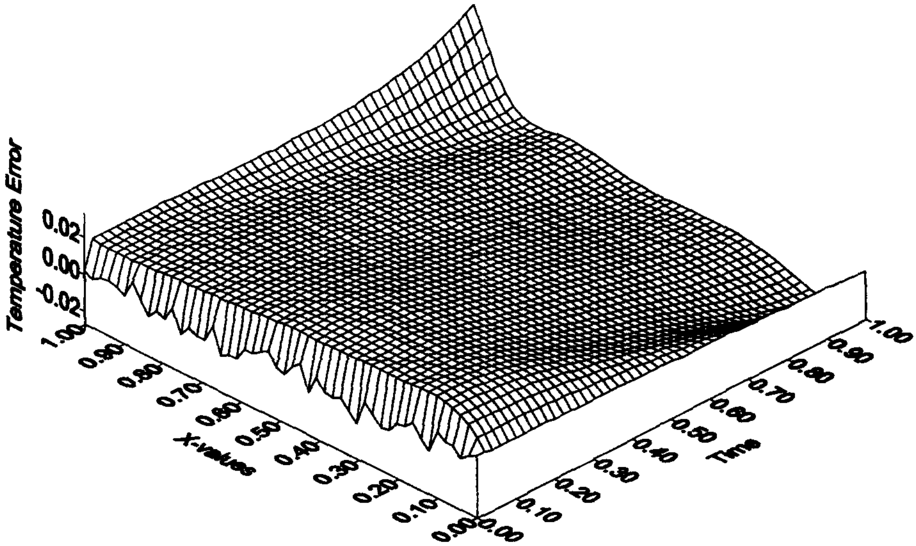

Figure 15. Example 3. Errors of reconstructed temperature in $[0,1] \times [0,1]$.

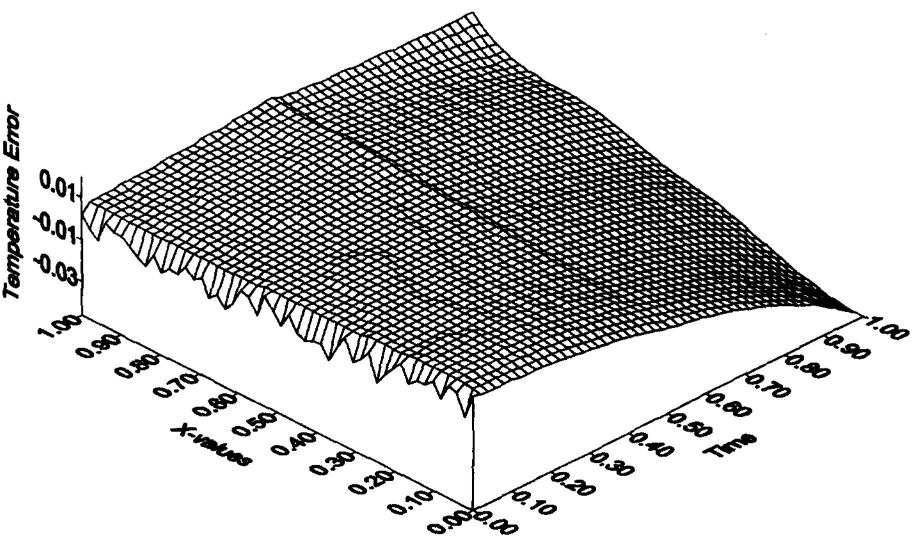

Figure 16. Example 4. Errors of reconstructed temperature in $[0,1] \times [0,1]$.

The errors of the recovered coefficients and the recovered heat flux at $x = 1$ and $t = 1$ are measured by weighted l^2-norms defined as follows.

Error in coefficient:

$$\left[\frac{1}{M}\sum_{j=0}^{M} |a(jh) - A_j|^2\right]^{1/2}.$$

Error in heat flux at $x = 1$:

$$\left[\frac{1}{N}\sum_{n=0}^{N} |a(1)u_x(1, nk) - Q_M^n|^2\right]^{1/2}.$$

Error in heat flux at $t = 1$:

$$\left[\frac{1}{M}\sum_{j=0}^{M} |a(jh)u_x(jh, 1) - Q_j^N|^2\right]^{1/2}.$$

All the tables were prepared with $\Delta t = k = 1/128$. No significant changes occur if we consider values of the time discretization parameter in the (tested) interval $[1/32, 1/256]$.

EXAMPLE 1. This example is designed to stress the behavior of the method when attempting to reconstruct a smooth parameter with strong concavity. We consider the following problem.

Find $a(x)$, $u(x,t)$, $u_x(x,t)$ satisfying

$$\begin{aligned} u_t &= (a(x)u_x)_x - \left(4(x-0.5)^2 + 8(x-0.5) + 2\right) e^{x-t}, \\ u(0,t) &= e^{-t}, \\ u_x(0,t) &= e^{-t}, \\ a(0) &= 2, \\ u_x(x,0) &= e^x. \end{aligned}$$

The exact solution for $a(x)$ is

$$a(x) = 1 + 4(x-0.5)^2.$$

Figures 1–3 and 13 give a clear qualitative indication of the approximate solutions obtained by this method. Further verifications of stability and accuracy are provided by the data in Table 1.

EXAMPLE 2. If $a(x)$ is smooth but changes concavity frequently, the results obtained by the scheme are very competitive. To illustrate this, we use the algorithm to solve the following problem.

Find $a(x)$, $u(x,t)$, $u_x(x,t)$ satisfying

$$\begin{aligned} u_t &= ((1.5 + \sin 20x)u_x)_x - (2.5 + 20\cos 20x + \sin 20x)\, e^{x-t}, \\ u(0,t) &= e^{-t}, \\ u_x(0,t) &= e^{-t}, \\ a(0) &= 1.5, \\ u_x(x,0) &= e^x. \end{aligned}$$

The exact solution for $a(x)$ is

$$a(x) = 1.5 + \sin 20x.$$

The results are plotted in Figures 4–6 and 14, which show the excellent agreement between the computed and the exact solutions. Table 2 further illustrates the stability properties and the practical accuracy of the method.

EXAMPLE 3. This example shows the numerical results obtained when attempting to reconstruct a nonsmooth coefficient associated with the following problem.

Find $a(x)$, $u(x,t)$, $u_x(x,t)$ satisfying

$$\begin{aligned} u_t &= (a(x)u_x)_x + f(x,t), \\ u(0,t) &= e^{-t}, \\ u_x(0,t) &= e^{-t}, \\ a(0) &= 1, \\ u_x(x,0) &= e^x, \end{aligned}$$

where

$$f(x,t) = \begin{cases} -2e^{x-t}, & 0 \le x < 0.25, \\ -(5+4x)e^{x-t}, & 0.25 \le x < 0.5, \\ (-2+2x)e^{x-t}, & 0.5 \le x < 0.75, \\ -2.5e^{x-t}, & 0.75 \le x \le 1. \end{cases}$$

The exact solution for the parameter $a(x)$ is

$$a(x) = \begin{cases} 1, & 0 \le x < 0.25, \\ 4x, & 0.25 \le x < 0.5, \\ 3 - 2x, & 0.5 \le x < 0.75, \\ 1.5, & 0.75 \le x \le 1. \end{cases}$$

Figures 7–9, 15, and Table 3 illustrate the stability and accuracy of the method in this case.

EXAMPLE 4. In practice, it is possible to encounter composite materials and $a(x)$ is usually discontinuous in this case. Assuming that there is no contact resistance at the interface location x_0 (i.e., at x_0, we have $q(x_0 - 0, t) = q(x_0 + 0, t)$ for all t and $u(x_0 - 0) = u(x_0 + 0)$), consider the following identification problem.

Find $a(x)$, $u(x,t)$, $u_x(x,t)$ satisfying

$$\begin{aligned} u_t &= (a(x)u_x)_x + f(x,t), \\ u(0,t) &= e^{-2-t}, \\ u_x(0,t) &= 4e^{-2-t}, \\ a(0) &= 1, \\ u_x(x,0) &= \begin{cases} 4e^{4(x-0.5)}, & 0 \le x < 0.5, \\ 3e^{3(x-0.5)}, & 0.5 \le x \le 1, \end{cases} \\ \lim_{x \to 0.5-} u(x,t) &= \lim_{x \to 0.5+} u(x,t), \\ \lim_{x \to 0.5-} a(x)u_x(x,t) &= \lim_{x \to 0.5+} a(x)u_x(x,t), \end{aligned}$$

where

$$f(x,t) = \begin{cases} -\left(32x^2 + 16x + 17\right) e^{4(x-0.5)-t}, & 0 \le x < 0.5, \\ \left(18x^2 - 6x - 20.5\right) e^{3(x-0.5)-t}, & 0.5 \le x \le 1. \end{cases}$$

The exact solution for $a(x)$ is

$$a(x) = \begin{cases} 1 + 2x^2, & 0 \le x < 0.5, \\ 2 - 2(x - 0.5)^2, & 0.5 \le x \le 1. \end{cases}$$

The numerical results obtained by the scheme are plotted in Figures 10–12, 16, and also described in Table 4.

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