Identification the Unknown Coefficient in Ordinary Differential Equations via Method of Variational Imbedding

T. T. Marinov * C. I. Christov †

Abstract

We explore the practicability of the Method of Variational Imbedding (MVI) for identification the coefficient in ordinary differential equation from over-posed boundary data. The inverse problem is replaced by the higher–order boundary value problem for the Euler equations for minimization of the quadratic functional of the original system. The imbedding problem is correct in the sense of Hadamard and consists of an explicit equation for the unknown coefficient. The existence and uniqueness of solution of the imbedding problem is demonstrated and a difference scheme is proposed for its numerical solution. The performance of the technique is demonstrated for three different problems. Comparisons with the "direct" and "inverse" solutions where available are quantitatively very good. Relevant numerical examples are included.

Key words: Inverse problems of ODE, Variational methods.

AMS subject classifications: 34A55, 76M30.

1 Introduction

Most mathematical problems in science, technology and medicine are inverse problems, which often are ill-posed in the sense of J. Hadamard [7]. The optimization of technological processes and identification of material properties yields as a rule mathematical problems in which initial or boundary conditions are missing (or overdetermined) while additional information is available for the supposed solution (or additional unknown functions are present). According to [1] "an initial-boundary-value problem is *inverse* if some information on the initial and/or boundary conditions needed for solution or/and on the parameters that characterize the model are missing and are replaced by suitable information on the solution of the mathematical problem".

The work of Hadamard spurred significant activity for creating regularizing procedures (see, e.g., [10]) 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 was proposed by the second author. 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.

*Dept. of El. Eng., SIT, 1690 Fusaiji, Okabe, Saitama 369-0293, Japan, E-mail: marinov@sit.ac.jp
†Dept. of Math., USL, Lafayette, LA 70504-1010, USA, E-mail: christov@usl.edu

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The first application of MVI was for identification of localized solutions (homoclinics of Lorenz system) [2]. Later on it was applied also to the more complicated case of homoclinics and heteroclinics [3] of Kuramoto-Sivashinsky equation. Note that the MVI does not require introduction of higher-order derivatives multiplied by artificial small parameter as it is the case with "quasi-reversibility method" [10, 8]. In the recent authors' work [6] a difference scheme and algorithm are created to apply MVI to the classical problem of identification of heat-conduction coefficient as function of the spatial coordinate from overdetermined boundary data which are functions of time. The most straightforward application of MVI for identification of boundary-layer thickness is proposed in [5] where the equation for the longitudinal component of the velocity is treated separately as a parabolic equation with unknown coefficient and the continuity equation is added in an explicit manner.

2 Posing the problem

Consider the one-dimensional problem:

(1) $$\mathcal{A}u = \frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right) = f(x)$$

(2) $$u(0) = \alpha_0, \qquad u(1) = \alpha_1,$$

(3) $$u'(0) = \beta_0, \qquad u'(1) = \beta_1.$$

If the coefficient σ is given the problem (1), (2), (3) is over-posed, i.e. for arbitrary $f(x)$, σ, α_0, α_1, β_0 and β_1, there may be no solution $u(x)$ satisfying all of the conditions (2) and (3). On the other hand, when

(4) $$\sigma(x) = \begin{cases} c_1 = \text{const} & \text{for} \quad 0 < x < \xi_0 \\ c_2 = \text{const} & \text{for} \quad \xi_0 < x < 1 \end{cases} .$$

where c_1 and c_2 are not known a priori and the point ξ_0 is given, then under certain conditions it may be possible to find a coefficient $\sigma(x)$ such that the problem (1) has a unique solution $u(x)$ and this solution also satisfies (2) and (3). In this case we say that the pair of functions (u, σ) constitute a solution to the inverse problem (1), (2) and (3).

3 Variational imbedding

Following the MVI we replace the original problem by the problem of minimization of the functional

(5) $$\mathcal{I}(u,\sigma) = \int_0^1 [\mathcal{A}u]^2\,\mathrm{d}x = \int_0^1 \left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right) - f(x)\right]^2 \mathrm{d}x \to \min ,$$

where u must satisfy the conditions (2), (3) and σ must be composed from two unknown constant (the break-point is known). 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 (1) and the minimization problem (5).

The necessary condition for minimization of (5) are the Euler(-Lagrange) equations for the functions $u(x)$ and σ. The equation for u reads

(6) $$\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right) - f(x)\right] = 0$$

This equation is of fourth order and its solution can satisfy the four conditions at the boundaries. In this reason the problem (6), (2), (3) is well-posed if coefficient σ is given.

The problem is coupled by the equation for σ. The interval $(0,1)$ is split into two parts $(0,\xi_0)$ and $(\xi_0,1)$. In the each of them

(7) $$\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}}{\mathrm{d}x} \equiv \sigma\frac{\mathrm{d}^2}{\mathrm{d}x^2},$$

which is not true in the whole interval. This allow us to write the functional (5) in the next form

(8) $$\mathcal{I} = \left(\int_0^{\xi_0} (u'')^2\mathrm{d}x\right) c_1^2 - \left(2\int_0^{\xi_0} u'' f\mathrm{d}x\right) c_1 + \left(\int_{\xi_0}^1 (u'')^2\mathrm{d}x\right) c_2^2 - \left(2\int_{\xi_0}^1 u'' f\mathrm{d}x\right) c_2 + \left(\int_0^1 f^2\mathrm{d}x\right) ,$$

The essence of the MVI in the problem under consideration is the equation for σ, which after fairly obvious manipulations involving adopts the form:

(9) $$c_1 = \frac{\int_0^{\xi_0} u'' f \mathrm{d}x}{\int_0^{\xi_0} (u'')^2 \mathrm{d}x}, \qquad c_2 = \frac{\int_{\xi_0}^1 u'' f \mathrm{d}x}{\int_{\xi_0}^1 (u'')^2 \mathrm{d}x}.$$

4 Existence and uniqueness of solution

Let us consider now the space $H([0,1])$ comprised by the functions $\alpha(x)$ which are defined for all $x \in [0,1]$ and satisfy the following conditions

(10) $$\alpha(0) = \alpha'(0) = \alpha(1) = \alpha'(1) = 0\,,$$

The following scalar product is introduced in $H([0,1])$

(11) $$[\alpha, \beta] = \int_0^1 \left(\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}\alpha}{\mathrm{d}x}\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}\beta}{\mathrm{d}x}\right)\mathrm{d}x\,.$$

The equation (11) is a scalar product since

(12) $$[\alpha, \alpha] = \int_0^1 \left(\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}\alpha}{\mathrm{d}x}\right)^2 \mathrm{d}x = c_1^2\int_0^{\xi_0}\left(\frac{\mathrm{d}^2\alpha}{\mathrm{d}x^2}\right)^2 \mathrm{d}x + c_2^2\int_{\xi_0}^1\left(\frac{\mathrm{d}^2\alpha}{\mathrm{d}x^2}\right)^2 \mathrm{d}x$$

and the only solution of the Cauchy's problems

(13) $$\sigma\frac{\mathrm{d}^2\alpha}{\mathrm{d}x^2} = 0\,, \qquad \alpha(0) = \alpha'(0) = 0\,, \qquad \text{for} \quad x \in [0, \xi_0]\,,$$

(14) $$\sigma\frac{\mathrm{d}^2\alpha}{\mathrm{d}x^2} = 0\,, \qquad \alpha(1) = \alpha'(1) = 0\,, \qquad \text{for} \quad x \in [\xi_0, 1]\,,$$

is the trivial one, i.e. $[\alpha, \alpha] = 0$ is true only when $\alpha(x) \equiv 0$.

The space $H([0,1])$ with scalar product (11) is a Hilbert space.

Let us introduce the sufficiently times differentiable functions $\chi(x)$ defined for $x \in [0,1]$ and satisfying the boundary conditions (2), (3). Then, a *generalized solution* of (6), (2), (3) is called any function u for which the following expression holds true

(15) $$[u, \Phi] = \int_0^1 \left(\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}\Phi}{\mathrm{d}x}\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right)\mathrm{d}x = -\int_0^1 \sigma\frac{\mathrm{d}\Phi}{\mathrm{d}x}\frac{\mathrm{d}f}{\mathrm{d}x}\mathrm{d}x$$

for all $\Phi \in H([0,1])$ and $(u - \chi) \in H([0,1])$. It is easily seen that the classical solution of (6), (2), (3) is also a generalized solution. We multiply equation (6) by Φ and integrate over the domain $[0,1]$ to obtain

$$0 = \int_0^1 \Phi\left\{\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right) - f(x)\right]\right\}\mathrm{d}x$$

$$= \left\{\sigma\Phi\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right) - f(x)\right]\right\}\Bigg|_0^1 - \int_0^1 \sigma\frac{\mathrm{d}\Phi}{\mathrm{d}x}\left\{\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right)\right]\right\}\mathrm{d}x + \int_0^1 \sigma\frac{\mathrm{d}\Phi}{\mathrm{d}x}\frac{\mathrm{d}f}{\mathrm{d}x}\mathrm{d}x$$

(16) $$= \left[\frac{\mathrm{d}(\sigma\Phi)}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right)\right]\Bigg|_0^1 + \int_0^1 \left(\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}\Phi}{\mathrm{d}x}\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\right)\mathrm{d}x + \int_0^1 \sigma\frac{\mathrm{d}\Phi}{\mathrm{d}x}\frac{\mathrm{d}f}{\mathrm{d}x}\mathrm{d}x = [u, \Phi] + \int_0^1 \sigma\frac{\mathrm{d}\Phi}{\mathrm{d}x}\frac{\mathrm{d}f}{\mathrm{d}x}\mathrm{d}x$$

where the boundary conditions for $\Phi \in H([0,1])$ are acknowledged.

The existence of a generalized solution follows from the Riesz Theorem because, as has been above shown, (11) defines a scalar product and therefore a functional.

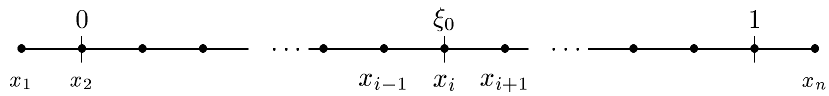


Figure 1: *The mesh*

In order to prove the uniqueness we consider the difference $\hat{u} = u_1 - u_2$ between two supposed solutions. It is obvious that $\hat{u} \in H([0,1])$. On the other hand equation (15) holds also for u_1 and u_2 and for the difference $\hat{u}$ we obtain $[\hat{u}, \Phi] = 0$. Then taking simply $\Phi \equiv \hat{u}$ we have $[\hat{u}, \hat{u}] = 0$ and then $\hat{u} \equiv (0, 0)$.

So far, it has been shown that the Euler equation (6) possess a unique solution under the boundary conditions (2), (3), provided that σ is given.

If the function u is given then the existence and uniqueness of solution of equations (9) is obvious.

It has already been shown that each of the equations (6), and (9) possesses a unique solution, when the other function is thought of as known. Hence the system (6), (9) has a unique solution. Thus the functional $\mathcal{J}$ has a stationary point because the equations (6) and (9) are necessary conditions for existing of a stationary point of a functional. On the other hand, the quadratic functional $\mathcal{J}$ is convex and this unique stationary point is the global minimum of the functional.

So far, we have proved the correctness of the linearized problem. The solution of the full nonlinear problem is obtained by means of iterations after replacing σ or u with the function calculated at the previous iteration.

5 Difference Scheme

We solving the above fourth-order boundary value problem with finite differences. The mesh (see Figure 1) is a regular and allow to approximate all operators with standard central differences with second order of approximation. It is important fact that the break-point ξ_0 must be one of grid-points.

For the grid spacing we have $h \equiv \frac{1}{n-3}$, where n is the total number of grid points. Then the gird points are defined as $x_i = (i-2)h$ for $i = 1, \ldots, n$. Let us introduce the notation $u_i = u(x_i)$ and $\sigma_i = \sigma(x)$ for $x_i \leq x < x_{i+1}$. We employ symmetric central differences for approximating the differential operator of forth order as follow:

$$\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\Big|_{x=x_i} = \frac{1}{h^4}\left[\sigma_{i-2}\sigma_i u_{i-2} - (\sigma_{i-2}\sigma_i + 2\sigma_{i-1}\sigma_i + \sigma_{i-1}\sigma_{i+1})u_{i-1}\right.$$
$$\left. +(2\sigma_{i-1}\sigma_i + \sigma_i^2 + \sigma_{i-1}\sigma_{i+1} + \sigma_{i-1}\sigma_{i+1})u_i - (\sigma_i^2 + 2\sigma_i\sigma_{i+1} + \sigma_{i+1}^2)u_{i-1} + \sigma_{i+1}^2 u_{i+2}\right] + O(h^2) \qquad (17)$$

for $i = 3, \ldots n-2$. The boundary conditions (2), (3) are approximated with second order.

The five–diagonal system is solved by means of a specialized solver [4] which is a generalization of what is called Thomas algorithm in the English-language literature or "progonka" in the Russian-language one.

In order to gather "experimental" data for the β_0 and β_1 from boundary condition (3) we solve numerically the "direct" problem (1), (2) with given $f(x)$ and σ. On the same mesh (see Figure 1) we approximate the second order differential operator as follow:

$$\frac{\mathrm{d}}{\mathrm{d}x}\sigma\frac{\mathrm{d}u}{\mathrm{d}x}\Big|_{x=x_i} = \frac{1}{h^2}\left[\sigma_{i-1}u_{i-1} - (\sigma_{i-1} + \sigma_i)u_i + \sigma_i u_{i+1}\right] + O(h^2) \qquad (18)$$

for $i = 2, \ldots n-1$. The solution algorithm allows for complete coupling of the boundary conditions (2).

General consequence of algorithm:

(I) With the obtained "experimentally observed" values of the β_0 and β_1 the fourth-order boundary value problem (6), (2), (3) is solved for function u.

(II) The current iteration for the σ is calculated from (9). If the difference between the new and old field for σ is less than ε_0 then the calculations are terminated, otherwise return to (I) with the new σ.

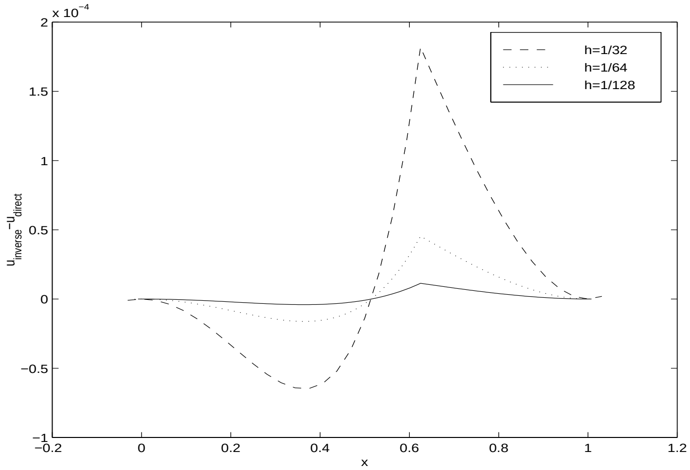


Figure 2: *Discretization error $u_{inverse} - u_{direct}$ for three different grid steps and the right–hand function $f(x) = 12x^2$ and $c_1 = c_2 = 1$.*

6 Numerical Experiments

To illustrate the numerical implementation of MVI we solve the "direct" problem for a given coefficient σ and thus we obtain self-consistent "experimental" over-posed boundary data (3). Then with the obtained in "experimentally observed" values of the β_0 and β_1 the fourth-order boundary value problem is solved. The tests show that the program works well then the jump in point ξ_0 is not a great then 300% from $\min\{c_1, c_2\}$. The accuracy of the developed here difference scheme and algorithm are checked with the mandatory tests involving different grid spacing h. We conducted a number of calculations with different values of mesh parameters and verified the practical convergence and the $O(h^2)$ approximation of the numerical solution.

In Figure 2 are shown the shapes of the difference between the numerical and the analytical solution (discretization error) for three different grid steps and the right–hand function $f(x) = 12x^2$ and $c_1 = c_2 = 1$. It is easy to seen that if $\alpha_1 = 1$ and $\alpha_2 = 2$ the solution is $u(x) = 1 + x^4$. The initial guess for this calculations is $c_1 = 1$, $c_2 = 2$ and $u(x) \equiv 1$. The values of constants c_1 and c_2 and number of iterations are given in a Table 1. It is well seen the fact that the numerical solution approximate to analytical with $O(h^2)$. The next test is with the same right side

$$f(x) = 12x^2, \qquad \alpha_0 = 0, \qquad \alpha_1 = 1, \qquad \text{and} \qquad \sigma = \begin{cases} c_1 = 1, & 0 < x < \frac{5}{8} \\ c_2 = 2, & \frac{5}{8} < x < 1 \end{cases}. \tag{19}$$

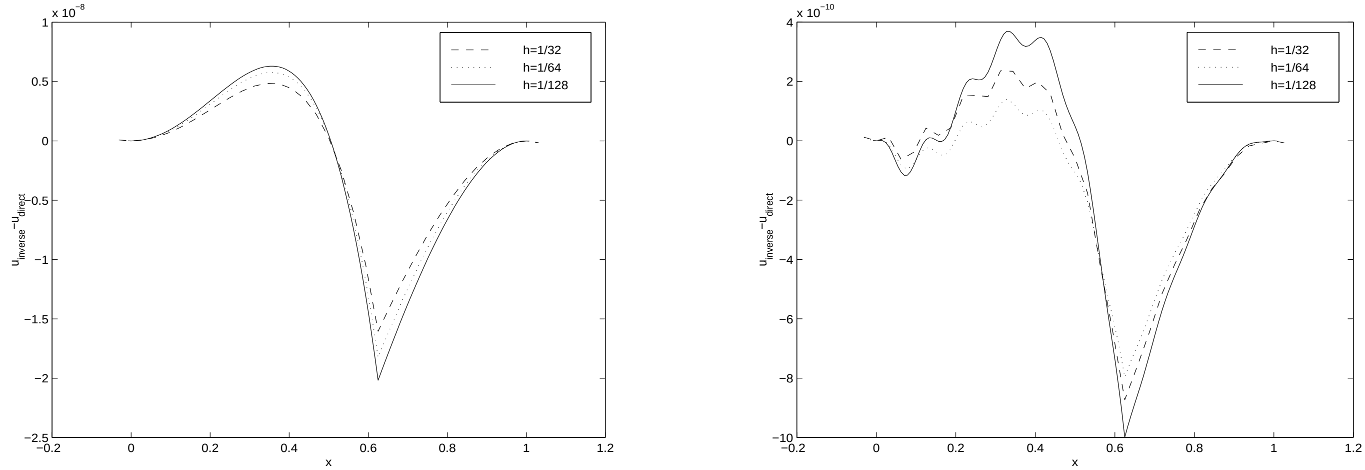
The shapes of the difference between the 'direct' and the 'inverse' solution for three different grid steps are shown in Figure 3 a). The initial guess for this calculations is $c_1 = c_2 = 1$ and $u(x) \equiv 1$. The last test is with right side and boundary conditions

$$f(x) = 5 + 4e^{-x^2} \sin 20\pi x, \qquad \alpha_0 = 0, \qquad \alpha_1 = 1 \qquad \text{and} \qquad \sigma = \begin{cases} c_1 = 1, & 0 < x < \frac{5}{8} \\ c_2 = 2, & \frac{5}{8} < x < 1 \end{cases}. \tag{20}$$

The profile of the difference between the 'direct' and the 'inverse' solution for three different grid steps are shown in Figure 3 b). The initial guess for this calculations is $c_1 = c_2 = 1$ and $u(x) \equiv 1$.

Table 1: *The values of constants c_1 and c_2 and the number of iterations for three different grid steps and the right–hand function $f(x) = 12x^2$ and $c_1 = c_2 = 1$.*

h	c_1	c_2	iterations
analytical	1	1	—
1/32	0.9963126105943	0.9995121712033	201
1/64	0.9990776818529	0.9998779325057	226
1/128	0.9997691381823	0.9999694557608	240



a) b)

Figure 3: *Discretization error for:* a) $f(x)$, α_1 *and* α_2 *given in (19);* b) $f(x)$, α_1 *and* α_2 *given in (20).*

7 Conclusions

In the present paper we have displayed the performance of the MVI for solving the inverse problem of coefficient identification in ordinary differential 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 equations for minimization comprise a fourth-order equation for the solution of original equation and an explicit 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. 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 different coefficients. The numerical results confirm that the solution of the imbedding problem coincides with the direct simulation of the original problem within the truncation error $O(h^2)$.

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