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A Numerical Study of Inverse Heat Conduction Problems

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Abstract—In this paper, two boundary element methods, a collocation method and a weighted method, are employed to solve a one-dimensional inverse heat conduction problem (IHCP). Inverse heat conduction problems are well known for being ill-posed. When numerical methods are directly applied on an IHCP, ill-conditioned linear systems will be involved. We show that the condition numbers for these systems increase as e^n where n is the number of the elements. We use a couple of Tikhonov's regularization methods to stabilize the matrix which is generated by the weighted method. An error bound for each method is analyzed. Finally, both methods are implemented and the result for the collocation method with the truncated singular value decomposition method is also shown in this article.

Keywords—Inverse heat conduction, Boundary element methods, Tikhonov's regularization, Condition numbers.

1. INTRODUCTION

Heat conduction phenomena appear in many situations in our lives. In fact, heat conduction phenomena do not exist only in a dead world. Engineers are applying the knowledge of heat conduction in many fields such as crystal growing [1], material structure control [2], and integrated circuit packaging [3]. The heat conduction behavior of a material is considered linear if its thermal conductivity and specific heat are not temperature dependent, and homogeneous if its thermal conductivity, specific heat, and density are the same everywhere. The time-varied temperature u should obey the linear heat equation $\nabla^2 u = (1/D)\frac{\partial}{\partial t}u$ if the heat conduction is linear and homogeneous where D is the thermal diffusivity. A well-posed boundary value problem in a heat equation requires that either temperature or heat flux (not both) is known on the boundary [4]. Sometimes the solution of inverse problems is required [5]. Being an ill-posed problem, an inverse heat conduction problem (IHCP) is difficult to deal with [6]. There are also many ill-posed problems arising from integral equations with smooth kernels, for example, the inverse radon transformation [7], but IHCP are more difficult than other kind of ill-posed problems. The inverse radon transformation was applied to computed tomography for decades [8] and has made a great success in medicine. An IHCP can be formulated into an integral equation with a very smooth kernel. Some numerical studies have been made through use of finite difference methods, for example [9], and other methods, for example, [10–12]. In order to know more about numerical solutions for IHCP, we investigate a simple one-dimensional problem through the boundary element methods (BEM). Recently, BEM have been applied to IHCP [13,14]. As

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a boundary element method is employed, i.e., the boundary integral equation is employed and the solution discretized on temporal space, a linear system is obtained. We will show that the matrix, which represents the linear system, has a condition number increasing exponentially with respect to the number of time steps if the time interval is fixed. Because of the ill-conditionality of the linear system, a special treatment is needed for the linear system.

Tikhonov's regularization methods and singular value decomposition (SVD) methods are most often used for ill-posed problems. A singular value decomposition method, such as that in [15], damps the vectors with respect to small singular values in the numerical solution. This kind of SVD method can also be seen as a Tikhonov regularization [15]. The truncated SVD method, such as that in [16,17], is similar to the generalized inverse. This SVD method removes the vectors with respect to small singular values from the numerical solutions. Tikhonov's regularization methods have been discussed intensively. Recently a book discussing the theories of Tikhonov's regularization methods was published by Tikhonov *et al.* [18]. The rate of convergence for the approximations generated by regularization methods and related topics have been discussed from different points of view (cf. [19]). In consideration of practical computation, the precision is restricted by the computer system. To reduce round-off errors and truncation errors to zero is impossible. In the computer system, we cannot distinguish $\mathbf{x}$ from $\mathbf{y}$ when $\|\mathbf{x}-\mathbf{y}\| < \varepsilon$. The positive number ε is called the precision of the computer system. In this study, fixed precision of the computer system is assumed. We use the truncated SVD method and a couple of Tikhonov's regularization methods to stabilize the ill-conditioned system. From the analysis, we find that there is no guarantee of accuracy for the methods. Numerical experiments become important to decide which methods are applicable. We also illustrate the numerical results in this paper. Considerably large numbers of time steps are used for these results to test the reliability of the methods.

The mathematical formulations for the heat equation and the numerical methods are reviewed or derived in Section 2. The Green's function and boundary integral equation are considered for the one-dimensional heat equation. Two boundary element methods, a weighted method and a collocation method, are described. We also show the numerical results without any regularization in this section. In the following section, the linear systems for these methods are shown to be ill-conditioned. The condition numbers increase exponentially with respect to the number of time steps. In the last section, regularization methods are discussed. The truncated SVD method is applied to the linear system obtained from the collocation method. An error bound for the generalized Tikhononv's regularization is also derived and two regularization methods for the weighted BEM are implemented for the example. The regularization parameter is automatically adjusted to the number of time steps.

In this study, we find that the weighted method is more stable than the collocation method, and regularization methods can improve the accuracy of the solutions for IHCP very well, especially when some prior knowledge is available. The results of the truncated SVD method are not superior to the results of Tikhonov's regularization. Because the truncated SVD method needs more computation than Tikhonov's regularization, using a weighted BEM with Tikhonov's regularization will be a better choice for ill-posed problems than using a collocation BEM with a SVD method.

2. THE BOUNDARY ELEMENT METHODS

Consider one-dimensional heat conduction problems. $T(x,t)$ denotes the time-varied temperature where x is the coordinate of the space and t is the time. $T(x,t)$ is assumed to obey the normalized heat equation on the half-space $x > 0$; i.e.,

$$\frac{\partial^2}{\partial x^2}T(x,t) = \frac{\partial}{\partial t}T(x,t), \qquad \text{for } x > 0. \tag{2.1}$$

There is a heat source at $x = 0$ and a thermal sensor at $x = 1$. Therefore, the temperature at $x = 1$ is measured on $t > 0$. Let $s(t)$ denote $T(1,t)$ and $f(t)$ denote for the heat flux at the boundary, $x = 0$, i.e.,

$$T(1,t) = s(t) \tag{2.2}$$

and

$$\frac{\partial}{\partial x}T(0,t) = f(t). \tag{2.3}$$

The initial condition is assumed to be zero; i.e.,

$$T(x,0) = 0, \qquad \text{for } x > 0. \tag{2.4}$$

The problem consists of using the measured data $s(t)$ to determine the heat flux $f(t)$.

Consider the forward problem first. The integral equation for $T(x,t)$ is

$$T(x,t) = \int_0^t G(x,t,0,\tau)f(\tau)\,d\tau + \int_0^\infty G(x,t,\xi,0)T(\xi,0)\,d\xi,$$

where $G(x,t,\xi,\tau)$ is Green's function for the heat equation corresponding to the boundary condition (2.3),

$$G(x,t,\xi,\tau) = \frac{1}{2\sqrt{\pi(t-\tau)}}\left(e^{-(x-\xi)^2/4(t-\tau)} + e^{-(x+\xi)^2/4(t-\tau)}\right)H(t-\tau), \tag{2.5}$$

and $H(t)$ is the unit step function. In our problem, $T(x,0) = 0$. The temperature at $x = 1$, $s(t)$, has to be

$$\begin{aligned} s(t) = T(1,t) &= \int_0^t \frac{1}{\sqrt{\pi(t-\tau)}}e^{-1/4(t-\tau)}f(\tau)\,d\tau \\ &= \int_0^t \frac{1}{\sqrt{\pi\tau}}e^{-1/4\tau}f(t-\tau)\,d\tau. \end{aligned} \tag{2.6}$$

More details about Green's function, G, can be found in [20]. Integration (2.6) defines a linear map from $f(t)$ to $s(t)$. $\mathcal{L}$ is used to denote this linear map; i.e.,

$$\mathcal{L}f(t) = s(t). \tag{2.7}$$

It is well known that linear operator $\mathcal{L}$ is ill-posed [6]. In order to find an approximate solution for $f(t)$, we employ a numerical method to solve the equation (2.6). The solution of the heat flux $f(t)$ on a finite interval $[0, T_0]$ is considered. There is a set of nodes $\{t_0, t_1, \dots, t_n\}$ where $t_0 = 0$, $t_n = T_0$, and $t_i = \Delta t\, i$. $\Delta t = T_0/n$ denotes the size of time steps.

The approximation $f^*(t)$ of heat flux $f(t)$ is chosen to be piecewise constant; i.e., $f^*(t)$ is constant in each time step (t_i, t_{i+1}). Therefore, the approximation $f^*(t)$ can be represented as

$$f^*(t) = \sum_{i=1}^{n} f_i\phi_i(t), \tag{2.8}$$

where

$$\phi_i(t) = \begin{cases} 1, & t_{i-1} \le t < t_i, \\ 0, & t < t_{i-1} \text{ or } t \ge t_i, \end{cases}$$

and f_i are real numbers. Substitute $f^*(t)$ into equation (2.7), then $\mathcal{L}f^*(t) = \sum_{i=1}^n f_i\mathcal{L}\phi_i(t)$ has to approximate the measured data $s(t)$. Let $\psi_i(t)$ denote $\mathcal{L}\phi_i$. Using the collocation method, we have

$$\mathcal{L}f^*(t_j) = s(t_j), \qquad \text{for } j = 1, 2, \dots, n,$$

or

$$\sum_{i=1}^{n} f_i \psi_i (t_j) = s(t_j), \tag{2.9}$$

where

$$\psi_i(t) = \psi(t-(i-1)\Delta t) - \psi(t - i\Delta t),$$
$$\psi(t) = \left[\frac{2}{\sqrt{\pi}}\sqrt{t}e^{-1/4t} - \left(1 - \operatorname{erf}\left(\frac{1}{2\sqrt{t}}\right)\right)\right] H(t)$$

and the error function $\operatorname{erf}(x)$ is defined as $(2/\sqrt{\pi})\int_0^x e^{-u^2}\,du$. Here the collocation point is chosen at the end of a time step. It is better than using the middle point as in [14], because the information received at the middle point does not reflect the heat flux in the whole time step. The equations (2.9) become a linear system that

$$\mathbf{C}_n \mathbf{f}_n^c = \mathbf{s}_n^c, \tag{2.10}$$

where

$$\mathbf{C}_n = [c_{ij}],$$
$$c_{ij} = \psi_j(t_i) = \psi(t_{i-j+1}) - \psi(t_{i-j}),$$
$$\mathbf{f}_n^c = \begin{pmatrix} f_1^c \\ f_2^c \\ \vdots \\ f_n^c \end{pmatrix} \quad \text{and} \quad \mathbf{s}_n^c = \begin{pmatrix} s(t_1) \\ s(t_2) \\ \vdots \\ s(t_n) \end{pmatrix}.$$

Matrix $\mathbf{C}_n$ is lower triangular.

A weighted method may also be used. We take

$$\langle \mathcal{L} f^*(t), \psi_j(t) \rangle = \langle s(t), \psi_j(t) \rangle, \qquad \text{for } j = 1, \dots, n,$$

or

$$\sum_{i=1}^{n} f_i \langle \psi_i, \psi_j \rangle = \langle s, \psi_j \rangle, \qquad \text{for } j = 1, \dots, n, \tag{2.11}$$

where the inner product of $s(t)$ and ψ_j, $\langle s, \psi_j \rangle = \int_0^{T_0} s(t)\psi_j(t)\,dt$.

The equations (2.11) form a linear system that

$$\mathbf{A}_n \mathbf{f}_n^w = \mathbf{b}_n, \tag{2.12}$$

where

$$\mathbf{A}_n = [a_{ij}], \qquad a_{ij} = \langle \psi_i, \psi_j \rangle = \int_0^t \psi_i(t)\psi_j(t)\,dt,$$
$$\mathbf{f}_n^w = \begin{pmatrix} f_1^w \\ f_2^w \\ \vdots \\ f_n^w \end{pmatrix}, \quad \mathbf{b}_n = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}, \quad \text{and} \quad b_i = \int_0^{T_0} s(t)\psi_i(t)\,dt.$$

Matrix $\mathbf{A}_n$ is symmetric and positive definite.

Because matrix $\mathbf{C}_n$ in equation (2.10) is lower triangular, the linear system may be solved directly. Here is an example.

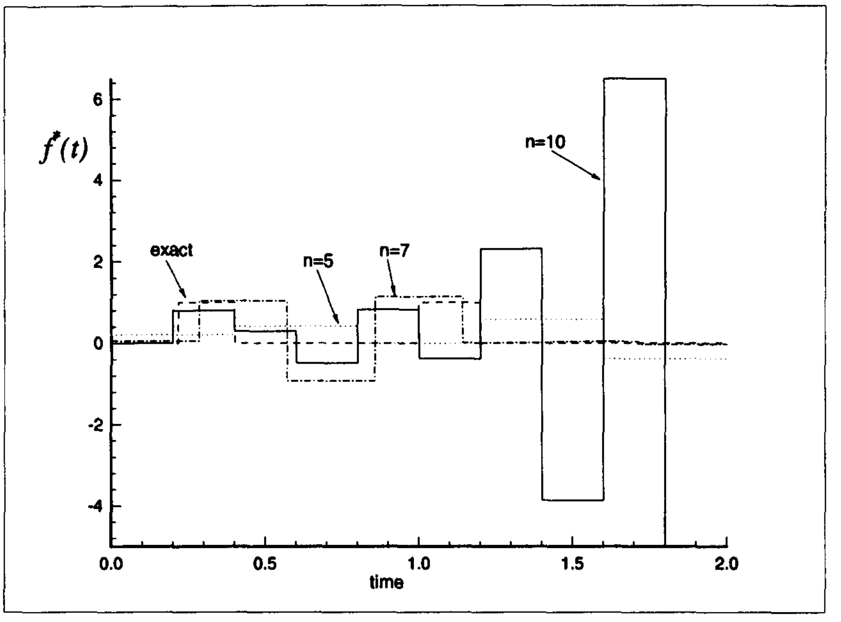

Figure 1. The results for the collocation method where n is the number of elements. For every n, the collocation method cannot attain significant result without regularization.

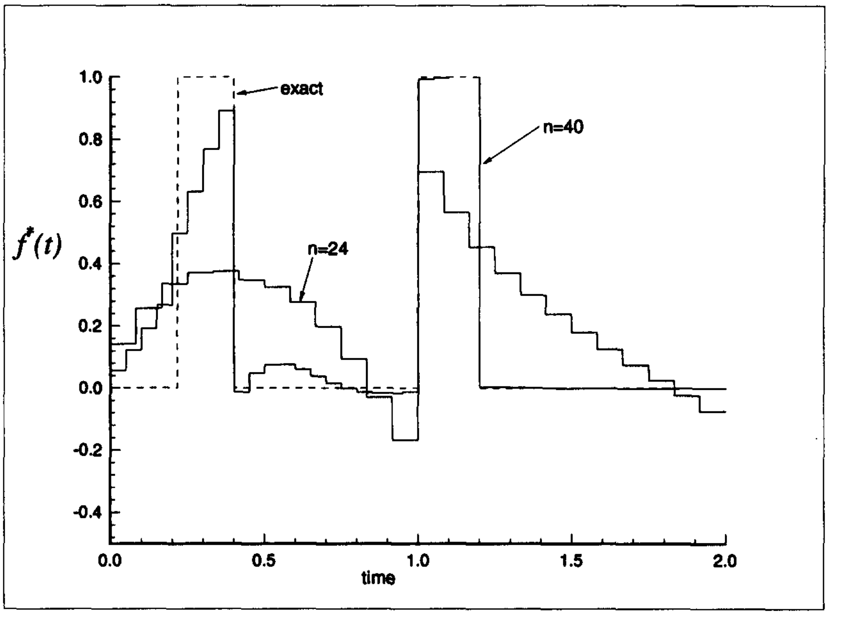

Figure 2. The results for the weighted method without any regularization.

The heat flux

$$f(t) = \begin{cases} 1, & \text{if } 0.2173 \leq t \leq 0.4 \text{ or } 1 \leq t \leq 1.2, \\ 0, & \text{else}, \end{cases} \tag{2.13}$$

and $T_0 = 2$.

The measured data $s(t)$ is calculated by a numerical integration. As n is 5, 7, and 10, the results are shown in Figure 1 with the exact solution. The numerical result overflows when n is greater than 20. Note that no artificial noise is put here, but the exact solution is not included in the approximation space. Obviously, the numerical errors greatly affect the results. An analysis of the condition numbers of the matrices appears in the next section.

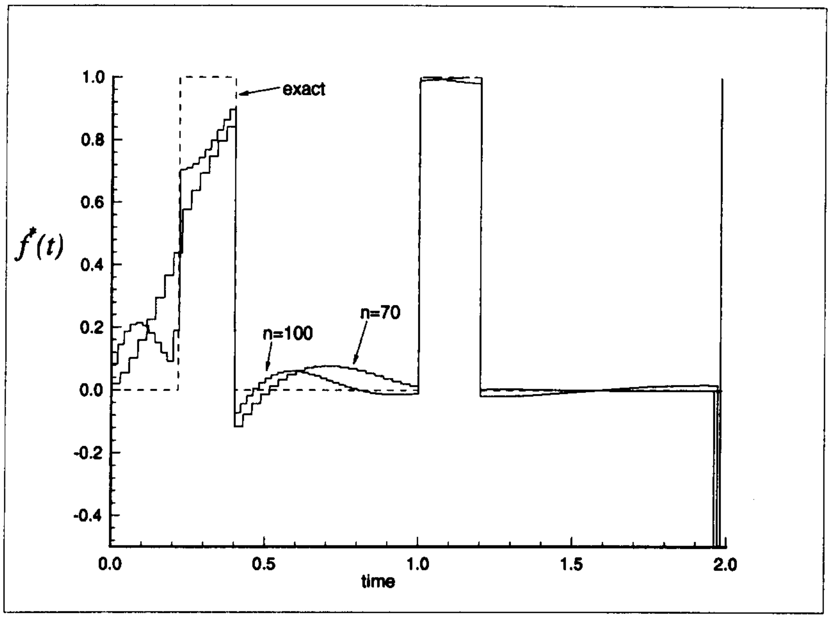

Figure 3. The results for the weighted method. At a time near 2, the values for $f^*(t)$ are about ($\pm$) 15.

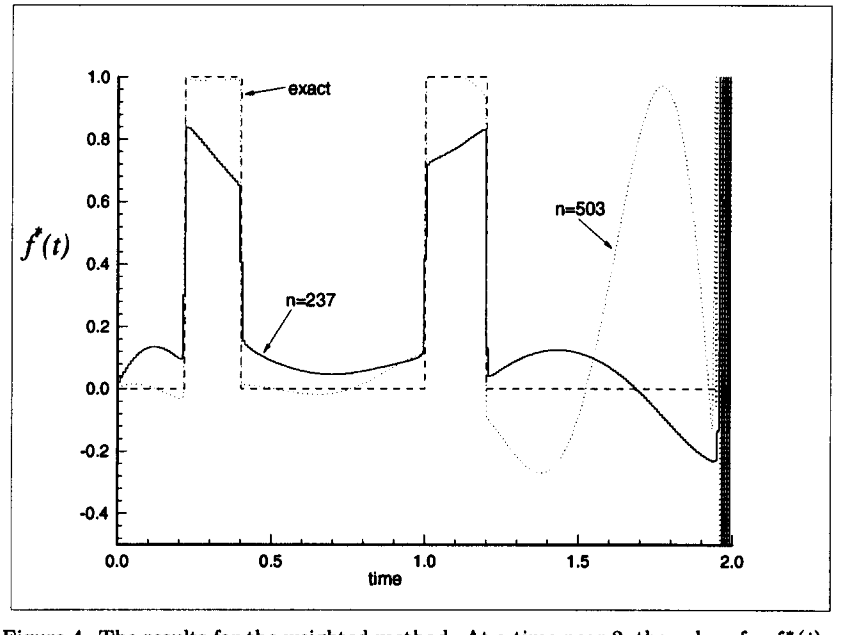

Figure 4. The results for the weighted method. At a time near 2, the values for $f^*(t)$ are about ($\pm$) 10^{23}.

For the weighted method, equation (2.12) can be solved through the Gaussian elimination. The results of the weighted method for problem (2.13) are shown in Figures 2–4 for $n = 24$ and 40, $n = 70$ and 100, and $n = 237$ and 503, respectively. The values for the last steps (near $t = 2$) of the results are about ($\pm$) 15 in Figure 3 and are about ($\pm$) 10^{23} in Figure 4. For larger ns, neither method attains a significant answer.

3. ILL-CONDITIONING

Consider a linear system

$$\mathbf{Ax} = \mathbf{b}, \tag{3.1}$$

where $\mathbf{A}$ is a $n \times n$ matrix and $\mathbf{x}$ and $\mathbf{b}$ are n-dimensional vectors. $\|\mathbf{x}\|$ denotes the two-norm of $\mathbf{x}$; i.e., $\|\mathbf{x}\| = (\mathbf{x} \cdot \mathbf{x})^{1/2}$. The operator norm of $\mathbf{A}$ is defined as

$$\|\mathbf{A}\| = \sup_{x \neq 0} \frac{\|\mathbf{Ax}\|}{\|\mathbf{x}\|}. \tag{3.2}$$

Assume $\mathbf{x}^*$ be a numerical solution for the linear system (3.1), and assume the difference between $\mathbf{Ax}^*$ and $\mathbf{b}$ to be controlled by

$$\frac{\|\mathbf{Ax}^* - \mathbf{b}\|}{\|\mathbf{b}\|} \leq \varepsilon, \tag{3.3}$$

where ε is a small positive real number which depends on the computer system. An inequality may be established [21, p. 114], that is,

$$\|\mathbf{x}^* - \mathbf{x}\| \leq \varepsilon \left\|\mathbf{A}^{-1}\right\| \|\mathbf{A}\| \|\mathbf{x}\|. \tag{3.4}$$

$\|\mathbf{A}^{-1}\| \|\mathbf{A}\|$ is defined as the condition number of $\mathbf{A}$ and denoted by $\mathrm{Con}(\mathbf{A})$. The inequality (3.4) shows that the relative error $\|\mathbf{x}^* - \mathbf{x}\| / \|\mathbf{x}\|$ will be smaller than $\varepsilon\,\mathrm{Con}(\mathbf{A})$. The poor performance due to large condition number is explained in detail in [22, Section 2.7]. When $\mathrm{Con}(\mathbf{A})$ is not very large, the numerical solution $\mathbf{x}^*$ is reliable. In this manner, the linear systems (2.10) and (2.12) can be analyzed.

Consider the matrix $\mathbf{C}_n$ in equation (2.10). Let

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{e}_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}.$$

Because $\|\mathbf{e}_1\|$ and $\|\mathbf{e}_n\|$ are 1, we have

$$\|\mathbf{C}_n\| \geq \|\mathbf{C}_n \mathbf{e}_1\| \quad \text{and} \quad \left\|\mathbf{C}_n^{-1}\right\| \geq \frac{1}{\|\mathbf{C}_n \mathbf{e}_n\|}.$$

Therefore, the condition number of $\mathbf{C}_n$ has to be larger than $\|\mathbf{C}_n \mathbf{e}_1\| / \|\mathbf{C}_n \mathbf{e}_n\|$.

$$\|\mathbf{C}_n \mathbf{e}_1\| = \left(\sum_{i=1}^{n} c_{i1}^2 \right)^{1/2} \geq \max_i \{|c_{i1}|\} \geq \frac{1}{n} \left| \sum_{i=1}^{n} c_{i1} \right|$$

and

$$\begin{aligned} \left| \sum_{i=1}^{n} c_{i1} \right| &= \sum_{i=1}^{n} \psi(t_i) - \psi(t_{i-1}) \\ &= \psi(n\Delta t) - \psi(0) = \psi(T_0). \end{aligned}$$

Thus,

$$\|\mathbf{C}_n \mathbf{e}_1\| \geq \frac{1}{n} \left(\frac{2}{\sqrt{\pi}} \sqrt{T_0} e^{-1/4T_0} - \left(1 - \operatorname{erf}\left(\frac{1}{2\sqrt{T_0}} \right) \right) \right).$$

$$\begin{aligned} \|\mathbf{C}_n \mathbf{e}_n\| &= \psi_n(t_n) = \psi(\Delta t) \\ &= \frac{2}{\sqrt{\pi}} \sqrt{\Delta t} e^{-1/4\Delta t} - \left(1 - \operatorname{erf}\left(\frac{1}{2\sqrt{\Delta t}} \right) \right). \end{aligned}$$

$(1 - \operatorname{erf}(1/2\sqrt{\Delta t}))$ may be estimated as follows:

$$e^{1/4\Delta t}\left(1 - \operatorname{erf}\left(\frac{1}{2\sqrt{\Delta t}}\right)\right) = e^{1/4\Delta t}\int_{1/2\sqrt{\Delta t}}^{\infty} \frac{2}{\sqrt{\pi}} e^{-u^2}\, du = \int_{u_0}^{\infty} \frac{2}{\sqrt{\pi}} e^{-(u^2-u_0^2)}\, du,$$

where $u_0 = 1/2\sqrt{\Delta t}$. Let $v = u^2 - u_0^2$, then

$$\begin{aligned} 1 - \operatorname{erf}\left(\frac{1}{2\sqrt{\Delta t}}\right) &= e^{-1/4\Delta t}\int_0^{\infty} \frac{1}{\sqrt{\pi}\sqrt{v+u_0^2}} e^{-v}\, dv \\ &\le e^{-1/4\Delta t}\frac{1}{\sqrt{\pi}u_0}\int_0^{\infty} e^{-v}\, dv = \frac{2\sqrt{\Delta t}}{\sqrt{\pi}} e^{-1/4\Delta t}. \end{aligned}$$

Furthermore,

$$0 \le 1 - \operatorname{erf}\left(\frac{1}{2\sqrt{\Delta t}}\right).$$

Therefore,

$$0 \le \psi(\Delta t) \le \frac{2\sqrt{\Delta t}}{\sqrt{\pi}} e^{-1/4\Delta t}. \tag{3.5}$$

We have

$$\|\mathbf{C}_n \mathbf{e}_n\| \le \frac{2\sqrt{T_0}}{\sqrt{n\pi}} e^{-n/4T_0}.$$

Therefore, the condition number of $\mathbf{C}_n$

$$\operatorname{Con}(\mathbf{C}_n) \ge \frac{\sqrt{\pi}\psi(T_0)}{2\sqrt{nT_0}} e^{n/4T_0}.$$

The condition number $\operatorname{Con}(\mathbf{C}_n)$ increases exponentially with respect to the number of steps n. In other words, regardless of how accurate the computer system is, the numerical solution $\mathbf{x}^*$ cannot maintain the accuracy when n increases.

Similarly, we may show that the condition number of the matrix $\mathbf{A}$ in equation (2.12) increase exponentially with respect to the number of steps n. Because of the symmetry of matrix $\mathbf{A}_n$ for any unit vector $\mathbf{u}$, there is an inequality

$$\frac{1}{\|\mathbf{A}_n^{-1}\|} \le \left|\mathbf{u}^\top \mathbf{A}_n \mathbf{u}\right| \le \|\mathbf{A}_n\|. \tag{3.6}$$

Let

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{e}_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}.$$

Using inequality (3.6), we have

$$\left\|\mathbf{e}_1^\top \mathbf{A}_n \mathbf{e}_1\right\| = |a_{11}| \le \|\mathbf{A}_n\|$$

and

$$\left\|\mathbf{e}_n^\top \mathbf{A}_n \mathbf{e}_n\right\| = |a_{nn}| \ge \frac{1}{\|\mathbf{A}_n^{-1}\|}$$

$$\begin{aligned} a_{11} &= \int_0^{T_0} \psi_1^2(t)\, dt = \int_0^{T_0} (\psi(t) - \psi(t-\Delta t))^2\, dt \\ &= (\Delta t)^2 \int_0^{T_0} \left(\frac{\psi(t) - \psi(t-\Delta t)}{\Delta t}\right)^2 dt \\ &= (\Delta t)^2 \int_0^{T_0} \psi'^2(\xi(t))\, dt, \end{aligned}$$

where $t - \Delta t \le \xi(t) \le t$. Because $\psi'(t)$ is increasing on $[0, 1/2)$ and decreasing on $(1/2, \infty)$,

$$\int_0^{1/2} \psi'^2(\xi(t))\,dt \ge \int_0^{1/2} \psi'^2(t - \Delta t)\,dt \ge \int_0^{1/2} \psi'^2(t)\,dt - \Delta t \psi'^2\left(\frac{1}{2}\right)$$

and

$$\int_{1/2}^{T_0} \psi'^2(\xi(t))\,dt \ge \int_{1/2+\Delta t}^{T_0} \psi'^2(t)\,dt \ge \int_{1/2}^{T_0} \psi'^2(t)\,dt - \Delta t \psi'^2\left(\frac{1}{2}\right).$$

Therefore, if $\Delta t \le 1/2$,

$$a_{11} \ge (\Delta t)^2 \int_0^{T_0} \psi'(t)\,dt - 2(\Delta t)^3 \psi'\left(\frac{1}{2}\right)$$

and

$$\begin{aligned} a_{nn} &= \int_0^{T_0} \psi_n^2(t)\,dt = \int_0^{T_0} \psi^2(t - (n-1)\Delta t)\,dt \\ &= \int_0^{\Delta t} \psi^2(t)\,dt \le \psi^2(\Delta t)\Delta t. \end{aligned}$$

Using inequality (3.5), we have

$$a_{nn} \le \frac{4T_0^2}{n^2\pi} e^{-n/2T_0}.$$

Consequently, the condition number of $\mathbf{A}_n$

$$\mathrm{Con}(\mathbf{A}_n) = \|\mathbf{A}_n\| \left\|\mathbf{A}_n^{-1}\right\| \ge \frac{|a_{11}|}{|a_{nn}|} \ge \frac{\pi}{4} \left(\int_0^{T_0} \psi'^2(t)\,dt - 2\frac{T_0}{n}\psi'^2\left(\frac{1}{2}\right) \right) e^{n/2T_0}. \tag{3.7}$$

The right-hand side of inequality (3.7) is in proportion to e^n.

4. REGULARIZATION METHODS

In the last section, we proved that the condition number of matrix $\mathbf{C}_n$ in equation (2.10) increases exponentially with respect to the number of time steps n. For a well-posed problem, we use finer time steps (or use a larger n) when we need a more accurate approximation. Because the original integral equation (2.7) is ill-posed, the ill-conditioned property of $\mathbf{C}_n$ in equation (2.10) and $\mathbf{A}_n$ in equation (2.12) is essential. In other words, no numerical method may solve every problem of equation (2.7) with arbitrary accuracy. Usually, a worse result is produced with finer time steps when the number of time step is large. The example in Section 2 demonstrates the effect of the ill-conditioned system. Several methods have been developed for solving ill-conditioned problems and applied to some numerical examples [16]. The most efficient methods are the singular value decomposition methods [17] and Tikhonov's regularization methods [23]. Nevertheless, an IHCP causes more difficulty than any other ill-posed problem does.

In this section, a SVD method and some regularization methods are employed to avoid getting worse results with a larger n. Because the matrix in equations (2.10) is not positive definite, the truncated singular value decomposition method is applied to the linear system (2.10). Consider the singular value decomposition of $\mathbf{C}_n$ in equation (2.10),

$$\mathbf{C}_n = \mathbf{U}\mathbf{D}\mathbf{V}^\top,$$

where $\mathbf{U}$ and $\mathbf{V}$ are orthogonal, and $\mathbf{D} = \mathrm{diag}(\sigma_i)$ with $\sigma_1 \ge \sigma_1 \ge \cdots \ge \sigma_n \ge 0$. σ_i are the singular values. The solution of equation (2.10) $\mathbf{f}_n^c$ has to be $\sum_{i=1}^n (s_i^*/\sigma_i)\mathbf{v}_i$, where $\mathbf{v}_i$ is the

i^{th} column of $\mathbf{V}$ and s_i^* is the i^{th} component of $\mathbf{U}^{\mathsf{T}}\mathbf{s}_n^c$. Unacceptable numerical error due to very small singular values may be removed. The solution of the truncated method

$$\mathbf{f}_{\text{svd}} = \sum_{i=1}^{k} \frac{s_i^*}{\sigma_i}\mathbf{v}_i,$$

where $k = \max\{j \mid \sigma_j \geq \delta\}$ and the positive number δ is the cut-off level. This method has been applied to IHCP before [16]. Figures 5 and 6 show the results for the example with $n = 237$ and 503 and $n = 1000$ and $n = 1001$, respectively. The cut-off level $\delta = \sigma_1 * 10^{-3}$ is used for these numerical results. In Figure 6, a significant difference is shown between the results for $n = 1000$ and $n = 1001$. It implies that the numerical method is very sensitive. In this method, the condition number is equivalent to σ_1/δ.

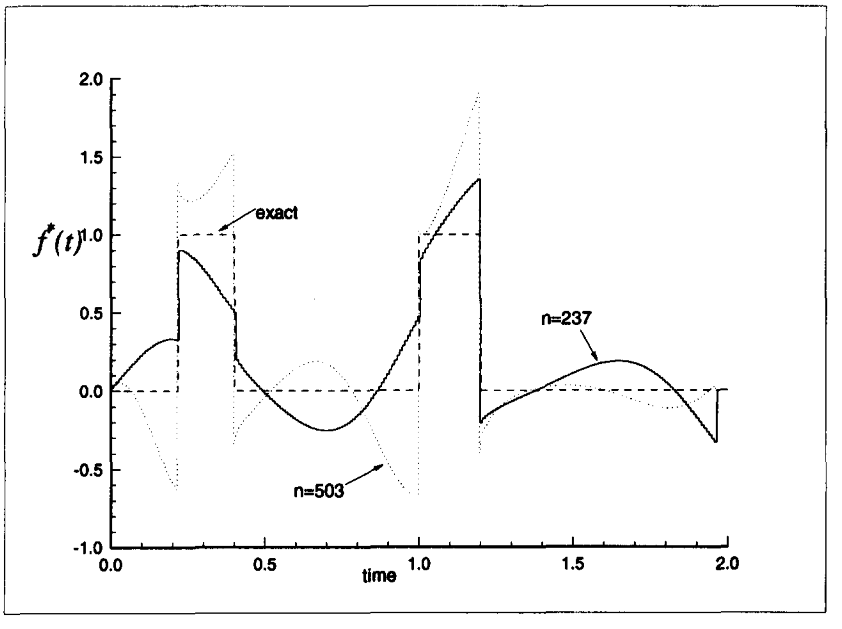

Figure 5. The results for the collocation method with singular value decomposition. The cut-off level $\delta = 10^{-3}\sigma_1$.

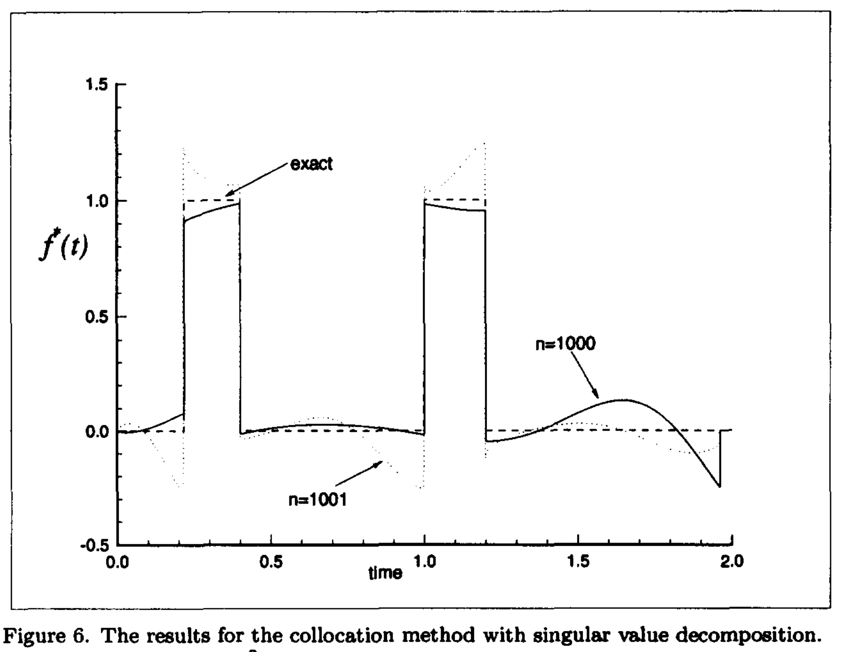

Figure 6. The results for the collocation method with singular value decomposition. The cut-off level $\delta = 10^{-3}\sigma_1$.

The truncated SVD method ignores oscillatory parts of the solution to avoid huge numerical error. A regularization method also sacrifices exactness to attain a well-conditioned linear system. A generalized Tikhonov's regularization is analyzed and implemented in this section. The analysis is starts from a linear system,

$$\mathbf{Ax} = \mathbf{b}, \tag{4.1}$$

where $\mathbf{A}$ is an ill-conditioned symmetric positive definite square matrix. Assume $\mathbf{x}^*$ to be the numerical solution for equation (4.1). Therefore,

$$\frac{\|\mathbf{x}^* - \mathbf{x}\|}{\|\mathbf{x}\|} \leq \varepsilon \,\mathrm{Con}(\mathbf{A}). \tag{4.2}$$

Here, Con$\mathbf{A}$ is a very large number. The exact solution $\mathbf{x}$ minimizes the inner product

$$E(\mathbf{u}) = \left(\mathbf{A}^{1/2}\mathbf{u} - \mathbf{A}^{-1/2}\mathbf{b}\right)^2.$$

Let $\mathbf{y}$ minimize the inner product

$$H(\mathbf{u}) = E(\mathbf{u}) + \mathbf{u}^{\mathrm{T}}\mathbf{Bu}, \tag{4.3}$$

where $\mathbf{B}$ is a positive semidefinite symmetric matrix; i.e., $\mathbf{u}^{\mathrm{T}}\mathbf{Bu} \geq 0$ for any $\mathbf{u}$.

Obviously, $(\mathbf{A} + \mathbf{B})$ is not singular. The minimizer $\mathbf{y}$ must satisfy the equation which is

$$(\mathbf{A} + \mathbf{B})\mathbf{y} = \mathbf{b}. \tag{4.4}$$

Consider equation (4.4). There is a numerical solution $\mathbf{y}^*$ for $\mathbf{y}$ where

$$\frac{\|(\mathbf{A} + \mathbf{B})\mathbf{y}^* - \mathbf{b}\|}{\|\mathbf{b}\|} \leq \varepsilon. \tag{4.5}$$

Substituting equation (4.4) into inequality (4.5), we have

$$\|\mathbf{y} - \mathbf{y}^*\| \leq \varepsilon \,\left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \|\mathbf{b}\|. \tag{4.6}$$

From equation (4.1) and equation (4.4), we have

$$(\mathbf{A} + \mathbf{B})\mathbf{y} = \mathbf{Ax}.$$

Therefore,

$$(\mathbf{A} + \mathbf{B})\mathbf{y} = (\mathbf{A} + \mathbf{B})\mathbf{x} - \mathbf{Bx},$$

and

$$(\mathbf{A} + \mathbf{B})(\mathbf{x} - \mathbf{y}) = \mathbf{Bx}.$$

We have

$$\|\mathbf{x} - \mathbf{y}\| \leq \left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \|\mathbf{Bx}\|. \tag{4.7}$$

From inequality (4.6) and inequality (4.7), we have

$$\|\mathbf{x} - \mathbf{y}\| + \|\mathbf{y} - \mathbf{y}^*\| \leq \varepsilon \,\left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \,\|\mathbf{b}\| + \left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \,\|\mathbf{Bx}\|$$

and then

$$\|\mathbf{x} - \mathbf{y}^*\| \leq \varepsilon \,\left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \,\|\mathbf{b}\| + \left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \,\|\mathbf{Bx}\|. \tag{4.8}$$

Applying the inequality: $\|\mathbf{x}\| \geq \|\mathbf{b}\|/\|\mathbf{A}\|$, we have

$$\frac{\|\mathbf{x} - \mathbf{y}^*\|}{\|\mathbf{x}\|} \leq \varepsilon \,\left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \,\|\mathbf{A}\| + \left\|(\mathbf{A} + \mathbf{B})^{-1}\right\| \frac{\|\mathbf{Bx}\|}{\|\mathbf{x}\|}. \tag{4.9}$$

In case $\mathbf{B} = \mu I$, where μ is a small positive number and I is the $n \times n$ identity matrix, the regularization (4.3) is the first-order Tikhonov's regularization. As $\mathbf{B} = \mu I$, $\|(\mathbf{A} + \mathbf{B})^{-1}\|$ is $1/(\lambda_n + \mu)$, where λ_n is the smallest eigenvalue of $\mathbf{A}$. The inequality (4.9) becomes

$$\frac{\|\mathbf{y}^* - \mathbf{x}\|}{\|\mathbf{x}\|} \leq \varepsilon \frac{\lambda_1}{\lambda_n + \mu} + \frac{\mu}{\lambda_n + \mu}, \tag{4.10}$$

where λ_1 is the largest eigenvalue of $\mathbf{A}$. Investigating inequality (4.10), we find that when λ_1/λ_n is very large ($\lambda_1/\lambda_n \gg 1/\varepsilon$), the error bound ($\varepsilon(\lambda_1/(\lambda_n + \mu)) + \mu/(\lambda_n + \mu)$) for $\mathbf{y}^*$ is much lower than the error bound ($\varepsilon(\lambda_1/\lambda_n)$) for $\mathbf{x}^*$. There is no guarantee of accuracy for ill-conditioned problems even when the regularization is applied. The second term of the right-hand side of inequality (4.10) is almost 1, which does not depend on the system error ε. It may be shown that the error bound in (4.10) cannot be reduced. When $\mathbf{x}$ is the eigenvector with respect to the smallest eigenvalue of the matrix $\mathbf{A}$ and $\varepsilon = 0$, $\mathbf{y}^*$ is $(\lambda_n/(\mu + \lambda_n))\mathbf{x}$ and the relative error is $\mu/(\mu + \lambda_n)$. Therefore, if Tikhonov's regularization is applied to a problem in the perfect computational environment, $\varepsilon = 0$, the accuracy may still be totally lost.

Tikhonov's regularization offers a good computability but risks the accuracy. For the inverse heat conduction problem, the condition number of the corresponding linear system increases as fast as e^n. The direct methods are shown being not applicable and Tikhonov's regularization method provides no guarantee for the accuracy either. Numerical experiments become a rule of thumb to decide which methods are applicable. As Tikhonov's regularization is applied to example (2.13), the regularization parameter μ has to be decided automatically first. We choose a μ which lets the condition number of $(\mathbf{A} + \mu\mathbf{I})$ be about 10^5. From Section 3, a_{11} is an estimated value for $\|\mathbf{A}\|$. Consequently, the estimated condition number of $(\mathbf{A} + \mu\mathbf{I})$ is a_{11}/μ. Therefore, we use $\mu = a_{11} \times 10^{-5}$ for any number of n. The results are shown in Figures 7–9 for $n = 237$ and 503, $n = 1000$ and 1001, and $n = 1555$ and 1989, respectively, with $\mu = a_{11} \times 10^{-5}$. The regularization parameter is much easier to choose than that of the method in [14]. Because $\Delta t = 2/n$, the round-off error for Δt depends on n. Therefore, we randomly choose the values of n.

In case $\mathbf{Bx} = 0$, i.e., some prior knowledge for the solution $\mathbf{x}$ exist. The inequality (4.9) implies

$$\frac{\|\mathbf{y}^* - \mathbf{x}\|}{\|\mathbf{x}\|} \leq \varepsilon \operatorname{Con}(\mathbf{A} + \mathbf{B}).$$

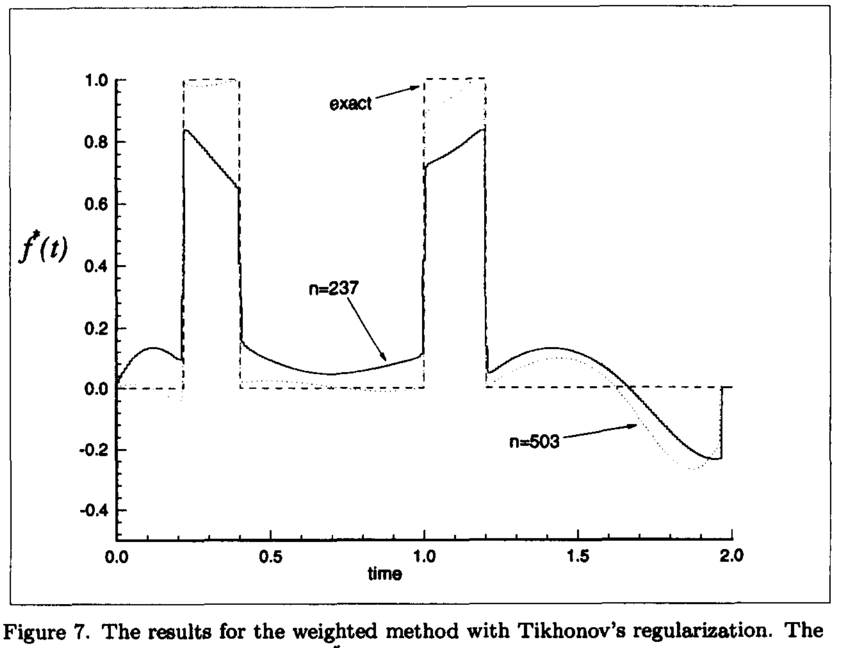

Figure 7. The results for the weighted method with Tikhonov's regularization. The regularization parameter $\mu = 10^{-5}a_{11}$.

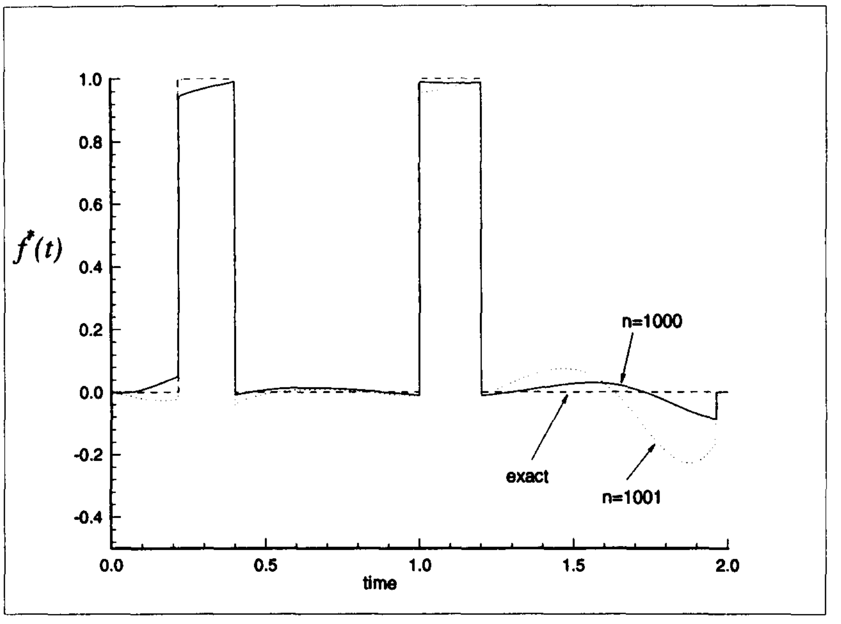

Figure 8. The results for the weighted method with Tikhonov's regularization. The regularization parameter $\mu = 10^{-5}a_{11}$.

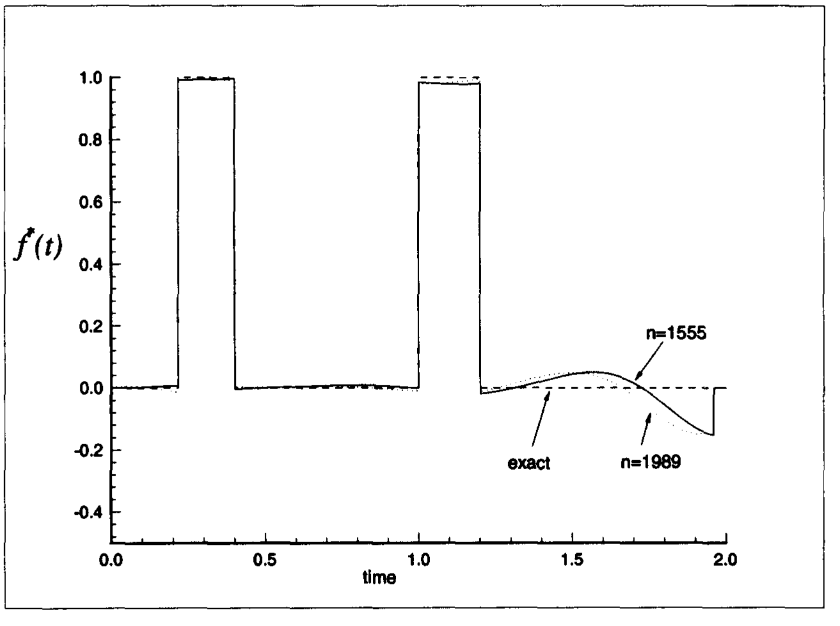

Figure 9. The results for the weighted method with Tikhonov's regularization. The regularization parameter $\mu = 10^{-5}a_{11}$.

Obviously, $\mathrm{Con}(\mathbf{A}+\mathbf{B}) \le \mathrm{Con}(\mathbf{A})$ under the assumption of $\mathbf{A}$ and $\mathbf{B}$ being nonnegative. In this case, the condition is very strong, but it may be available for the example. Assuming a prior knowledge that $f(t)$ is zero for $1.5 < t \le 2.0$ for problem (2.13), we may choose $\mathbf{B}$ as

$$\mathbf{B} = \mathrm{diag}\,(b_1, b_2, \dots, b_n),$$

where

$$b_i = \begin{cases} 0, & \text{if } i\Delta t \le 1.5, \\ 5, & \text{if } 1.5 < i\Delta t \le 2.0. \end{cases}$$

The results are shown in Figures 10–12 when $n = 237$ and 503, $n = 1000$ and 1001, and $n = 1555$ and $n = 1989$, respectively. The dashed line represents the exact solution. This method produces

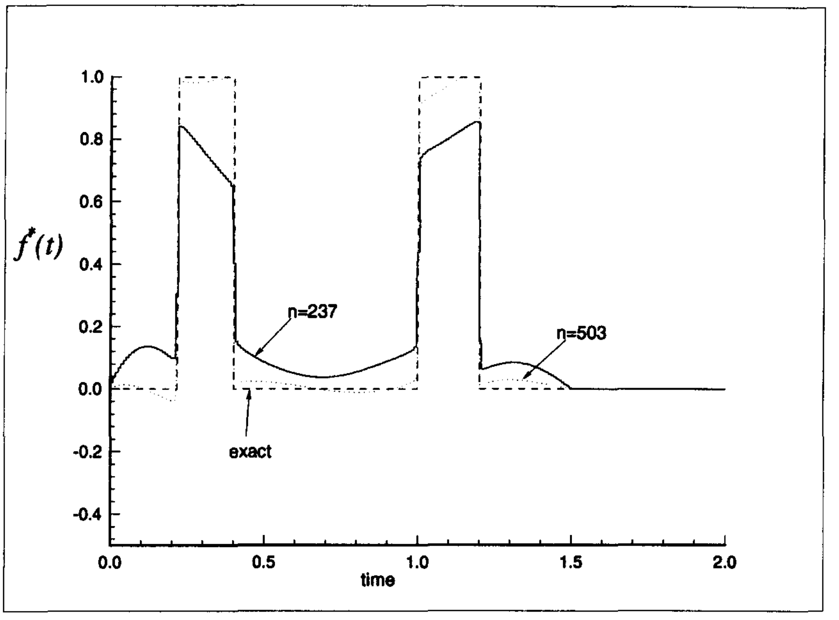

Figure 10. The results for the weighted method with generalized Tikhonov's regularization. The information that $f(t) = 0$ for $1.5 < t \le 2$ is assumed to be the prior knowledge.

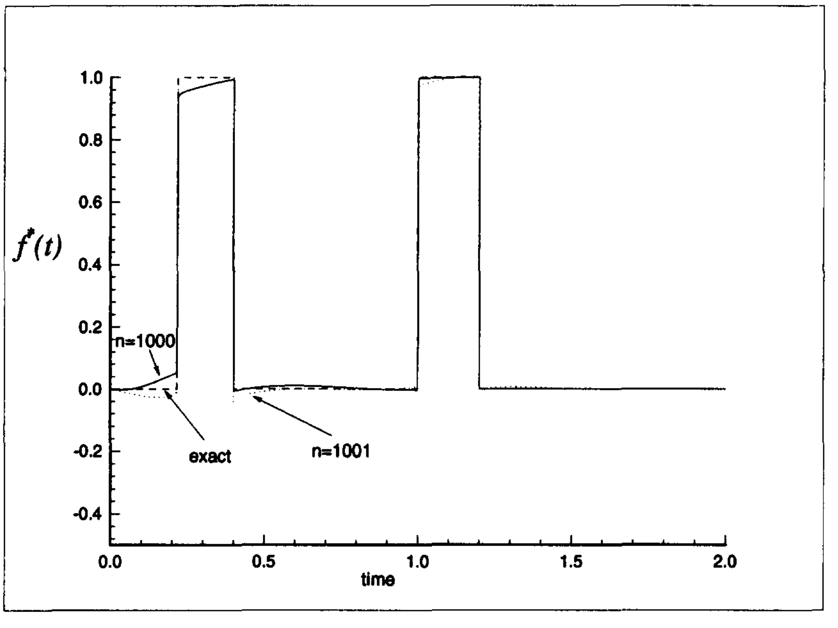

Figure 11. The results for the weighted method with generalized Tikhonov's regularization. The information that $f(t) = 0$ for $1.5 < t \le 2$ is assumed to be the prior knowledge.

stable and accurate results. The number of elements, n, which is 1989 is considered large enough. Since the restriction of the size of main memory in our computer, we do not use larger n.

5. CONCLUSIONS

The boundary integral representation (2.5), which provides a direct relation between the flux $f(t)$ and measured data $s(t)$, is applied to calculate the numerical solutions. In addition, the initial condition is assumed to be zero and the bases are integrated analytically. The noise in the computation is reduced as low as possible. Because the condition number of the corresponding linear systems increases as e^n, the condition number can be very large when a large n is used to

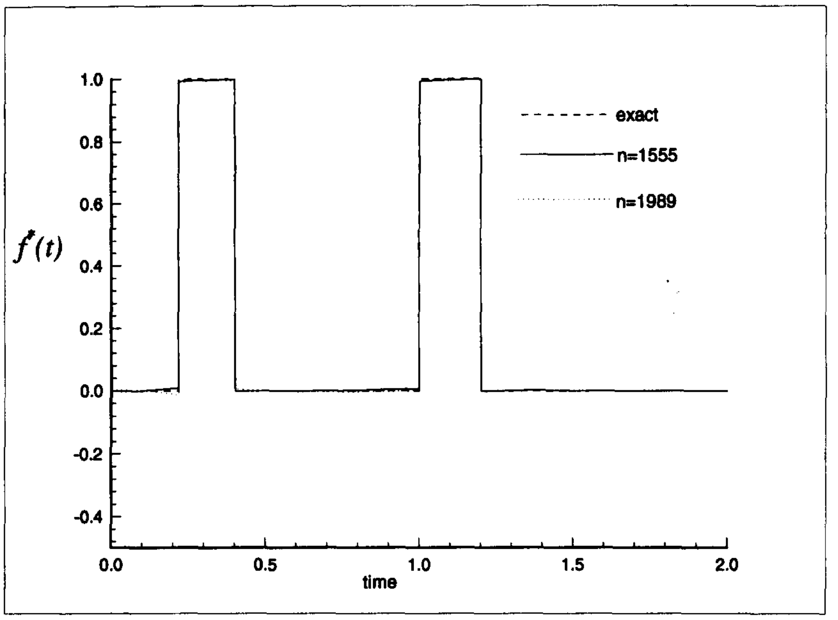

Figure 12. The results for the weighted method with generalized Tikhonov's regularization. The information that $f(t) = 0$ for $1.5 < t \leq 2$ is assumed to be the prior knowledge.

generate a precise approximation. Tikhonov's regularization reduced the condition number but still offers no guarantee of accuracy. Therefore, numerical experiments provide a more practical criterion (than analysis) to decide which methods are applicable. In the example, the thermal diffusivility and the distance from the boundary to the sensor point are unity. Thus, in this normalized problem, the time unit is equivalent to L^2/D for a practical problem, where D is the diffusivity and L is the distance from the boundary to the sensor point.

We have shown that the direct methods are not applicable even for a small n. The truncated singular value decomposition method needs much more computations than the regularization methods; but the results for the regularization are better than those for the singular value decomposition method. It may be concluded that the regularization methods are superior to the truncated SVD method. If an information, $\mathbf{Bx} = 0$, is available, the regularization method, $(\mathbf{A} + \mathbf{B})\mathbf{x} = \mathbf{b}$, could provide stable and accurate approximations.

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