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The Lie-Group Shooting Method for Quasi-Boundary Regularization of Backward Heat Conduction Problems

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Summary

By using a quasi-boundary regularization we can formulate 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 $\mathbf{G}(\mathsf{T})$ and the formation of a generalized mid-point Lie group element $\mathbf{G}(\mathsf{r})$. Then, by imposing $\mathbf{G}(\mathsf{T}) = \mathbf{G}(\mathsf{r})$ we can seek the missing initial conditions through a minimum discrepancy of the target in terms of the weighting factor $\mathsf{r} \in (0, 1)$. A numerical example is worked out to persuade that this novel approach has good efficiency and accuracy.

keywords: Backward heat conduction problem, Lie-group shooting method, Strongly ill-posed problem, Quasi-boundary regularization, Two-point boundary value problem

Introduction

The goal of this paper is to study an ill-posed problem that emerges from one-dimensional backward heat conduction equation, but before proceeding we recollect 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 solve than the direct one.

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 appear several methods making certain progress in this issue, including the boundary element method [Han, Ingham and Yuan (1995)], the iterative boundary element method [Mera, Elliott, Ingham and Lesnic (2001); Mera, Elliott and Ingham (2002); Jourhmane and Mera (2002)], the regularization technique [Muniz, de Campos Velho and Ramos (1999); Muniz, Ramos and de Campos Velho (2000)], the operator-splitting method [Kirkup and Wadsworth (2002)], the implicit inversion method [Liu (2002)], the lattice-free high-order finite difference method [Iijima (2004)], the contraction group technique [Liu (2004)], the method

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of fundamental solutions [Mera (2005)] and the backward group preserving scheme [Liu, Chang and Chang (2006)]. A recent review of the numerical BHCP was provided by Chiwiacowsky and de Campos Velho (2003).

After transforming the BHCP into a two-point boundary value problem (BVP) by using the quasi-boundary regularization, our approach is based on the group preserving scheme (GPS) developed by Liu (2001) for the integration of initial vale problems (IVPs). The GPS is very effective to deal with ordinary differential equations (ODEs) with special structures as shown by Liu (2005) for stiff equations and Liu (2006a) for ODEs with constraints. The degree of the 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, Liu and Chang (2005) with the GPS.

The present paper will provide a Lie-group shooting method (LGSM) for the BHCP. Our approach is based on the study by Liu (2006b) with an extension applied to the solutions of multiple-dimensional and multiple targets BVPs. It is clear that our method can be applied to the BHCP, since we are able to search the missing initial condition through an iterative solution of r in a compact space of $\mathsf{r} \in (0, 1)$, where the factor r is used in a generalized mid-point rule for the Lie group of the 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.

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 $\mathsf{u(x, t)}$, where $\mathsf{t} < \mathsf{T}$, of which the temperature is presumed to be known at a given final time T. Here, we consider the following problem:

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

$$u(0,t) = u(\ell,t) = 0,\ 0 \le t \le T, \tag{2}$$

$$u(x,T) = h(x),\ 0 \le x \le \ell. \tag{3}$$

This is the so-called 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 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 [Liu (2004); Chang, Liu and Chang (2005)], which replaces Eq. (1) by a set of ODEs:

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

where $\Delta x = \ell/(n+1)$,$x_i = i\Delta x$ 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 (1969), and a hyperbolic regularization proposed by Ames and Cobb (1997). It seems that Showalter (1983) 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 (1994) for heat conduction inverse problem. Ames and Payne (1999) have investigated those regularizations from the continuous dependence of solution on the regularized parameter.

A new method for BHCP

Let us write

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

Then for $i = 1, \ldots, n$ Eq. (4) can be expressed as a vector form:

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

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

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

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 LGSM [Liu (2006b)] for finding the initial value $\mathbf{u}(0)$, such that the numerical solution $\mathbf{u}(\mathsf{T})$ can match Eq. (8) very well for arbitrary $\alpha > 0$.

The GPS

Liu (2001) has embedded Eq. (7) into the following n+1-dimensional augmented system:

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

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

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

with

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

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

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

Therefore, a group-preserving numerical scheme can be developed as follows [Liu (2001)]:

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

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

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

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

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

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

Generalized mid-point rule

Applying scheme (14) to Eq. (10) with a specified initial condition $\mathbf{X}(\mathbf{0}) = \mathbf{X}^{\mathbf{0}}$, 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 we use in GPS is $\Delta t = T/K$, and starting from an initial augmented condition $\mathbf{X}^{\mathbf{0}} = ((\mathbf{u}^{\mathbf{0}})^{\mathsf{T}},\ \|\mathbf{u}^{\mathbf{0}}\|)^{\mathsf{T}}$, we may calculate the value $\mathbf{X}^{\mathrm{f}} = ((\mathbf{u}(T))^{\mathsf{T}},\ \|\mathbf{u}(T)\|)^{\mathsf{T}}$ 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 recall 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 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

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

This is a one-step transformation from $\mathbf{X}^0$ to $\mathbf{X}^{\mathrm{f}}$; see, e.g., Liu, Chang and Chang (2006).

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:

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

where

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

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

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

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

Here, we employ the initial $\mathbf{u}^0 = (u_1(0),\ldots,u_n(0))$ and the final $\mathbf{u}^{\mathrm{f}}=(u_1(T),\ldots,u_n(T))$ 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 a generalized mid-point rule on the calculation of $\mathbf{G}$, and the result is a single-parameter Lie group element denoted by $\mathbf{G}(r)$.

A Lie group mapping between two points

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

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

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

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

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

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

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

where

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

Substituting

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

into Eq. (30), we obtain

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

where

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

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

are obtained by inserting Eq. (32) for **F** into Eqs. (27) and (28).

Let

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

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

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

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

By defining

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

we obtain a quadratic equation for Z from Eq. (38):

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

The solution is found to be

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

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

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

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

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

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

The Lie-group shooting method

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

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

By Eq. (8) we attain

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

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 originated from by letting the two $\mathbf{F}$ 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 $\mathbf{G}(\mathsf{T}) = \mathbf{G}(\mathsf{r})$.

For a specified r, Eq. (46) can be used to generate the new $\mathbf{u}^0$, until $\mathbf{u}^0$ converges according to a given stopping criterion:

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

which means that the norm of the difference between the i + 1-th and the i-th 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 r, which leads to the smallest error of Eq. (8). That is,

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

Numerical example

In order to compare our numerical results with those acquired by Lesnic, Elliott and Ingham (1998), Mera, Elliott, Ingham and Lesnic (2001), Mera, Elliott and Ingham (2002), Mera (2005) and Liu, Chang and Chang (2006), let us consider a one-dimensional benchmark BHCP:

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

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

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

The one-dimensional spatial domain [0, 1] is discretized by $N = n + 2$ points including two end 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 sec were employed such that when the final data are in the order of $O(10^{-7})$-$O(10^{-13})$ we attempt to use LGSM to retrieve the desired initial data $\sin \pi x$, which is in the order of $O(1)$. For this very difficult problem, the method proposed by Lesnic, Elliott and Ingham (1998) was unstable when $T > 1$ sec. Conversely, the results given by LGSM with $\Delta x = 1/80$ for T = 1.5 sec and $\Delta x = 1/100$ for T = 2.5, 3 sec were rather promising. In all the calculations, we can also employ $\alpha = 0$ without any difficulty because Eq. (46) is still applicable.

In Fig. 1, we present the numerical errors for these three cases. The maximum error for the case of T = 3 sec is about 2.8×10^{-3}. Liu, Chang and Chang (2006) 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 sec, they have provided a stable and accurate solution with the maximum error occurring at x = 0.5 is about 0.008. The present results are better than that paper, even for the severe case up to T = 3 sec, the maximum error occurring at x = 0.5 is about 0.0028.

To the authors' best knowledge, there has 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 (2005) with the method of fundamental solution (MFS) together with Tikhonov regularization technique (see Figure 5 of the above cited paper), we can say that LGSM is much better than MFS.

Conclusions

The heat conduction problems are calculated by the formulation with a semi-discretization of the spatial coordinate of heat conducting equations in conjunction with the Lie-group shooting method along the time direction. In order to evaluate the missing initial conditions for the quasi-boundary value problems of the BHCP, we have employed the equation $\mathbf{G}(T) = \mathbf{G}(r)$ to derive algebraic equations. Hence, we can solve them through a minimum solution in a compact space of $r \in (0,\ 1)$. A Numerical example of the BHCP was 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, which usually required only a small number of iterations. 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.

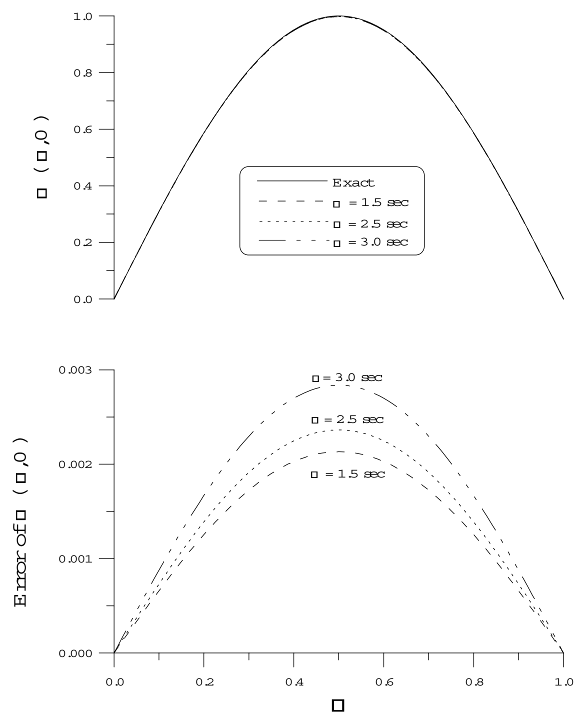

Figure 1: Comparisons of exact solutions and numerical solutions with final times T = 1.5, 2.5, 3 sec, and the corresponding numerical errors.

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