
METHOD OF VARIATIONAL IMBEDDING
FOR IDENTIFICATION OF HEAT-CONDUCTION
COEFFICIENT FROM OVERPOSED BOUNDARY DATA

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We consider the inverse problem of identifying a spatially varying coefficient in diffusion equation from overspecified boundary conditions. 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 presenting the necessary conditions for minimization of the quadratic functional of the original equations. The latter is well-posed for redundant data at boundaries. The equivalence of the two problems is demonstrated. In the recent authors' works difference scheme and algorithm have been created to apply MVI to the problem under consideration. In the present work we show that the number of boundary conditions can be decreased, replacing them with the so-called "natural conditions" for minimization of a functional. A difference scheme of splitting type is employed and featuring examples are elaborated numerically.

Keywords: inverse problem, coefficient identification, diffusion equation

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1. INTRODUCTION

The attention attracted by the ill-posed (inverse, incorrect, etc.) problems constantly increases during the last decade because of their practical importance. The optimization of technological processes and identification of material properties

yield as a rule mathematical problems in which initial or boundary conditions are missing (or overdetermined), while additional information is available for the needed solution (or additional unknown functions are present).

At the same time the incorrect problems have a great potential for inciting the development of the applied mathematics itself. According to [1]: "The analysis of inverse problems is of relevant importance for mathematical modelling and, in general, for applied mathematics. With this in mind, the applied mathematician should attempt the solution of problems without artificial simplification, which may obscure the information he hopes to obtain from the real system."

Naturally, the whole variety of the mentioned "non-standard" problems goes well beyond the framework of the Hadamard's [10] definition of incorrect problem. His definition does not cover all of them and is pertinent only to stability of a solution. For this reason, when we speak of "inverse problems," we mean the whole set of problems which are unusually or inconveniently posed. To distinguish from the problems for which Hadamard's definition applies, we shall call the latter "incorrect in the sense of Hadamard." In this instance we shall follow the classification from [1].

The work of Hadamard spurred significant activity for creating regularizing procedures (see, e.g., [15]) for the problems that are incorrect in the sense of Hadamard, e.g. for smoothing the data in order to evade the instability provoked by the pollution of the data. Such an approach has an important implication for the practical problems. At the same time the very notion of replacing the ill-formulated (e.g., ill-specified and inverse) or ill-posed by a well-formulated mathematical problem is of not lesser importance. Indeed, if one succeeds in doing so, one arrives at a problem that is also correct in the sense of Hadamard and then it is automatically regularizing the data if some pollution is present. To this end the Method of Variational Imbedding (MVI — for brevity) was proposed by the second author of the present paper. The idea of MVI is to replace an incorrect problem with the well-posed problem for minimization of quadratic functional of the original equations, i.e. we "embed" the original incorrect problem in a higher-order boundary value problem which is well-posed. For the latter a difference scheme and numerical algorithm for its implementation can easily be constructed.

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); 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 [14, 11], called "quasi-reversibility method" (see also [15]). Apart from being inverse, the second and the third problems are also incorrect in the sense of Hadamard (see [10]). 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. This is the aim of

the present paper. We make use of the above mentioned MVI technique, 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.

The first application of MVI was to the problem of identification of homoclinic trajectories as an inverse problem [2] (see also the ensuing works [8, 7]). The way to treat the classical inverse problems by means of MVI was sketched in [3-5]. In the recent authors' work [9] difference scheme and algorithm have been created to apply MVI to the problem under consideration. In the present work we show that the number of boundary conditions can be decreased replacing them with the so-called "natural conditions" for minimization of a functional. 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 the (1+1)-D equation of heat conduction

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

in the domain, shown in Fig. 1. The initial and boundary conditions are

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

$$u(t, 0) = f(t), \quad u(t, l) = g(t), \quad (2.3)$$

that are to match continuously, i.e.

$$f(0) = u_0(0), \quad g(0) = u_0(l). \quad (2.4)$$

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 a known positive function.

Suppose that the coefficient λ is unknown. In order to identify it, one needs more information. We consider here the case when a "terminal" condition is known:

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

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. In the recent authors' work [9] we consider the case when the heat fluxes at boundaries are known functions of time, namely,

$$\lambda(0) \frac{\partial u}{\partial x} \Big|_{x=0} = \psi(t), \quad \lambda(l) \frac{\partial u}{\partial x} \Big|_{x=l} = \phi(t). \quad (2.6)$$

The goal of the present work is to show that the number of boundary conditions can be decreased as compared to (2.6). More precisely, we shall consider here the problem when only the values of the unknown coefficient $\lambda(x)$:

$$\lambda(0) = \lambda^0, \quad \lambda(l) = \lambda^l, \quad (2.7)$$

are prescribed in the boundary points.

3. METHOD OF VARIATIONAL IMBEDDING

We replace the original problem (2.1) by the problem of minimization of the following functional:

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

where u must satisfy the conditions (2.2), (2.3). The 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 conditions for minimization of (3.1) are the Euler-Lagrange equations for the functions $u(t, x)$ and $\lambda(x)$. The equation for u reads

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

This 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 $t = T$. It is of fourth order with respect to the spatial variable x and its solution must satisfy the four conditions at the spatial boundaries — the original boundary conditions (2.3) and the so-called *natural conditions* for minimization of the functional \mathcal{I} :

$$\mathcal{A}u \equiv -\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left[\lambda(x) \frac{\partial u}{\partial x} \right] = 0 \quad \text{for } x = 0, l. \quad (3.3)$$

The problem is coupled by the Euler-Lagrange equation for λ , namely (see [4]):

$$\frac{d}{dx} F(x) \frac{d\lambda}{dx} + G(x)\lambda = K(x), \quad (3.4)$$

where

$$F(x) \equiv \int_0^T u_x^2 dt, \quad G(x) \equiv \int_0^T u_x u_{xxx} dt, \quad K(x) \equiv \int_0^T u_{tx} u_x dt, \quad (3.5)$$

with the boundary conditions (2.7).

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 Fig. 2). For the grid spacings we have $h = l/(N - 3)$, $\tau = T/(M - 1)$, where N is the total number of grid lines in the spatial direction, $M - 1$ in the temporal direction, and the grid lines are defined as follows:

$$x_j = (j - 2)h, \quad j = 1, \dots, N; \quad t_i = (i - 1)\tau, \quad i = 1, \dots, M, \quad (4.1)$$

We employ symmetric central differences for the operators

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

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

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 to the second order of accuracy as follows:

$$\begin{aligned} F_j &\stackrel{\text{def}}{=} \tau \left[\frac{1}{2} \left(\frac{u_{1,j+2} - u_{1,j}}{2h} \right)^2 + \frac{1}{2} \left(\frac{u_{M,j+2} - u_{M,j}}{2h} \right)^2 + \sum_{i=2}^{M-1} \left(\frac{u_{i,j+2} - u_{i,j}}{2h} \right)^2 \right] \\ &= \int_0^T (u_x)^2 + O(\tau^2 + h^2), \quad j = 1, 2, \dots, N-2; \end{aligned} \quad (4.4)$$

$$\begin{aligned} G_j &\stackrel{\text{def}}{=} \tau \left[\frac{1}{2} \left(\frac{u_{1,j+1} - u_{1,j}}{h} \right) \left(\frac{u_{1,j+2} - 3u_{1,j+1} + 3u_{1,j} - u_{1,j-1}}{h^3} \right) \right. \\ &+ \frac{1}{2} \left(\frac{u_{M,j+1} - u_{M,j}}{h} \right) \left(\frac{u_{M,j+2} - 3u_{M,j+1} + 3u_{M,j} - u_{M,j-1}}{h^3} \right) \\ &+ \left. \sum_{i=2}^{M-1} \left(\frac{u_{i,j+1} - u_{i,j}}{h} \right) \left(\frac{u_{i,j+2} - 3u_{i,j+1} + 3u_{i,j} - u_{i,j-1}}{h^3} \right) \right] \\ &= \int_0^T u_x u_{xxx} + O(\tau^2 + h^2), \quad j = 2, 3, \dots, N-2; \end{aligned} \quad (4.5)$$

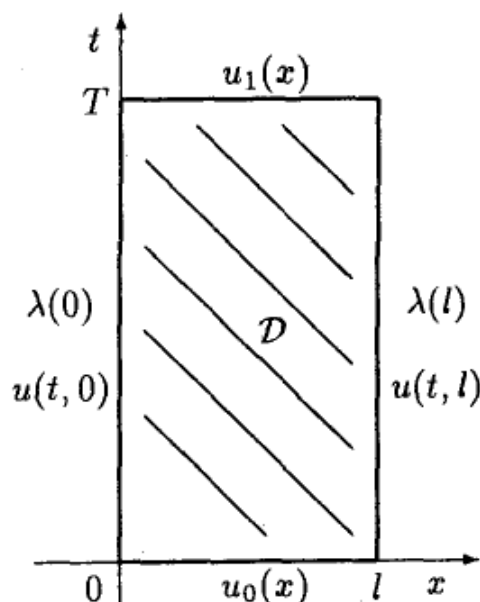


Fig. 1. Sketch of the domain

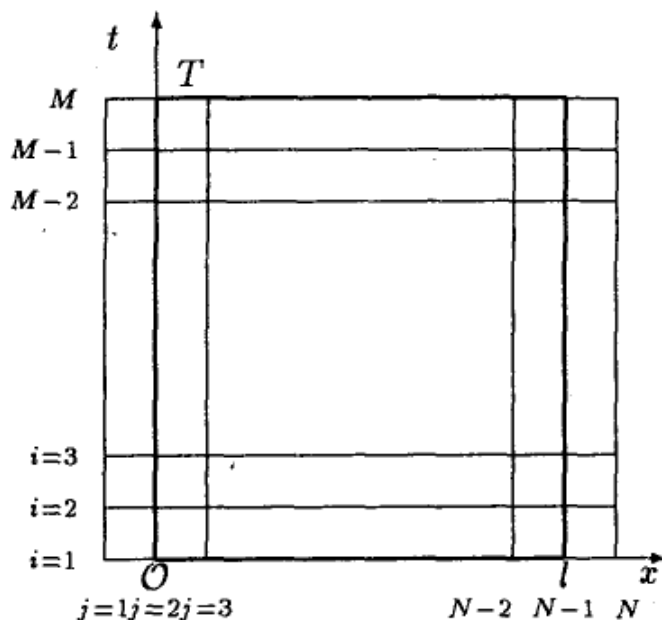


Fig. 2. Grid pattern

$$K_j \stackrel{\text{def}}{=} \frac{1}{2} \left[\left(\frac{u_{M,j+1} - u_{M,j}}{h} \right)^2 - \left(\frac{u_{1,j+1} - u_{1,j}}{h} \right)^2 \right], \quad j = 2, 3, \dots, N-2. \quad (4.6)$$

4.2. THE SCHEME FOR THE "DIRECT" PROBLEM

In order to gather "experimental" data for the "terminal" condition (2.5), 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,

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

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

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

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:

$$-\frac{1}{\tau^2} (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + \Lambda_{xxxx} u_{i,j} = 0. \quad (4.9)$$

Upon introducing a fictitious time, the equation (4.9) adopts the form of a parabolic difference equation for which the implicit time stepping reads

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\sigma} = \Lambda_{tt} u_{i,j}^n - \Lambda_{xxxx} u_{i,j}^n, \quad (4.10)$$

where the notation Λ_{tt} stands for the second time difference, which enters (4.9). Then the splitting is enacted as follows:

$$\frac{\tilde{u}_{i,j} - u_{i,j}^n}{\sigma} = \Lambda_{tt} \tilde{u}_{i,j} - \Lambda_{xxxx} u_{i,j}^n, \quad \frac{u_{i,j}^{n+1} - \tilde{u}_{i,j}}{\sigma} = -\Lambda_{xxxx} [u_{i,j}^{n+1} - u_{i,j}^n], \quad (4.11)$$

where $\tilde{u}_{i,j}$ is called "half-time-step variable." The latter can be readily excluded, which yields the following $O(\sigma^2)$ approximation of (4.10):

$$B \frac{u_{i,j}^{n+1} - u_{i,j}^n}{\sigma} = \Lambda_{tt} u_{i,j}^n - \Lambda_{xxxx} u_{i,j}^n, \quad (4.12)$$

where $B = (E - \sigma^2 \Lambda_{tt} \Lambda_{xxxx})$ is an operator whose norm is always greater than one. This means that the splitting scheme is even more stable than the general implicit scheme (4.10).

4.4. THE SCHEME FOR THE COEFFICIENT

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

$$\frac{1}{h^2} [F_j \lambda_{j+1} - (F_j + F_{j-1}) \lambda_j + F_{j-1} \lambda_{j-1}] + G_j \lambda_j = K_j, \quad (4.13)$$

where F_j , G_j and K_j , are defined in (4.4), (4.5) and (4.6), respectively.

4.5. GENERAL CONSEQUENCES OF THE 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 obtained in (I) "experimentally observed" values of the $u_1(x)$, the fourth-order boundary value problem (4.11) is solved for the function u . The iterations with respect to the fictitious time are terminated when

$$\max_{i,j} |(u_{i,j}^{n+1} - u_{i,j}^n)/u_{i,j}^n| < \varepsilon.$$

- (III) The current iteration for the function $\lambda(x)$ is calculated from (4.13). If the difference between the new and the old $\lambda(x)$ is less than ε , then the calculations are terminated, otherwise one returns to (II).

5. NUMERICAL EXPERIMENTS

The first numerical experiment was to verify that the fourth-order elliptic problem for a given coefficient and consistent boundary data has the same solution as the "direct problem." We found that the iterative solution of the fourth-order problem does not depend on the magnitude of the increment σ of the artificial time. The optimal value turned out to be $\sigma = 0.05$. After 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 a 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 above discussed intermediate steps. For boundary data, which are not self-consistent, the "global" iteration can converge to a solution which has little in common with a solution of the heat-conduction equation.

To illustrate the numerical implementation of MVI, we solved the "direct" problem for a given diffusion coefficient and thus we obtained the self-consistent "experimental" over-posed terminal profile (2.5) at $t = T$.

The accuracy of the developed here difference scheme and algorithm were 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 results confirmed the full approximation of the scheme (no dependence on σ) and the $O(h^2 + \tau^2)$ approximation.

To illustrate the accuracy and efficiency of the scheme, we considered the heat-conduction coefficient

$$\lambda(x) = x^2 + 1, \quad (5.1)$$

whose profile is shown in Fig. 3a. For smaller τ and h the differences are graphically indistinguishable. In Fig. 3b the ratio of the identified and "true" coefficient is shown, i.e.

$$r = \frac{\lambda_{\text{identified}}}{\lambda_{\text{true}}} \quad (5.2)$$

for different grids: $h = \tau = 1/64, 1/128, 1/256$.

A very serious test for the algorithm was the identification of a broken heat-conduction coefficient

$$\lambda(x) = \begin{cases} c_1 = \text{const} = 1 & \text{for } 0 < x < 0.3, \\ c_2 = \text{const} = 1.1 & \text{for } 0.3 < x < 0.7, \\ c_1 = \text{const} = 1 & \text{for } 0.7 < x < 1. \end{cases} \quad (5.3)$$

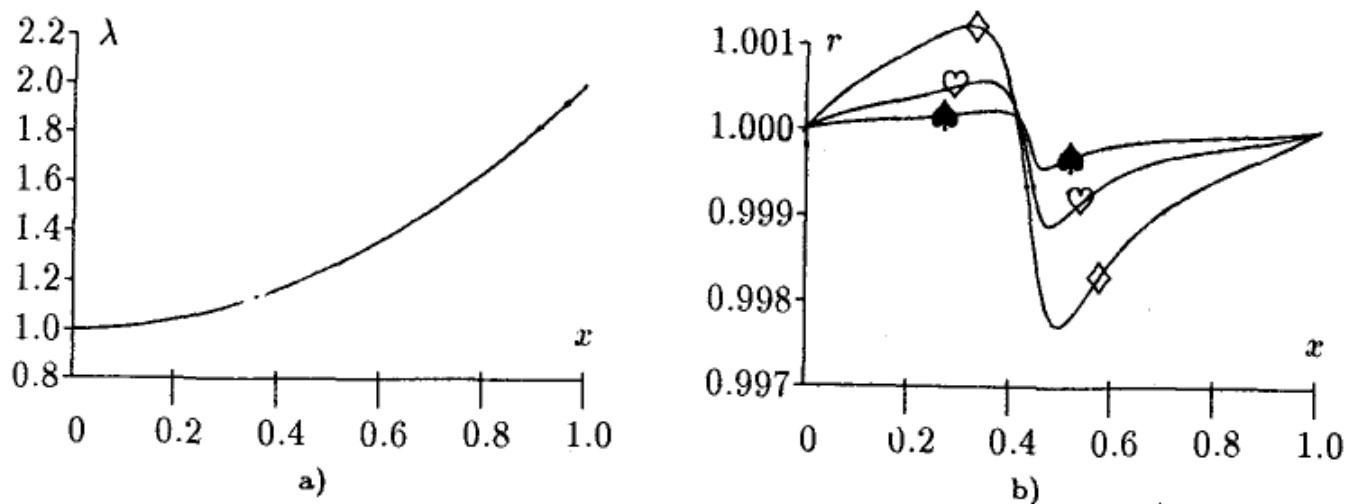


Fig. 3. Results of identification with $T = 1$, $l = 1$, $\varepsilon = 5 \cdot 10^{-8}$ for three different grid steps: a) the identified shape of the coefficient $\lambda(x)$; b) the ratio between the identified and the true coefficient: $\diamond - h = \tau = 1/64$, $\heartsuit - h = \tau = 1/128$, $\spadesuit - h = \tau = 1/256$

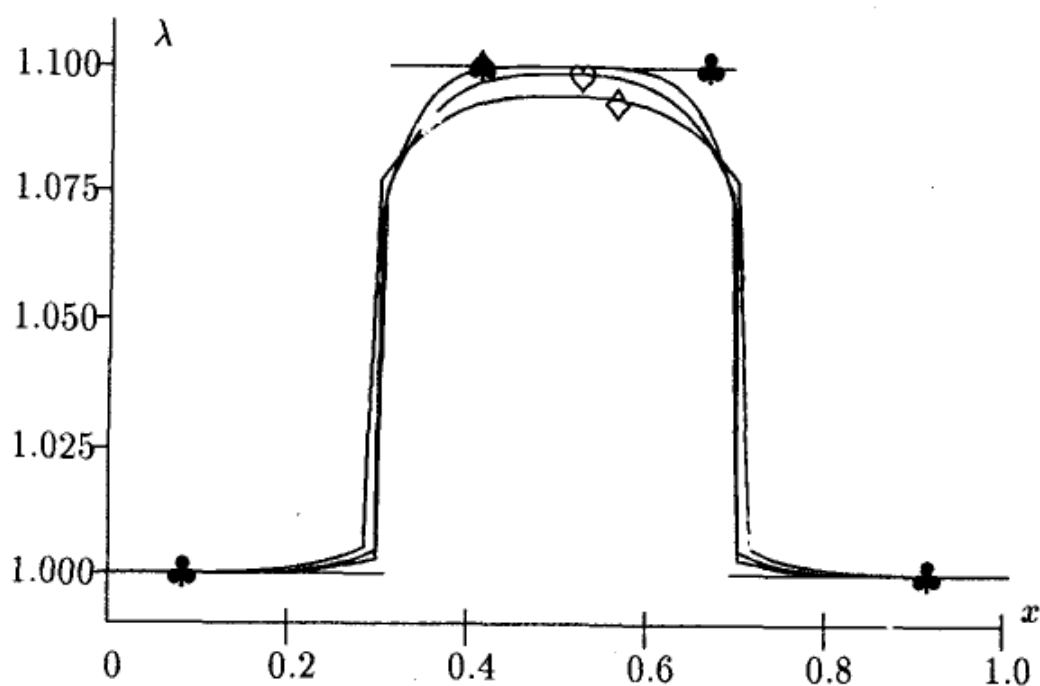


Fig. 4. Shapes of the identified and the true coefficient (5.3) for three different grid steps: \clubsuit - the true coefficient, $\diamond - \tau = 1/128$, $h = 1/64$, $\heartsuit - \tau = 1/256$, $h = 1/128$, $\spadesuit - \tau = 1/512$, $h = 1/256$

In Fig. 4 the shape of the "true" coefficient and the shapes of the three identified with different mesh-spaces coefficients are shown. The values of these coefficients are $\tau = 1/128$, $h = 1/64$, $\tau = 1/256$, $h = 1/128$ and $\tau = 1/512$, $h = 1/256$, respectively.

In Fig. 5 the ratios of the identified and "true" coefficient are shown.

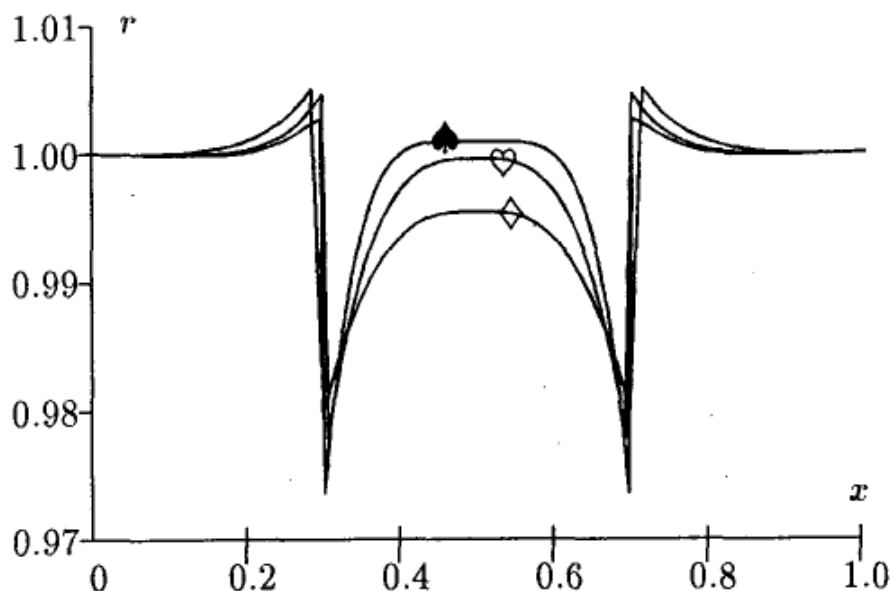


Fig. 5. Ratio between the identified and the true coefficient (5.3) for three different grid steps:
 $\diamond - \tau = 1/128, h = 1/64$, $\heartsuit - \tau = 1/256, h = 1/128$, $\spadesuit - \tau = 1/512, h = 1/256$

6. CONCLUSIONS

In the present paper we have displayed the performance of 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 imbedded into a higher-order but well posed elliptic boundary value problem ("imbedding problem"). In the present work we show that the number of boundary conditions can be decreased replacing them with the so-called "natural conditions" for minimization of a functional. Featuring examples are elaborated numerically with two different coefficients through solving the direct problem with a 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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