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A new shooting method for quasi-boundary regularization of backward heat conduction problems

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Abstract

A quasi-boundary regularization leads to a two-point boundary value problem of the backward heat conduction equation. The ill-posed problem is analyzed by using the semi-discretization numerical schemes. Then the resulting ordinary differential equations in the discretized space are numerically integrated towards the time direction by the Lie-group shooting method to find the unknown initial conditions. The key point is based on the erection of a one-step Lie group element $\mathbf{G}(T)$ and the formation of a generalized mid-point Lie group element $\mathbf{G}(r)$. Then, by imposing $\mathbf{G}(T) = \mathbf{G}(r)$ we can search for the missing initial conditions through a minimum discrepancy of the targets in terms of the weighting factor $r \in (0, 1)$. Several numerical examples were worked out to persuade that this novel approach has good efficiency and accuracy. Although the final temperature is almost undetectable and/or is disturbed by large noise, the Lie group shooting method is stable to recover the initial temperature very well.

Keywords: Backward heat conduction problem; Lie-group shooting method; Strongly ill-posed problem; Quasi-boundary regularization; Two-point boundary value problem; Group preserving scheme

1. Introduction

The aim of this paper is to study an ill-posed problem that emerges from the one-dimensional backward heat conduction equation, but before proceeding we recall what is meant by an ill-posed problem in partial differential equations. One may view a problem as being well-posed if a unique solution exists which depends continuously on the data; otherwise, it is an ill-posed problem. Mathematically speaking, the inverse problem is much more difficult to deal with than the direct one. In addition, the ill-posed problem is very sensitive to the measurement errors.

The backward heat conduction problem (BHCP) is a severely ill-posed problem in the sense that the solution is unstable for a given final data. In order to calculate the BHCP, there appears certain progress in this issue, including the boundary element method [1], the iterative boundary element method [2–4], the regularization technique [5,6], the operator-splitting method [7], the implicit inversion method [8], the lattice-free high-order finite difference method [9], the contraction group technique [10], the method of fundamental solutions [11] and the backward group preserving scheme [12]. A recent review of the numerical BHCP was provided by Chiwiacowsky and de Campos Velho [13].

After reformulating the BHCP by a quasi-boundary value regularization, it results in a two-point boundary-value problem (BVP) in the time-domain. Our approach of BVPs is based on the group preserving scheme (GPS) developed by Liu [14] for the integration of initial value problems (IVPs). The GPS is very effective to deal with the ordinary differential equations (ODEs) with special structures as shown by Liu [15] for stiff equations and Liu [16] for ODEs with constraints. The degree of the

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Nomenclature

$\mathbf{A}$	augmented matrix
a, b	coefficients used in Eqs. (23), (24), (27), (28), (34), (35)
$\cos\theta$	coefficient defined in Eq. (36)
$\mathbf{f}$	n-dimensional vector field
$\hat{\mathbf{f}}$	n-dimensional vector field used in Eq. (20)
$\mathbf{F}$	a vector defined in Eq. (25)
$\mathbf{g}$	$n+1$-dimensional Minkowski metric
$\mathbf{G}$	an element of Lorentz group
$\mathbf{G}_i$, $i = 1,\ldots,K$	elements of Lorentz group
G_0^0	the 00th component of $\mathbf{G}$
$h(x)$	the final data
$\mathbf{h}$	a vector defined in Eq. (9)
$\mathbf{I}_n$	n-dimensional unit matrix
l	length of a homogeneous rod
L^2	set of square-integrable functions
$\Vert\cdot\Vert$	Euclidean norm
n	number of interior grid points
$\mathbb{R}$	the set of real numbers
$\mathbb{R}^n$	n-dimensional real space
$R(i)$	random numbers
s	noise level
S	coefficient defined in Eq. (37)
$SO_o(n,1)$	$n+1$-dimensional Lorentz group
$so(n,1)$	the Lie algebra of $SO_o(n,1)$
t	time
$\hat{t}$	time used in Eq. (22)
t_k	discretized time of kth step
Δt	time increment
T	final time
u	temperature distribution
u_i	numerical value of u at the ith grid point
$\mathbf{u}$	n-dimensional vector
$\hat{\mathbf{u}}$	n-dimensional vector used in Eq. (21)
$\mathbf{u}^0$	initial temperature distribution
$\mathbf{u}^{\mathrm{f}}$	temperature distribution at final time T
$\mathbf{u}_i^0$	numerical value of $\mathbf{u}^0$ at the ith iteration
x	space variable
Δx	lattice spacing length of x
$\mathbf{X}$	$n+1$-dimensional augmented vector
$\mathbf{X}^0$	the value of $\mathbf{X}$ at the initial time
$\mathbf{X}^{\mathrm{f}}$	the numerical value of $\mathbf{X}$ at final time T
Z	coefficient defined in Eq. (39)

Greek symbols

α	regularized parameter
α_1	a positive integer
ε	a given stopping criterion
η	a coefficient defined in Eq. (31)

Subscripts and superscripts

k	index
T	transpose

ill-posedness of BHCP is over other inverse heat conduction problems including the sideways heat conduction problem, which is dealt with the reconstruction of unknown boundary conditions. The main motivation is placed on an effective solution of the BHCP, which is one of the inverse problems, and is different from the sideways heat conduction problem recently reviewed and calculated by Chang et al. [17] with the GPS.

The present paper will provide a new shooting method for the BHCP. Our approach is based on the study by Liu [18–20] with an extension applied to the solutions of multiple-dimensional and multiple targets BVPs. In [18–20] a Lie group shooting method (LGSM) is first developed by the second author to solve the BVPs of the second order ODEs. It is clear that our method can be applied to the BHCP, since we are able to search for the missing initial condition through an iterative solution of r in a compact space of $r \in (0,1)$, where the factor r is used in a generalized mid-point rule for the Lie group of one-step GPS. Another advantage is that with the application of the Lie group we can develop an effective numerical scheme, whose accuracy is much better than other numerical methods. Through this study, we may have an easy-implementation and accurate LGSM used in the calculations of the BHCP.

2. Backward heat conduction problems

We consider a homogeneous rod of length l. The rod is sufficiently thin such that the temperature is uniformly distributed over the cross section of the rod at time t. The surface of the rod is insulated and thus, there is no heat loss through the boundary. In many practical engineering application areas, we may want to recover all the past temperature distribution $u(x,t)$, where $t < T$, of which the temperature is presumed to be known at a given final time T. Here, we consider the following problem:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < l, \quad 0 < t < T, \tag{1}$$

$$u(0,t) = u_0(t), \quad u(l,t) = u_l(t), \quad 0 \leqslant t \leqslant T, \tag{2}$$

$$u(x,T) = h(x), \quad 0 \leqslant x \leqslant l. \tag{3}$$

Here these three quantities of u, x and t are normalized, such that they are dimensionless.

Eqs. (1)–(3) are called a one-dimensional backward heat conduction problem, which is known to be highly ill-posed, namely, the solution does not depend continuously on the input data $u(x,T)$. Actually, the rapid decay of temperature with time results in the fast fading memory of initial conditions. Thus, the numerical recovery of initial temperature from the data measured at time T is a rather difficult issue because of the influence of noise and computational error.

Here, we are going to calculate the BHCP by a semi-discretization method [10,17], which replaces Eq. (1) by a set of ODEs:

$$\dot{u}_i(t) = \frac{1}{(\Delta x)^2}[u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)], \tag{4}$$

where $\Delta x = l/(n+1)$, $x_i = i\Delta x$ and $u_i(t) = u(x_i, t)$. One way to solve the ill-posed problem is to perturb it into a well-posed one. A number of perturbing techniques have been proposed, including a biharmonic regularization developed by Lattés and Lions [21], and a hyperbolic regularization proposed by Ames and Cobb [22]. It seems that Showalter [23] first regularized the BHCP by considering a quasi-boundary-value approximation to the final value problem, that is, to supersede Eq. (3) by

$$\alpha u(x,0) + u(x,T) = h(x). \tag{5}$$

The problems (1), (2) and (5) can be shown to be well-posed for each $\alpha > 0$ as that done by Clark and Oppenheimer [24] for the heat conduction inverse problem. Ames and Payne [25] have investigated those regularizations from the continuous dependence of solution on the regularized parameter.

3. A new method for BHCP

Let us write

$$\mathbf{u} := \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}, \quad \mathbf{f} := \frac{1}{(\Delta x)^2}\begin{bmatrix} u_2(t) - 2u_1(t) + u_0(t) \\ u_3(t) - 2u_1(t) + u_1(t) \\ \vdots \\ u_{n+1}(t) - 2u_n(t) + u_{n-1}(t) \end{bmatrix}. \tag{6}$$

The dependence of $\mathbf{f}$ on t is owing to $u_0(t)$ and $u_{n+1}(t)$. Then Eq. (4) for $i = 1, \ldots, n$ can be expressed as a vector form:

$$\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u}, t), \quad \mathbf{u} \in \mathbb{R}^n, \quad t \in \mathbb{R}, \tag{7}$$

in which Eq. (5) as being a constraint is written to be

$$\alpha\mathbf{u}(0) + \mathbf{u}(T) = \mathbf{h}, \tag{8}$$

where

$$\mathbf{h} := \begin{bmatrix} h(x_1) \\ h(x_2) \\ \vdots \\ h(x_n) \end{bmatrix}. \tag{9}$$

We are going to develop a multi-dimensional LGSM, which aims to find the initial value $\mathbf{u}(0)$, such that the numerical solution $\mathbf{u}(T)$ can match Eq. (8) very well for arbitrary $\alpha > 0$.

3.1. The GPS

Liu [14] has embedded Eq. (7) into the following $n+1$-dimensional augmented system:

$$\dot{\mathbf{X}} := \frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{n\times n} & \frac{\mathbf{f}(\mathbf{u},t)}{\|\mathbf{u}\|} \\ \frac{\mathbf{f}^{\mathrm{T}}(\mathbf{u},t)}{\|\mathbf{u}\|} & 0 \end{bmatrix}\begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix} := \mathbf{A}\mathbf{X}, \tag{10}$$

where $\mathbf{A}$ is an element of the Lie algebra $so(n,1)$ satisfying

$$\mathbf{A}^{\mathrm{T}}\mathbf{g} + \mathbf{g}\mathbf{A} = \mathbf{0}, \tag{11}$$

with

$$\mathbf{g} = \begin{bmatrix} \mathbf{I}_n & \mathbf{0}_{n\times 1} \\ \mathbf{0}_{1\times n} & -1 \end{bmatrix} \tag{12}$$

a Minkowski metric. Here, $\mathbf{I}_n$ is the identity matrix of order n, and the superscript $^{\mathrm{T}}$ denotes the transpose. The augmented variable $\mathbf{X}$ satisfies the cone condition:

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X} = \mathbf{u}\cdot\mathbf{u} - \|\mathbf{u}\|^2 = 0. \tag{13}$$

Therefore, Liu [14] has developed a group-preserving numerical scheme as follows:

$$\mathbf{X}_{k+1} = \mathbf{G}(k)\mathbf{X}_k, \tag{14}$$

where $\mathbf{X}_k$ denotes the numerical value of $\mathbf{X}$ at the discrete time t_k, and $\mathbf{G}(k) \in SO_o(n,1)$ satisfies

$$\mathbf{G}^{\mathrm{T}}\mathbf{g}\mathbf{G} = \mathbf{g}, \tag{15}$$

$$\det\mathbf{G} = 1, \tag{16}$$

$$G_0^0 > 0, \tag{17}$$

where G_0^0 is the 00th component of $\mathbf{G}$.

3.2. Generalized mid-point rule

Applying scheme (14) to Eq. (10) with a specified initial condition $\mathbf{X}(0) = \mathbf{X}^0$, we can compute the solution $\mathbf{X}(t)$ by GPS. Assuming that the total time T is divided by K steps, that is, the time stepsize used in GPS is $\Delta t = T/K$, and starting from an initial augmented condition $\mathbf{X}^0 = ((\mathbf{u}^0)^{\mathrm{T}}, \|\mathbf{u}^0\|)^{\mathrm{T}}$, we may calculate the value $\mathbf{X}^{\mathrm{f}} = ((\mathbf{u}(T))^{\mathrm{T}}, \|\mathbf{u}(T)\|)^{\mathrm{T}}$ at time $t = T$.

By applying Eq. (14) step-by-step, we can obtain

$$\mathbf{X}^{\mathrm{f}} = \mathbf{G}_K(\Delta t)\ldots\mathbf{G}_1(\Delta t)\mathbf{X}^0, \tag{18}$$

where $\mathbf{X}^{\mathrm{f}}$ approximates the exact $\mathbf{X}(T)$ with a certain accuracy depending on Δt. However, let us recollect that each $\mathbf{G}_i$, $i = 1, \ldots, K$, is an element of the Lie group $SO_o(n,1)$, and by the closure property of the Lie group, $\mathbf{G}_K(\Delta t)\ldots\mathbf{G}_1(\Delta t)$ is also a Lie group denoted by $\mathbf{G}$. Hence, we have

$$\mathbf{X}^{\mathrm{f}} = \mathbf{G}\mathbf{X}^0. \tag{19}$$

This is a one-step transformation from $\mathbf{X}^0$ to $\mathbf{X}^{\mathrm{f}}$ [26,27], where Liu has applied the above method to estimate the temperature-dependent heat conductivity and heat capacity, and showed that the new method has high accuracy and efficiency.

We can calculate $\mathbf{G}$ by a generalized mid-point rule, which is obtained from an exponential mapping of $\mathbf{A}$ by taking the values of the argument variables of $\mathbf{A}$ at a generalized mid-point. The Lie group generated from $\mathbf{A} \in so(n,1)$ by an exponential admits a closed-form representation as follows:

$$\mathbf{G} = \begin{bmatrix} \mathbf{I}_n + \frac{(a-1)}{\|\hat{\mathbf{f}}\|^2}\hat{\mathbf{f}}\hat{\mathbf{f}}^{\mathrm{T}} & \frac{b\hat{\mathbf{f}}}{\|\hat{\mathbf{f}}\|} \\ \frac{b\hat{\mathbf{f}}^{\mathrm{T}}}{\|\hat{\mathbf{f}}\|} & a \end{bmatrix}, \tag{20}$$

where

$$\hat{\mathbf{u}} = r\mathbf{u}^0 + (1-r)\mathbf{u}^{\mathrm{f}}, \tag{21}$$

$$\hat{\mathbf{f}} = \mathbf{f}(\hat{\mathbf{u}}, \hat{t}), \tag{22}$$

$$a = \cosh\left(\frac{T\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{u}}\|}\right), \tag{23}$$

$$b = \sinh\left(\frac{T\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{u}}\|}\right). \tag{24}$$

Here, we employ the initial $\mathbf{u}^0 = (u_1(0), \dots, u_n(0))$ and the final $\mathbf{u}^{\mathrm{f}} = (u_1(T), \dots, u_n(T))$ through a suitable weighting factor r to calculate $\mathbf{G}$, where $r \in (0,1)$ is a parameter and $\hat{t} = rT$. The above method is applied by a generalized mid-point rule on the calculation of $\mathbf{G}$, and the result is a single-parameter Lie group element denoted by $\mathbf{G}(r)$.

3.3. A Lie group mapping between two points on the cone

Let us define a new vector

$$\mathbf{F} := \frac{\hat{\mathbf{f}}}{\|\hat{\mathbf{u}}\|}, \tag{25}$$

such that Eqs. (20), (23) and (24) can also be expressed as

$$\mathbf{G} = \begin{bmatrix} \mathbf{I}_n + \frac{(a-1)}{\|\mathbf{F}\|^2}\mathbf{F}\mathbf{F}^{\mathrm{T}} & \frac{b\mathbf{F}}{\|\mathbf{F}\|} \\ \frac{b\mathbf{F}^{\mathrm{T}}}{\|\mathbf{F}\|} & a \end{bmatrix}, \tag{26}$$

$$a = \cosh(T\|\mathbf{F}\|), \tag{27}$$

$$b = \sinh(T\|\mathbf{F}\|). \tag{28}$$

From Eqs. (19) and (26) it follows that

$$\mathbf{u}^{\mathrm{f}} = \mathbf{u}^0 + \eta\mathbf{F}, \tag{29}$$

$$\|\mathbf{u}^{\mathrm{f}}\| = a\|\mathbf{u}^0\| + b\frac{\mathbf{F}\cdot\mathbf{u}^0}{\|\mathbf{F}\|}, \tag{30}$$

where

$$\eta := \frac{(a-1)\mathbf{F}\cdot\mathbf{u}^0 + b\|\mathbf{u}^0\|\|\mathbf{F}\|}{\|\mathbf{F}\|^2}. \tag{31}$$

Substituting

$$\mathbf{F} = \frac{1}{\eta}(\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0) \tag{32}$$

into Eq. (30), we obtain

$$\frac{\|\mathbf{u}^{\mathrm{f}}\|}{\|\mathbf{u}^0\|} = a + b\frac{(\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0)\cdot\mathbf{u}^0}{\|\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0\|\|\mathbf{u}^0\|}, \tag{33}$$

where

$$a = \cosh\left(\frac{T\|\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0\|}{\eta}\right), \tag{34}$$

$$b = \sinh\left(\frac{T\|\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0\|}{\eta}\right) \tag{35}$$

are obtained by inserting Eq. (32) for $\mathbf{F}$ into Eqs. (27) and (28).

Let

$$\cos\theta := \frac{(\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0)\cdot\mathbf{u}^0}{\|\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0\|\|\mathbf{u}^0\|}, \tag{36}$$

$$S := T\|\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0\|, \tag{37}$$

and from Eqs. (33)–(35) it follows that

$$\frac{\|\mathbf{u}^{\mathrm{f}}\|}{\|\mathbf{u}^0\|} = \cosh\left(\frac{S}{\eta}\right) + \cos\theta\sinh\left(\frac{S}{\eta}\right). \tag{38}$$

By defining

$$Z := \exp\left(\frac{S}{\eta}\right), \tag{39}$$

we obtain a quadratic equation for $\mathbf{Z}$ from Eq. (38):

$$(1+\cos\theta)Z^2 - \frac{2\|\mathbf{u}^{\mathrm{f}}\|}{\|\mathbf{u}^0\|}Z + 1 - \cos\theta = 0. \tag{40}$$

The solution is found to be

$$Z = \frac{\frac{\|\mathbf{u}^{\mathrm{f}}\|}{\|\mathbf{u}^0\|} + \sqrt{\left(\frac{\|\mathbf{u}^{\mathrm{f}}\|}{\|\mathbf{u}^0\|}\right)^2 - 1 + \cos^2\theta}}{1+\cos\theta}, \tag{41}$$

and then from Eqs. (39) and (37) we obtain

$$\eta = \frac{T\|\mathbf{u}^{\mathrm{f}} - \mathbf{u}^0\|}{\ln Z}. \tag{42}$$

Thus, between any two points $(\mathbf{u}^0, \|\mathbf{u}^0\|)$ and $(\mathbf{u}^{\mathrm{f}}, \|\mathbf{u}^{\mathrm{f}}\|)$ on the cone, there exists a single-parameter Lie group element $\mathbf{G}(T) \in SO_o(n,1)$ mapping $(\mathbf{u}^0, \|\mathbf{u}^0\|)$ onto $(\mathbf{u}^{\mathrm{f}}, \|\mathbf{u}^{\mathrm{f}}\|)$, which is given by

$$\begin{bmatrix} \mathbf{u}^{\mathrm{f}} \\ \|\mathbf{u}^{\mathrm{f}}\| \end{bmatrix} = G\begin{bmatrix} \mathbf{u}^0 \\ \|\mathbf{u}^0\| \end{bmatrix}, \tag{43}$$

where $\mathbf{G}$ is uniquely determined by $\mathbf{u}^0$ and $\mathbf{u}^{\mathrm{f}}$ through Eqs. (26)–(28), (32) and (42).

3.4. The Lie-group shooting method

From Eqs. (25) and (32) it follows that

$$\mathbf{u}^{\mathrm{f}} = \mathbf{u}^0 + \eta\frac{\hat{\mathbf{f}}}{\|\hat{\mathbf{u}}\|}. \tag{44}$$

By Eq. (8) we attain

$$\alpha\mathbf{u}^0 + \mathbf{u}^{\mathrm{f}} = \mathbf{h}. \tag{45}$$

Eqs. (44) and (45) can be utilized to solve $\mathbf{u}^0$ as follows:

$$\mathbf{u}^0 = \frac{1}{1+\alpha}\left[\mathbf{h} - \eta\frac{\hat{\mathbf{f}}}{\|\hat{\mathbf{u}}\|}\right], \tag{46}$$

where η is calculated by Eq. (42).

The above derivation of the governing equations (44)–(46) is stemmed from by letting the two $\mathbf{F}$'s in Eqs. (25) and (32) be equal, which, in terms of the Lie group elements $\mathbf{G}(T)$ and $\mathbf{G}(r)$, is essentially identical to the specification of $\mathbf{G}(T) = \mathbf{G}(r)$. For a specified r, Eqs. (46) can be used to generate the new $\mathbf{u}^0$, until $\mathbf{u}^0$ converges according to a given stopping criterion:

$$\|\mathbf{u}^0_{i+1} - \mathbf{u}^0_i\| \leqslant \varepsilon, \tag{47}$$

which means that the norm of the difference between the $i+1$th and the ith iterations of $\mathbf{u}^0$ is smaller than a given stopping criterion ε. If $\mathbf{u}^0$ is available, we can return to Eq. (7) and integrate it to obtain $\mathbf{u}(T)$. The above process can be done for all r in the interval of $r \in (0, 1)$. Among these solutions we pick up the best r, which leads to the smallest error of Eq. (8). That is,

$$\min_{r\in(0,1)} \|\alpha\mathbf{u}^0 + \mathbf{u}^{\mathrm{f}} - \mathbf{h}\|. \tag{48}$$

In the present paper, we will use the GPS to do those integrating works.

4. Numerical examples

4.1. Example 1

In order to compare our numerical results with those obtained by Lesnic et al. [28], Mera et al. [2,3,11] and Liu et al. [12], let us first consider a one-dimensional benchmark BHCP:

$$u_t = u_{xx}, \quad 0 < x < 1,\ 0 < t < T, \tag{49}$$

with the boundary conditions

$$u(0, t) = u(1, t) = 0, \tag{50}$$

and the final time condition

$$u(x, T) = \sin(\pi x)\exp(-\pi^2 T). \tag{51}$$

The data to be retrieved is given by

$$u(x, t) = \sin(\pi x)\exp(-\pi^2 t), \quad T > t \geqslant 0. \tag{52}$$

The one-dimensional spatial domain $[0, 1]$ is discretized by $N = n + 2$ points including two boundary points, at which the two boundary conditions $u_0(t) = u_{n+1}(t) = 0$ are imposed on the totally n differential equations obtained from Eq. (4). We apply the LGSM developed in Section 3 for this backward problem of n differential equations with the final data given by Eq. (51).

Let us investigate some very severely ill-posed cases of this benchmark BHCP, where $T = 1.5, 2.5, 3$ were employed such that when the final data are in the order of $O(10^{-7})$–$O(10^{-13})$, we attempt to use the LGSM to retrieve the desired initial data of $\sin\pi x$, which is in the order of $O(1)$. Before that we use this example to demonstrate how to pick up the best r as specified by Eq. (48). We plot the error of mis-matching the target with respect to r in Fig. 1. It can be seen that there is a minimum point as marked by the black point. When the range for searching the minima is identified, we can pick up a more correct value of r by searching for the minima in a more refined range. On the other hand, we should stress that in all the calculations, we can also employ $\alpha = 0$ without any difficulty because Eq. (46) is still applicable.

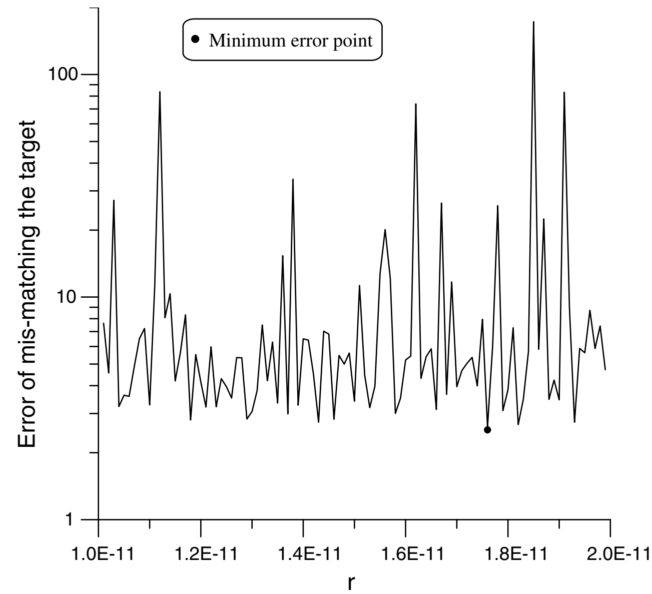

Fig. 1. For Example 1 we plot the error of mis-matching the target with respect to r.

For this very difficult problem, the method proposed by Lesnic et al. [28] was unstable when $T > 1$. Conversely, the results given by the LGSM with $\Delta x = 1/80$ and $\Delta t = 0.01$ for $T = 1.5$, and $\Delta x = 1/100$ and the same stepsize for $T = 2.5,\ 3$ were rather promising.

In Fig. 2, we present the numerical errors for these three cases. The maximum error for the case of $T = 3$ is about 2.8×10^{-3}. Liu et al. [12] have made a great progress for the computations of BHCPs by the backward group preserving scheme. For a severe case up to $T = 2.4$, they have provided a stable and accurate solution with the maximum error occurring at $x = 0.5$ about 0.008. The present results are better than that paper, even for the severe case up to $T = 3$, the maximum error occurring at $x = 0.5$ is about 0.0028.

To the authors' best knowledge, there is no open report that the numerical methods for this severely ill-posed BHCP can provide more accurate results than us. Upon compared with the numerical results computed by Mera [11] with the method of fundamental solution (MFS) together with the Tikhonov regularization technique (see Fig. 5 of the above cited paper), we can say that the LGSM is much better than the MFS.

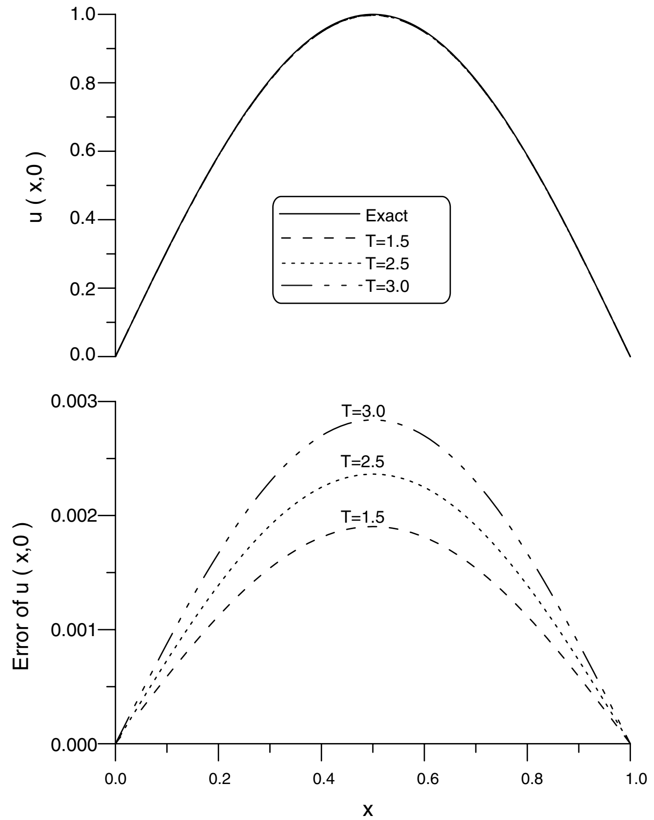

Fig. 2. Comparisons of the exact solutions and numerical solutions with final times $T = 1.5, 2.5, 3$, and the corresponding numerical errors.

4.2. Example 2

Let us then consider the one-dimensional BHCP:

$$u_t = u_{xx}, \quad 0 < x < 1, \quad 0 < t < T, \tag{53}$$

with the boundary conditions

$$u(0,t) = u(1,t) = 0, \tag{54}$$

and the initial condition

$$u(x,0) = \begin{cases} 2x, & \text{for } 0 \leqslant x \leqslant 0.5, \\ 2(1-x), & \text{for } 0.5 \leqslant x \leqslant 1. \end{cases} \tag{55}$$

The exact solution is given by

$$u(x,t) = \sum_{k=0}^{\infty} \frac{8}{\pi^2(2k+1)^2} \cos\frac{(2k+1)\pi(2x-1)}{2} e^{[-\pi^2(2k+1)^2 t]}. \tag{56}$$

The backward numerical solution is subjected to the final condition at time T:

$$u(x,T) = \sum_{k=0}^{\infty} \frac{8}{\pi^2(2k+1)^2} \cos\frac{(2k+1)\pi(2x-1)}{2} e^{[-\pi^2(2k+1)^2 T]}. \tag{57}$$

In practice, the data is attained by taking the sum of the first one hundred terms, which guarantees the convergence of the above series.

The difficulty of this problem is stemmed from that we attempt to use a smooth final data to retrieve a non-smooth initial data. In the literature, this one-dimensional BHCP is called a triangular test [5,6,13]. For this computational example, we have taken $T = 1$, $\Delta t = 0.01$ and $\Delta x = 1/50$. The accuracy as can be seen from Fig. 3(a) is rather good besides that at the turning point $x = 0.5$.

Muniz et al. [6] have calculated this example by different regularization techniques. They have shown that the explicit inversion method does not give satisfactory results even with a small terminal time with $T = 0.008$ [5]. In addition, they have calculated the initial data with a terminal time $T = 0.01$ by the Tikhonov regularization, maximum entropy principle and truncated singular value decomposition, and good results were obtained as shown in Figs. 4 and 5 of the above cited paper. However, when we apply the LGSM to this problem with $T = 0.01$, $\Delta t = 0.0001$ and $\Delta x = 1/50$, good result can be seen from Fig. 3(b). In the case of considering the temperature obtained through a measurement, we are also concerned with the stability of our method, which is investigated by adding the level of random noise on the final data: $h(x_i) \times [1 + sR(i)]$ where we use the function RANDOM_NUMBER given in Fortran to generate the noisy data $R(i)$, which are random numbers in $[-1, 1]$. The results are compared with the numerical result without considering the random noise in Fig. 4. The noise is obtained by multiplying $R(i)$ by a factor $s = 0.000039$.

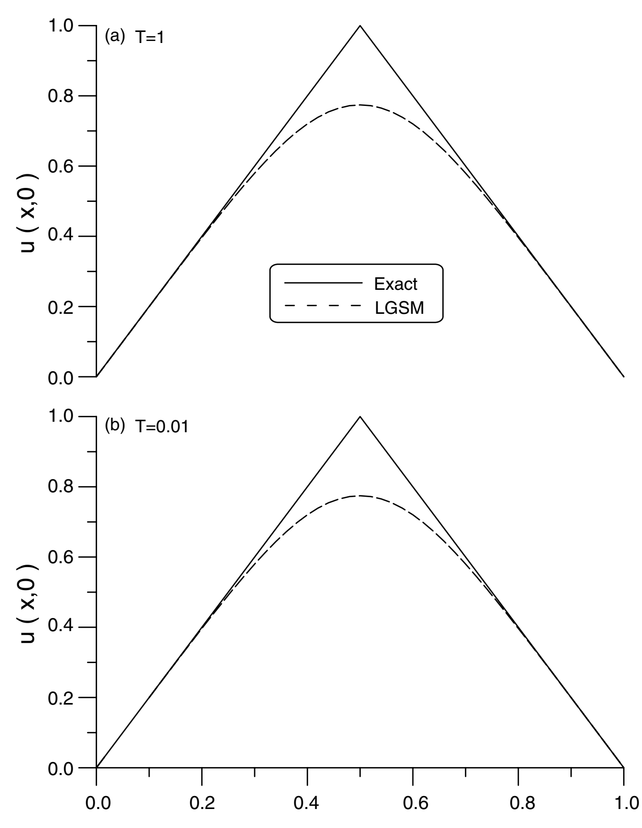

Fig. 3. For Example 2 we compare the LGSM and exact solutions with $T = 1$ in (a), and with $T = 0.01$ in (b).

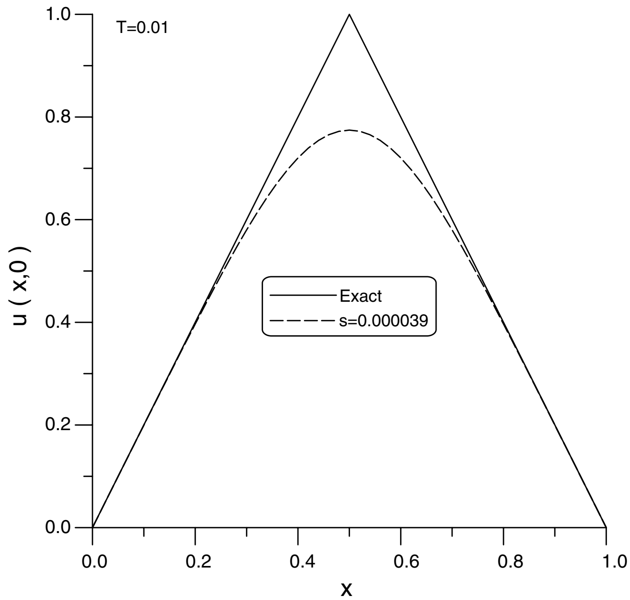

Fig. 4. For Example 2 we compare the LGSM solution under the level of noise $s = 0.000039$ with the exact solution for $T = 0.01$.

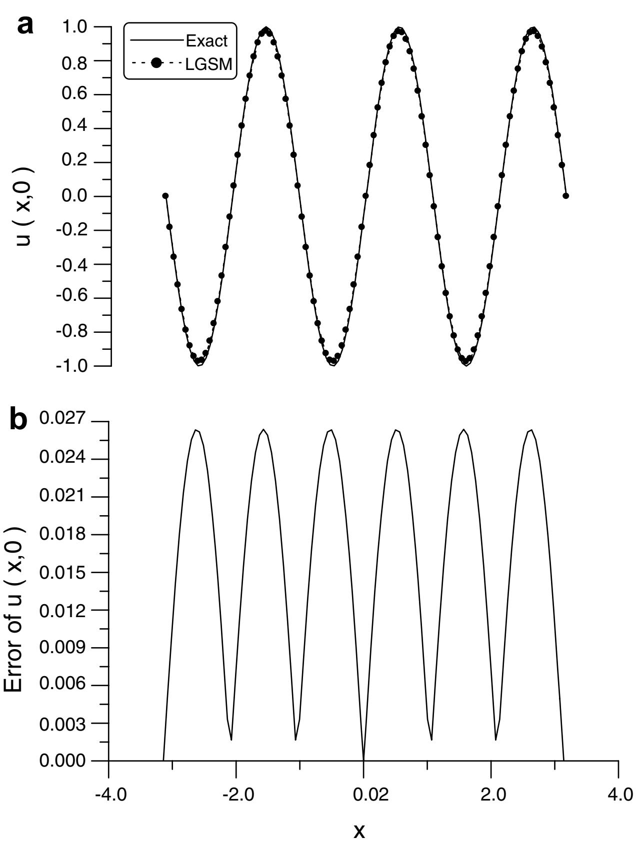

Fig. 5. For Example 3 we compare the LGSM with exact solution with $T = 1$ in (a), and plot the numerical error of $u(x, 0)$ in (b).

This example is a hard benchmark problem of BHCP to test the numerical performance of new numerical methods. From Fig. 3 it can be seen that at the middle point our method leads to bad solution. All that showing the present method still has room to ameliorate its accuracy, and we will propose another approach to attain a better result in a forthcoming paper.

4.3. Example 3

Let us further consider another one-dimensional benchmark BHCP:

$$u_t = u_{xx}, \quad -\pi < x < \pi, \quad 0 < t < T, \tag{58}$$

with the boundary conditions

$$u(-\pi, t) = u(\pi, t) = 0, \tag{59}$$

and the final time condition

$$u(x, T) = e^{-\alpha_1^2 T} \sin(\alpha_1 x). \tag{60}$$

The exact solution is given by

$$u(x, t) = e^{-\alpha_1^2 t} \sin(\alpha_1 x), \tag{61}$$

where $\alpha_1 \in \mathbb{N}$ is a positive integer.

We can demonstrate this ill-posed problem further by considering the L^2-norms of u and its final data:

$$\begin{aligned}\|u(x,t)\|_{L^2}^2 &= \int_0^T \int_{-\pi}^{\pi} [e^{-\alpha_1^2 t} \sin(\alpha_1 x)]^2 \, dx \, dt \\ &= \frac{1}{2\alpha_1^2}(e^{2\alpha_1^2 T} - 1) \int_{-\pi}^{\pi} [e^{-\alpha_1^2 T} \sin(\alpha_1 x)]^2 \, dx.\end{aligned} \tag{62}$$

Since for any $C > 0$ there exists $\alpha_1 \in \mathbb{N}$ such that $\sqrt{e^{2\alpha_1^2 T} - 1}/(\sqrt{2}\alpha_1) > C$, an inequality $\|u(x,t)\|_{L^2} > C\|u_F\|_{L^2}$ holds for any $C > 0$. This means that the solution does not depend on the final data continuously. Thus, the BHCP is unstable for a given final data with respect to the L^2-norm. The larger α_1 is, the worse is the final data depending on the solution. In other words, the problem is more ill-posed when α_1 is larger.

In Fig. 5, we present the numerical results which being compared with the exact solution (61) at time $t = 0$ for the case of $\alpha_1 = 3$ and $T = 1$. In the calculation, the grid length was taken to be $\Delta x = 2\pi/100$ and the time stepsize was taken to be $\Delta t = 0.01$.

Owing to the rather small final data in the order of $O(10^{-4})$ when comparing with the desired initial data $\sin \alpha_1 x$ of order $O(1)$ to be retrieved, Mera [11] has mentioned that it is impossible to cope with this strongly ill-posed problem by using the classical numerical approaches and requires some special techniques to be employed. However, by using the LGSM we can treat this problem very good as shown in Fig. 5(a), and the numerical error is very small in the order $O(10^{-2})$ as shown in Fig. 5(b). The current results are better than those of Liu et al. [12].

The numerical results under noise on the final data: $h(x_i) + sR(i)$ are compared with the exact result in Fig. 6, where the grid length $\Delta x = 2\pi/100$, the time stepsize $\Delta t = 0.001$, and $T = 0.5$ were chosen. It can be seen that the noise levels with $s = 0.00005$ and $s = 0.00006$ disturb the numerical solutions deviating from the exact solution

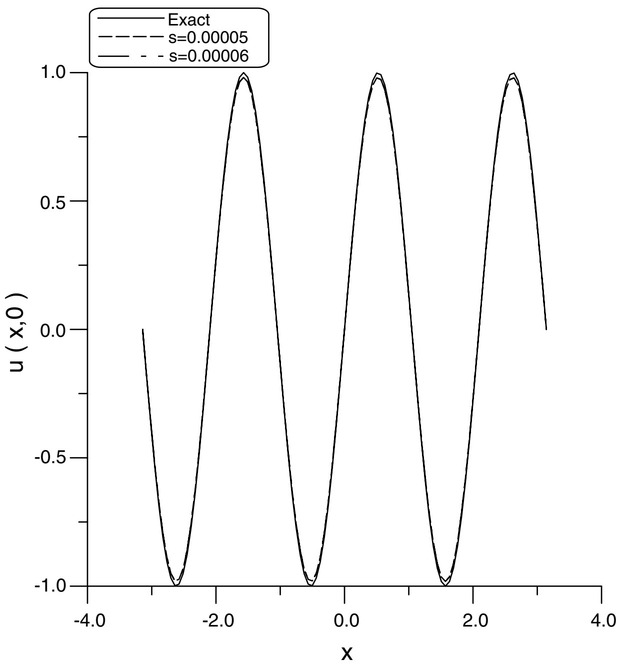

Fig. 6. For Example 3 we compare the LGSM solutions under different levels of noise $s = 0.00005, 0.00006$ with the exact solution for $T = 0.5$.

very small. However, we must stress that the noise levels as compared with the data itself are large up to 7%.

5. Conclusions

The backward heat conduction problems are formulated with a semi-discretization version. In order to evaluate the missing initial conditions for the quasi-boundary value problems of the BHCP, we have employed the Lie-group shooting method towards the time direction to derive the algebraic equations. Hence, we can solve them through a minimum solution in a compact space of $r \in (0, 1)$. Several numerical examples of the BHCP were examined to ensure that the new algorithm has a fast convergence speed on the solution of r in a pre-selected range smaller than $(0, 1)$ by using the minimum norm to fit the target equations, which usually requires only a small number of trials to select the best r. The new method is robust to against the noise disturbance. Through this paper, it can be concluded that the new shooting method is accurate, effective and stable. Its numerical implementation is very simple and the computation speed is very fast.

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