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Identification of Heat-Conduction Coefficient via Method of Variational Imbedding

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Abstract—The inverse parabolic problem of coefficient identification from over-posed data is embedded into a fourth order in space and second order in time elliptic boundary value problem. The latter is well posed for redundant data at boundaries. The equivalence of the two problems is demonstrated. A difference scheme of splitting-type is employed, and featuring examples are elaborated numerically.

Keywords—Ill-posed problems, Heat conduction, Coefficient identification, Variational problems.

1. INTRODUCTION

The inverse problems for diffusion equation can be roughly separated into three principal classes. The first is the coefficient identification from over-posed data at the boundary, the second is the identification of the thermal regimes at one of the spatial boundaries from over-posed data at the other one (the parabolic version of the so-called analytical continuation), and the third is the reversed-time problem for identification of initial temperature distribution from the known distribution at certain later moment of time. The second problem appears to be the most studied due to the successful technique proposed in [1,2] called "quasi-reversibility method" (see, also, [3]). Apart from being inverse, the second and third problems are also incorrect in the sense of Hadamard (see [4]). The first one is merely inverse without being incorrect in the strict sense of amplifying the disturbances. The problem then is how to create the appropriate algorithm. The present paper is devoted to this aim. We make use of a technique called Method of Variational Imbedding (MVI) which consists in replacing the original inverse problem by the boundary value problem for the Euler-Lagrange equations for minimization of the quadratic functional of the original equations.

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The first application of MVI was to the problem of identification of homoclinic trajectories as inverse problem [5] (see also the ensuing works [6,7]). The way to treat the classical inverse problems by means of MVI was sketched in [8–10]. In the present work, we are concerned with the numerical implementation of [9]. We heavily draw on the unpublished work [11]. A similar case has already been treated in [12], where the identification of the boundary-layer thickness was done by means of MVI.

2. PROBLEM OF COEFFICIENT IDENTIFICATION

Consider $(1+1)D$ equation of heat conduction

$$\mathcal{A}u \equiv -\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left[\lambda(x)\frac{\partial u}{\partial x}\right] = 0, \tag{2.1}$$

with initial and boundary conditions

$$u|_{t=0} = u_0(x), \tag{2.2}$$

$$u(t,0) = f(t), \qquad u(t,l) = g(t), \tag{2.3}$$

which match continuously, i.e., $f(0) = u_0(0)$, $g(0) = u_0(l)$.

The initial-boundary value problem (2.1)–(2.3) is correctly posed for the temperature $u(t,x)$ provided that the heat-conduction coefficient $\lambda(x)$ is known positive function.

Suppose that the coefficient λ is unknown. In order to identify it, one needs more information. There can be different sources of such an information, e.g., the temperature in some interior point(s) as function of time, fluxes at the boundaries, etc. We consider here the case when the heat fluxes at boundaries are known functions of time, namely,

$$\lambda(0)\left.\frac{\partial u}{\partial x}\right|_{x=0} = \psi(t), \qquad \lambda(l)\left.\frac{\partial u}{\partial x}\right|_{x=l} = \phi(t), \tag{2.4}$$

and when a "terminal" condition is also available

$$u|_{t=T} = u_1(x). \tag{2.5}$$

3. METHOD OF VARIATIONAL IMBEDDING (MVI)

We replace the original problem by the problem of minimization of the following functional:

$$\mathcal{I} = \int_0^T \int_0^l [\mathcal{A}u]^2 \, dx\, dt \equiv \int_0^T \int_0^l \left[-\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{\partial \lambda}{\partial x} + \lambda(x)\frac{\partial^2 u}{\partial x^2}\right]^2 dx\, dt = \min, \tag{3.1}$$

where u must satisfy the conditions (2.2)–(2.4). Functional $\mathcal{I}$ is a quadratic and homogeneous function of $\mathcal{A}u$, and hence, it attains its minimum if and only if $\mathcal{A}u \equiv 0$. In this sense there is one-to-one correspondence between the original equation (2.1) and the minimization problem (3.1).

The necessary condition for minimization of (3.1) are the Euler-Lagrange equations for the functions $u(t,x)$ and $\lambda(x)$. The equation for u reads

$$-\frac{\partial^2 u}{\partial t^2} + \frac{\partial}{\partial x}\lambda(x)\frac{\partial^2}{\partial x^2}\lambda(x)\frac{\partial u}{\partial x} = 0. \tag{3.2}$$

This equation is of fourth order with respect to the spatial variable x and its solution can satisfy the four conditions at the spatial boundaries. It is an elliptic equation of second order with respect to time, and hence, it requires two conditions at the two ends of the time interval under consideration. These are the initial condition (2.2) at $t = 0$ and the "terminal" condition (2.5) at $t = T$.

The problem is coupled by the Euler-Lagrange equation for λ, namely (see [9]),

$$\frac{d}{dx}F(x)\frac{d\lambda}{dx} + \lambda \int_0^T u_x u_{xxx}\, dt = \int_0^T u_{tx} u_x\, dt \equiv \left[\frac{u_x^2}{2}\right]_{t=0}^{t=T}, \qquad F(x) \equiv \int_0^T u_x^2\, dt. \tag{3.3}$$

For the sake of self-containedness of the present paper, we present here the essence of the result of [9] with the necessary modifications needed to absorb the "terminal" boundary condition.

Consider the Hilbert space $H(\mathcal{D})$ of functions $a(t,x)$ defined in $\mathcal{D} = (0 \le x \le l) \times (0 \le t \le T)$ (see Figure 1) and satisfying the boundary conditions

$$a(0,x) = 0, \qquad a(T,x) = 0, \tag{3.4}$$

$$a(t,0) = a(t,l) = \lambda(0)\left.\frac{\partial a}{\partial x}\right|_{x=0} = \lambda(l)\left.\frac{\partial a}{\partial x}\right|_{x=l} = 0, \tag{3.5}$$

where $\lambda(x)$ is sufficiently times differentiable function in the entire region $[0 \le x \le l]$.

The scalar product of two functions a, b from H is defined as follows:

$$[a,b] = \int_0^T \int_0^l \left[\frac{\partial a}{\partial t}\frac{\partial b}{\partial t} + \left(\frac{\partial}{\partial x}\lambda\frac{\partial a}{\partial x}\right)\left(\frac{\partial}{\partial x}\lambda\frac{\partial b}{\partial x}\right)\right] dt\, dx, \tag{3.6}$$

which is indeed a scalar product because $[a,a]$ reduces to sum of squares, and hence, $[a,a] = 0$ is possible only when $a \equiv 0$.

Consider now the sufficiently times differentiable function $\chi(t,x)$ that satisfies the boundary conditions (2.3),(2.4), i.e., χ is a continuation of functions $f(t)$, $g(t)$ into the interior of $\mathcal{D}$ with prescribed values of the normal derivative at the lateral boundaries in accordance with the fluxes $\psi(t)$, $\phi(t)$. Then a generalized solution to the imbedding problem is called any function $u(t,x)$ for which

$$[u, \Phi] = 0, \tag{3.7}$$

with $\Phi \in H(\mathcal{D})$ and $(u - \chi) \in H(\mathcal{D})$.

It is readily shown that the classical solution (if it exists) is also a generalized (weak) solution, namely,

$$\begin{aligned} 0 &= \int_0^T \int_0^l \Phi\left(-\frac{\partial^2 u}{\partial t^2} + \frac{\partial}{\partial x}\lambda(x)\frac{\partial^2}{\partial x^2}\lambda(x)\frac{\partial u}{\partial x}\right) dt\, dx \\ &= \int_0^T \int_0^l \left[\frac{\partial u}{\partial t}\frac{\partial \Phi}{\partial t} + \left(\frac{\partial}{\partial x}\lambda\frac{\partial u}{\partial x}\right)\left(\frac{\partial}{\partial x}\lambda\frac{\partial \Phi}{\partial x}\right)\right] dt\, dx. \end{aligned}$$

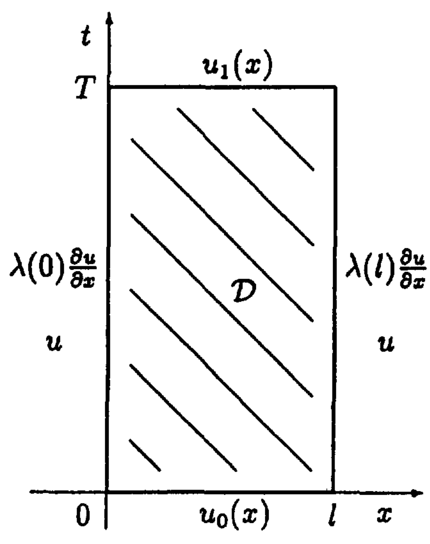


Figure 1. Sketch of domain.

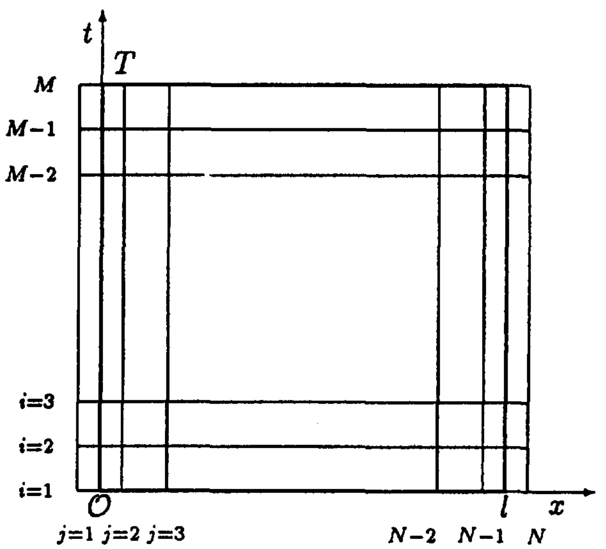


Figure 2. Grid pattern.

The last equality is derived upon acknowledging the b.c. for the members of the space $H(\mathcal{D})$, e.g., for the function Φ.

Now the existence of the generalized solution follows directly from Riesz theorem because (3.6) defines a scalar product and therefore a functional. In order to prove the uniqueness of solution to imbedding problem, we consider the difference $v = (u_1 - u_2)$ between two supposed solutions u_1 and u_2. It is clear that $v \in H(\mathcal{D})$ and equation (3.6) holds also for v as well. Then we take $\Phi \equiv v$ and arrive at $[v, v] = 0$ which means that $v \equiv 0$.

Thus we have shown that for arbitrary sufficiently smooth function $\lambda(x)$ there exists a unique solution to the fourth-order elliptic imbedding problem. Let us turn now to the problem for $\lambda(x)$. Here we focus on the practical case when the coefficient is known at the boundaries (natural boundary conditions for the unknown coefficient were treated in [9]). Hence we consider the Hilbert space $H^\lambda([0,l])$ of functions $\alpha(x)$ satisfying the conditions $\alpha(0) = \alpha(l) = 0$. The scalar product in H^λ is defined as

$$[\alpha, \beta] = \int_0^l \left(\alpha_x \beta_x \int_0^T u_x^2 \, dt - \alpha\beta \int_0^T u_x u_{xxx} \, dt \right) dx, \tag{3.8}$$

for which it is easily shown that $[\alpha, \alpha] = 0$ yields $\alpha \equiv 0$.

Up to this point, we have shown that the two Euler-Lagrange equations (3.2) and (3.3) for u and λ, respectively, possess unique solutions provided that in each of them the other function is thought of as known. This means that there exists a unique solution to the system as a whole and the functional $\mathcal{I}$ possesses only one stationary point. On the other hand, $\mathcal{I}$ is convex and then the only stationary point is its minimum. To show that the mentioned minimum has value equal to zero, we multiply (3.2) by $u(x)$ and integrate it with respect to t and x. Respectively, (3.3) is multiplied by $\lambda(x)$, integrated with respect to x, and added to the previous equation.

4. DIFFERENCE SCHEME

4.1. Grid Pattern and Approximations

In order to get second-order approximations of the boundary conditions we employ a staggered mesh in the spatial direction, while the mesh in the temporal direction is standard (see Figure 2). For the grid spacings we have $h = l/(N-2)$, $\tau = T/(M-1)$, where N is total number of grid lines in the spatial direction, M—in the temporal direction, and the grid lines are defined as follows:

$$x_j = (j - 1.5)h, \quad \text{for } j = 1, \dots, N, \qquad t_i = (i-1)\tau, \quad \text{for } i = 1, \dots, M. \tag{4.1}$$

We employ symmetric central differences for the operators

$$\Lambda_{xx} u_{i,j} \stackrel{\text{def}}{=} \frac{\lambda_{j-1}}{h^2} u_{i,j-1} - \frac{\lambda_{j-1} + \lambda_j}{h^2} u_{i,j} + \frac{\lambda_j}{h^2} u_{i,j+1} = \frac{\partial}{\partial x} \lambda(x) \frac{\partial}{\partial x} u(t,x) + O\left(h^2\right), \tag{4.2}$$

$$\begin{aligned} \Lambda_{xxxx} u_{i,j} \stackrel{\text{def}}{=} & \frac{\lambda_{j-2}\lambda_{j-1}}{h^4} u_{i,j-2} - \frac{\left(\lambda_{j-2} + 2\lambda_{j-1} + \lambda_j\right)\lambda_{j-1}}{h^4} u_{i,j-1} \\ & + \frac{\left(\lambda_{j-1} + \lambda_j\right)^2 + \lambda_{j-1}^2 + \lambda_j^2}{h^4} u_{i,j} - \frac{(\lambda_{j-1} + 2\lambda_j + \lambda_{j+1})\lambda_{j+1}}{h^4} u_{i,j+1} \\ & + \frac{\lambda_{j+1}\lambda_j}{h^4} u_{i,j+2} \\ = & \frac{\partial}{\partial x} \lambda(x) \frac{\partial^2}{\partial x^2} \lambda(x) \frac{\partial}{\partial x} u(t,x) + O\left(h^2\right), \end{aligned} \tag{4.3}$$

where $u_{i,j} = u(t_i, x_j)$ and $\lambda_j = \lambda(x_j + h/2)$.

The integrals entering the equation for the diffusion coefficient are approximated with second order as follows:

$$F_j \stackrel{\text{def}}{=} \tau \left[\frac{1}{2} \left(\frac{u_{1,j+2} - u_{1,j}}{2h} \right)^2 + \frac{1}{2} \left(\frac{u_{M,j+2} - u_{M,j}}{2h} \right)^2 + \sum_{i=2}^{M-1} \left(\frac{u_{i,j+2} - u_{i,j}}{2h} \right)^2 \right]$$
$$= \int_0^T (u_x)^2 + O\left(\tau^2 + h^2\right), \qquad \text{for } j = 1, 2, \ldots, N-2, \tag{4.4}$$

$$k_j \stackrel{\text{def}}{=} \tau \left[\frac{1}{2} \left(\frac{u_{1,j+1} - u_{1,j}}{h} \right) \left(\frac{u_{1,j+2} - 3u_{1,j+1} + 3u_{1,j} - u_{1,j-1}}{h^3} \right) \right.$$
$$+ \frac{1}{2} \left(\frac{u_{M,j+1} - u_{M,j}}{h} \right) \left(\frac{u_{M,j+2} - 3u_{M,j+1} + 3u_{M,j} - u_{M,j-1}}{h^3} \right)$$
$$\left. + \sum_{i=2}^{M-1} \left(\frac{u_{i,j+1} - u_{i,j}}{h} \right) \left(\frac{u_{i,j+2} - 3u_{i,j+1} + 3u_{i,j} - u_{i,j-1}}{h^3} \right) \right]$$
$$= \int_0^T u_x u_{xxx} + O\left(\tau^2 + h^2\right), \qquad \text{for } j = 2, 3, \ldots, N-2, \tag{4.5}$$

$$g_j \stackrel{\text{def}}{=} \frac{1}{2} \left[\left(\frac{u_{M,j+1} - u_{M,j}}{h} \right)^2 - \left(\frac{u_{1,j+1} - u_{1,j}}{h} \right)^2 \right], \qquad \text{for } j = 2, 3, \ldots, N-2. \tag{4.6}$$

4.2. Scheme for the "Direct" Problem

In order to gather "experimental" data for the fluxes at the boundaries, we solve numerically the "direct" initial-boundary value problem (2.1)–(2.3). To this end we use a two-layer (Crank-Nicolson type) implicit difference scheme with second order of approximation in time and space, namely,

$$\frac{u_{i+1,j} - u_{i,j}}{\tau} = \frac{1}{2} \left(\Lambda_{xx} u_{i+1,j} + \Lambda_{xx} u_{i,j} \right), \tag{4.7}$$

for $i = 1, \ldots, M-1$ and $j = 2, \ldots, N-1$. The algebraic problem is coupled with the difference approximations of the initial and boundary conditions

$$u_{1,j} = u_0(x_j), \qquad u_{i+1,1} + u_{i+1,2} = 2f(t_{i+1}), \quad u_{i+1,N-1} + u_{i+1,N} = 2g(t_{i+1}). \tag{4.8}$$

After the difference problem (4.7),(4.8) is solved, the "experimental" values of the fluxes are calculated with second order of approximation as follows:

$$u_1(x_j) \stackrel{\text{def}}{=} u_{M,j}, \qquad \psi(t_{i+1}) \stackrel{\text{def}}{=} \lambda_1 \frac{u_{i+1,2} - u_{i+1,1}}{h}, \quad \phi(t_{i+1}) \stackrel{\text{def}}{=} \lambda_{N-1} \frac{u_{i+1,N} - u_{i+1,N-1}}{h}, \tag{4.9}$$

where due to the staggerness of the grid in spatial direction, the discrete values of the diffusion coefficient λ_1 and λ_{N-1} correspond to the boundary values $\lambda(0)$ and $\lambda(l)$, respectively.

4.3. The Splitting Scheme for the Fourth-Order Elliptic Equation

The particular choice of scheme for the fourth-order equation is not essential for the purposes of the present work. We use the iterative procedure based on the coordinate-splitting method because of its computational efficiency. The most straightforward approximation is the following:

$$-\frac{1}{\tau^2} \left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j} \right) + \Lambda_{xxxx} u_{i,j} = 0. \tag{4.10}$$

Upon introducing a fictitious time, the equation (4.10) adopts the form of a parabolic difference equation for which the implicit time stepping reads

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\sigma} = \Lambda_{tt} u_{i,j}^n - \Lambda_{xxxx} u_{i,j}^n, \tag{4.11}$$

where the notation Λ_{tt} stands for the second time difference which enters (4.10). Then the splitting is enacted as follows:

$$\frac{\tilde{u}_{i,j} - u^n_{i,j}}{\sigma} = \Lambda_{tt}\tilde{u}_{i,j} - \Lambda_{xxxx}u^n_{i,j}, \qquad \frac{u^{n+1}_{i,j} - \tilde{u}_{i,j}}{\sigma} = -\Lambda_{xxxx}\left[u^{n+1}_{i,j} - u^n_{i,j}\right], \tag{4.12}$$

where $\tilde{u}_{i,j}$ is called "half-time-step variable". The latter is readily excluded to obtain the following $O(\tau^2)$ approximation of (4.11):

$$B\frac{u^{n+1}_{i,j} - u^n_{i,j}}{\sigma} = \Lambda_{tt}u^n_{i,j} - \Lambda_{xxxx}u^n_{i,j}, \tag{4.13}$$

where $B = (E - \sigma^2\Lambda_{tt}\Lambda_{xxxx})$ is an operator whose norm is always greater than unity. This means that the splitting scheme is even more stable than the general implicit scheme (4.11).

4.4. Scheme for the Coefficient

If the solution $u_{i,j}$ of the imbedding problem is thought of as known, then the coefficient can be computed on the base of the following scheme that is of second order of approximation:

$$\frac{1}{h^2}\left[F_j\lambda_{j+1} - (F_j + F_{j-1})\lambda_j + F_{j-1}\lambda_{j-1}\right] + k_j\lambda_j = g_j, \tag{4.14}$$

where F_j, k_j, and g_j, are defined in (4.4)–(4.6), respectively.

4.5 General Consequence of Algorithm

(I) With given $\lambda(x)$, $u_0(x)$, $f(t)$, and $g(t)$, the "direct" problem (4.7),(4.8) is solved.

(II) With the "experimentally observed" values of the $u_1(x)$, $\psi(t)$, and $\phi(t)$ obtained in (I), the fourth-order boundary value problem (4.12) is solved for function u. The iterations with respect to the fictitious time are terminated when $\max_{i,j}|(u^{n+1}_{i,j} - u^n_{i,j})/u^n_{i,j}| < \varepsilon$.

(III) The current iteration for the function $\lambda(x)$ is calculated from (4.14). If the difference between the new and old $\lambda(x)$ is less than ε, then the calculations are terminated, otherwise return to (II).

5. NUMERICAL EXPERIMENTS

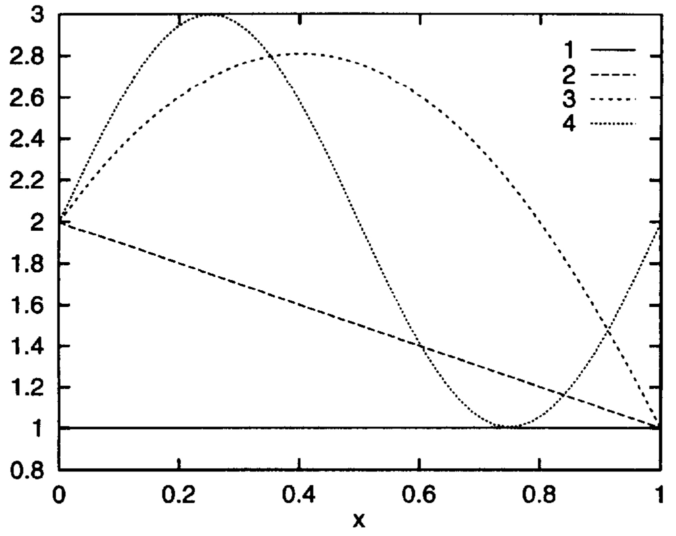
To illustrate the numerical implementation of MVI, we solve the "direct" problem for a given diffusion coefficient and thus we obtain self-consistent "experimental" over-posed boundary data (4.9) and terminal profile. We consider four different heat-conduction coefficients:

$$\lambda_1(x) = \text{const} = 1, \qquad \lambda_2(x) = 2 - x, \qquad \lambda_3(x) = 2 + 4x - 5x^2, \qquad \lambda_4(x) = 2 + \sin x, \tag{5.1}$$

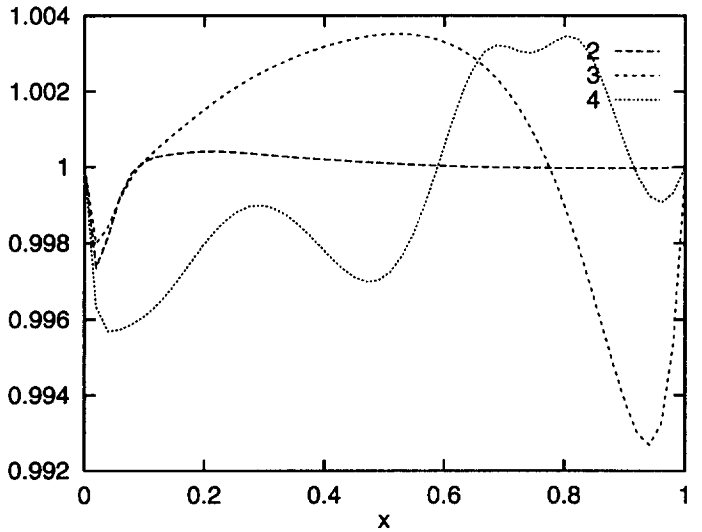
and they are shown in Figure 3a.

The accuracy of the difference scheme and algorithm developed here are checked with the mandatory tests involving different grid spacing τ and h, and different increments of the artificial time σ. We conducted a number of calculations with different values of mesh parameters and verified the practical convergence and the $O(\tau^2 + h^2)$ approximation of the difference scheme.

The first numerical experiment was to verify that the fourth-order elliptic problem for a given coefficient and consistent boundary data had the same solution as the "direct problem". We found that the iterative solution of the fourth-order problem did not depend on the magnitude of the increment σ of the artificial time. The optimal value turned out to be $\sigma = 0.05$. After



(a) The identified shape of the coefficient $\lambda(x)$.



(b) Ratio between the identified and the true coefficient.

Figure 3. Results of identification with $T = 1$, $l = 1$, $h = 0.02$, $\tau = 0.02$, $\varepsilon = 5 \cdot 10^{-8}$ for four different coefficients (5.1): $1 - \lambda_1(x)$, $2 - \lambda_2(x)$, $3 - \lambda_3(x)$, $4 - \lambda_4(x)$.

the convergence of the "inner" iteration of the coordinate-splitting scheme, the obtained solution coincided with the "direct" solution within the truncation error of the scheme.

The second numerical experiment was to verify the approximation of the scheme for identification of the coefficient with the field u considered as known from the solution of the "direct" problem. Once again, the result was in very good agreement within the truncation error.

Then the global iterative process can be started. The convergence of the "global" iterations does not necessarily follow from the correctness of the intermediate steps discussed above . For boundary data which is not self-consistent, the "global" iteration can converge to a solution which has little in common with a solution of the heat-conduction equation.

Figure 3b is shown to be the ratio of the identified and "true" coefficient. The differences for $\lambda_1 = 1$ are very small and are not shown in the figure. For smaller τ and h, the differences are graphically indistinguishable.

6. CONCLUSIONS

In the present paper, we have displayed the performance of the technique called Method of Variational Imbedding (MVI) for solving the inverse problem of coefficient identification in parabolic equation from over-posed data. The original inverse problem is replaced by the minimization problem for the quadratic functional of the original equation. The Euler-Lagrange equations for minimization comprise a fourth order in space and second order in time elliptic equation for the temperature, and a second order in space equation for the unknown coefficient. For this system, the boundary data is not over-posed. It is shown that the solution of the original inverse problem is among the solutions of the variational problem, i.e., the inverse problem is embedded into a higher order but well-posed elliptic boundary value problem ("imbedding problem"). The imbedding problem possesses a unique solution which means that when the imbedding functional is zero, the over-posed data is consistent, and the solution of the imbedding problem coincides with the sought solution of the inverse problem. Featuring examples are elaborated numerically with four different coefficients through solving the direct problem with given coefficient and preparing the over-posed boundary data for the imbedding problem. The numerical results confirm that the solution of the imbedding problem coincides with the direct simulation of the original problem within the truncation error $O(\tau^2 + h^2)$.

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