Solving an Inverse Diffusion Problem Using Tikhonov Regularization Method

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Abstract: This paper is concerned with the evaluation of the diffusion coefficient based on the measurement obtained at the boundary by using a numerical approach. We consider the problem of recovering the diffusion coefficient of a rod that is a function of space. The approach is based on finite-difference method and the least-squares scheme. At the beginning of the algorithm, the finite-difference method is used to discretize the problem domain. The present approach is to rearrange the matrix forms of the differential governing equations and estimate unknown diffusion coefficient. The least-squares method is adopted to find the solution. This solution is unstable, hence the problem is ill-posed. This instability is overcome using the Tikhonov regularization method with the gcv criterion for the choice of the regularization parameter. The stability and accuracy of the scheme presented is evaluated by comparison with the Singular Value Decomposition method (SVD). Results show that a good estimation on the diffusion coefficient can be obtained within a couple of minutes CPU time at pentium IV-2.4 GHz PC.

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1 Introduction

Inverse problems appear in many important scientific and technological fields. Hence analysis, design implementation and testing of inverse algorithms are also are great scientific and technological interest.

Several functions and parameters can be estimate from the inverse problem: static and moving heating sources, material properties, initial conditions, boundary conditions, optimal shape etc.

Fortunately, many methods have been reported to solve (IHCPs) [1]-[5], [6], [13], [14], [16]-[19], and among the most versatile methods the following can be mentioned: Tikhonov regularization [22], iterative regularization [1], mollification [15], BFM (Base Function Method) [16], SFDM (Semi Finite Difference Method) [13], and the FSM (Function Specification Method) [2].

Beck and Murio [4] presented a new method that combines the function specification method of Beck with the regularization technique of Tikhonov. Murio and Paloschi [14] propose a combined procedure based on a data filtering interpretation of the mollification method and FSM. Beck et al. [3] compare the FSM, the Tikhonov regularization and the iterative regularization, using experimental data. Another effective technique to solve ill-posed problems is based in the Singular Value Decomposition (SVD) of an ill condition matrix [8].

The plan of this paper is as follows: In section 2, we formulate an inverse diffusion problem. A method consists of Tikhonov regularization to the matrix form of least-squares method for solving this inverse problem will be presented in section 3. Finally some numerical experiment will be given in section 4.

2 Mathematical formulation

Consider a one-dimensional rod whose thermal conductivity $k(x)$ is a function of space. The conduction of heat is governed by the equation given by

$$T_t = (k(x)T_x)_x, \quad 0<x<1, \ 0<t<t_M \tag{1}$$

$$T(x,0) = f(x), \quad 0 \le x \le 1, \tag{2}$$

$$T(0,t) = p(t), \quad 0 \le t \le t_M, \tag{3}$$

$$T(1,t) = \phi(t), \quad 0 \le t \le t_M, \tag{4}$$

and the overspecified condition

$$T(a,t) = q(t), \quad 0 \le t \le t_M, \tag{5}$$

where $0 \le a \le 1$ is a fixed point, t_M is a given constant, $f(x)$ is the initial temperature of rod, $p(t)$ is the temperature at the left-hand side and $\phi(t)$ is the temperature at the right-hand side. In this context we consider that the functions $f(x)$, $p(t)$, and $\phi(t)$ are known functions, while $k(x) > 0$ and $T(x,t)$ are unknown functions which remain to be determined. Note that, for an unknown positive function $k(x)$ we must therefore provide additional information (5) to provide a unique solution $(T(x,t),k(x))$ to the inverse problem (1).

The inverse problem for the above system is then to recover the unknown function $k(x)$ based on the knowledge of the initial temperature, $f(t)$, temperature $p(t)$ at the boundary $x=0$, temperature $\phi(t)$ at the boundary $x=1$, and the measured temperature of the rod $q(t)$ [19].

3. Overview of the Method

Consider an inverse diffusion problem described by the equations (1). The application of the present numerical method will find a solution of problem (1), by using the following steps.

3.1. Finite difference method for discretizing

The explicit finite differences approximation for discretizing problem (1) may be written as follows [20]

$$\frac{1}{\delta t}(T_{i\,j+1}-T_{i\,j})=\frac{1}{\delta x^2}\left(k_{i+\frac{1}{2}}(T_{i+1j}-T_{i\,j})-k_{i-\frac{1}{2}}(T_{i\,j}-T_{i-1j})\right) \quad (6)$$

$$T_{i,0}=f(x_i), \qquad i=0,\ldots N, \quad (7)$$

$$T_{0,j}=p(t_j), \qquad j=0,\ldots,M, \quad (8)$$

$$T_{N,j}=\phi(t_j), \qquad j=0,\ldots,M, \quad (9)$$

where $x_i=i\delta x, t_j=j\delta t, i=0,1,\ldots,N$ and $j=0,1,\ldots,M$. Equation (6) for $i=1,\ldots,(N-1)$ may be written in the following matrix form

$$T_{j+1}=AT_j+C_j \quad (10)$$

$$A=\begin{pmatrix} \gamma_1 & \alpha_1 & \ldots & 0 & 0 & 0 \\ \beta_2 & \gamma_2 & \alpha_2 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & \beta_{N-2} & \gamma_{N-2} & \alpha_{N-2} \\ 0 & 0 & \ldots & 0 & \beta_{N-1} & \gamma_{N-1} \end{pmatrix},$$

and

$$T_j^t=(T_{1j}\ T_{2j}\ \ldots\ T_{N-1j})$$

$$T_{j+1}^t=(T_{1j+1}T_{2j+1}\ldots\ T_{N-1j+1})$$

$$C_j^t=(r\beta_1 T_{0j}\ \ 0 \ldots\ 0\ r\alpha_{N-1}T_{N\,j})$$

where, for $\nu=1,2,\ldots,N-1$,

$$\gamma_\nu=1-r\,(k_{\nu-\frac{1}{2}}+k_{\nu+\frac{1}{2}}),\ \alpha_\nu=rk_{\nu+\frac{1}{2}},\ \beta_\nu=rk_{\nu-\frac{1}{2}}$$

Theorem. If k_μ be the maximum value of $|k_{\nu+b_i}|;\nu=1,\ldots,N-1, b_i=(-1)^i\frac{1}{2}; i=1,\ldots,$ t then the finite difference scheme (10) is stable for $r<\frac{1}{2k_\mu}$.

Proof. In system (10), the matrix determining the propagation of the error is A. Therefore scheme (10) will be stable when the modulus of every eigenvalue of A does not exceed one. Application of Gerschgorins circle theorem to the matrix A shows that its eigenvalues λ lie on or within the circle

$$|\lambda-a_{ss}|\le\sigma_s,$$

where σ_s is the sum of the moduli of the elements along the sth row excluding the diagonal element a_{ss}.

Hence, for row 1 we obtain $r<\frac{2}{3k_\mu}$.

Similarly for row $N-1$ we require $r<\frac{2}{3k_\mu}$.

For rows $2,\ldots,N-2$ we obtain $r<\frac{1}{2k_\mu}$.

For overall stability, we obtain $r<\frac{1}{2k_\mu}$.

By solving the equation (10), we obtain

$$T_{j+1}^t=(T_{1j+1}T_{2j+1}\ldots\ T_{N-1j+1}) \quad (11)$$

These updated values of T_{j+1} are used to calculate A, T_j, and C_j for iteration. This computational procedure is performed repeatedly until desired convergence is achieved.

Remark: In this work the polynomial form proposed for the unknown $k(x)$ before performing the calculation. Therefore $k(x)$ approximated as

$$k(x)=a_0+a_1x+a_2x^2+\ldots+a_\lambda x^\lambda, \quad (12)$$

where $\{a_0, a_1, ..., a_\lambda\}$ are constants which remain to be determined.

The unknown function $k(x)$ is difficult to be approximated by a polynomial function for the whole time domain considered. Therefore the time domain $t_0 \le t \le t_M$ will be divided into some intervals where t_0 is the initial measurement time. Each of the intervals is assumed to be $t_{m-1} \le t \le t_m$ where $t_m = t_0 + m\Delta t$, $m = 1,...,M$ and

$$\Delta t = \frac{t_M - t_0}{M}.$$

For linearized nonlinear terms in equations (11) we use Taylor's series expansion. Let $\Psi(\xi_1,...,\xi_n)$ be a many differentiable nonlinear function of $\xi_1,...,\xi_n$ then its Taylor's series expansion is given as

$$\Psi(\xi_1,...,\xi_n) = \Psi(\bar{\xi}_1,...,\bar{\xi}_n) + \sum_{\lambda=1}^{n} \frac{\partial \Psi}{\partial \xi_\lambda}(\bar{\xi}_1,...,\bar{\xi}_n)(\xi_\lambda - \bar{\xi}_\lambda) + O\left((\xi_\lambda - \bar{\xi}_\lambda)^2\right) \quad (13)$$

where the overbar denotes the previously iterated solution. Therefore we obtain

$$\hat{T}_{\frac{a}{\delta x}, j+1}(a_0,...,a_\lambda) = \hat{T}_{\frac{a}{\delta x}, j+1}(\bar{a}_0,...,\bar{a}_\lambda) + \sum_{i=0}^{\lambda} \frac{\partial \hat{T}_{\frac{a}{\delta x}, j+1}}{\partial a_i}(\bar{a}_0,...,\bar{a}_\lambda)(a_i - \bar{a}_i), \quad (14)$$

where $(\bar{a}_0,...,\bar{a}_\lambda)$ denotes the previously iterated solution.

3.2. Least-squares minimization technique and the Tikhonov regularization method

The estimated coefficients $a_{ii}; ii = 0,1,\ldots,\lambda$ can be determined by using least squares method when the sum of the squares of the deviation between the calculated $T_{\frac{a}{\delta x}, j+1}$ and the measured $q((j+1)k))$ at $x = a$ is less than a small number. The error in the estimates $E(a_0, a_1,...,a_\lambda)$ can be expressed as

$$E(a_0, a_1,...,a_\lambda) = \sum_{j=0}^{i} \left(T_{\frac{a}{\delta x}, j+1} - q((j+1)k)\right)^2, \; i = 1,2,\ldots \quad (15)$$

which is to be minimized for each interval $t_{m-1} \le t \le t_m$, $m = 1,\ldots,M$. To obtain the minimum value of $E(a_0, a_1,...,a_\lambda)$, with respect to $a_0, a_1,...,a_\lambda$, differentiation of $E(a_0, a_1,...,a_\lambda)$, with respect to $a_0, a_1,...,a_\lambda$, will be performed. Thus the linear system corresponding to the values of a_i can be expressed as

$$\Lambda\Theta = B. \quad (16)$$

The Matrix Λ is ill-conditioned. On the other hand, as q is affected by measurement errors, the estimate of Θ by (16) will be unstable so that the Tikhonov regularization method must be used to control this measurement errors. The Tikhonov regularized solution ([21], [10] and [11]) to the system of linear algebraic equation (16) is given by

$$F_\alpha(\Theta) = \|\Lambda\Theta - B\|_2^2 + \alpha \|R^{(s)}\Theta\|_2^2$$

On the case of the zeroth order Tikhonov regularization method the matrix $R^{(s)}$, for $s = 0$, is given by, see e.g. [12]:

$$R^{(0)} = I_{M\times M} \in R^{M\times M},$$

Therefore, we obtain the Tikhonov regularized solution of the regularized equation as

$$\Theta_\alpha = [\Lambda^T\Lambda + \alpha (R^{(s)})^T R^{(s)}]^{-1}\Lambda^T B.$$

In our computation, we use the gcv scheme to determine a suitable value of α ([7], [9] and [23]).

4. Numerical Results and Discussion

In this section, we are going to demonstrate numerically, some of results for the unknown diffusion coefficient in the inverse problem (1). The propose of this section is to illustrate the applicability of the present method described in section 0 for solving inverse diffusion problem (1). As expected the inverse problems is ill-posed and therefore it is necessary to investigate the stability of the present method by giving a test problem.

In an IHCP, there are two sources of error in the estimation. The first source is the unavoidable bias deviation (or deterministic error). The second source of error is the variance due to the amplification of measurement errors (stochastic error). The global effect of deterministic and stochastic errors is considered in the mean squared error or total error, [5].

We also compare Tikhonov method and SVD method by considering total error S defined by

$$S = \left[\frac{1}{N-1}\sum_{i=1}^{N}(\hat{q}_i - q_i)^2\right]^{\frac{1}{2}} \quad (17)$$

where N is the total number of estimated values.

Example.

In this example, let us consider following inverse diffusion problem,

$$T_t = (k(x)T_x)_x, \quad 0 < x < 1, \quad 0 < t < t_M \qquad (18)$$

$$T(x,0) = x, \quad 0 \le x \le 1, \qquad (19)$$

$$T(0,t) = 2t, \quad 0 \le t \le t_M, \qquad (20)$$

$$T(1,t) = 1 + 2t, \quad 0 \le t \le t_M, \qquad (21)$$

and the overspecified condition

$$T(a,t) = 0.5 + 2t, \quad 0 \le t \le t_M. \qquad (22)$$

The exact solution of this problem is

$$T(x,t) = x + 2t, \quad k(x) = 2x$$

Tables 1 and 3 show the comparison between the exact solution and approximate solution result from our method by Tikhonov regularization 0th and SVD regularization with noiseless data. Table 2 and 4 and figures 1 and 2 show these comparisons with noisy data. Finally, we compare two methods with computation total error by (17)

Table 1. The comparison between exact and Tikhonov and SVD solutions for $k(i\delta x)$ with noiseless data when $\delta x = 0.1$.

i	Exact	SVD	Tikhonov 0
	$k(i\delta x)$	$\tilde{k}(i\delta x)$	$\tilde{k}(i\delta x)$
1	0.200000	0.200000	0.200000
2	0.400000	0.400000	0.400000
3	0.600000	0.600000	0.600000
4	0.800000	0.800000	0.800000
5	1.000000	1.000000	1.000000
6	1.200000	1.200000	1.200000
7	1.400000	1.400000	1.400000
8	1.600000	1.600000	1.600000
9	1.800000	1.800000	1.800000
S		$7.9e-015$	$7.6e-015$

Table 2. The comparison between exact and Tikhonov and SVD so lutions for $k(i\delta x)$ with noisy data when $\delta x = 0.1$.

i	Exact	SVD	Tikhonov 0
	$k(i\delta x)$	$\tilde{k}(i\delta x)$	$\tilde{k}(i\delta x)$
1	0.200000	0.206294	0.206294
2	0.400000	0.412587	0.412587
3	0.600000	0.618881	0.618881
4	0.800000	0.825175	0.825175
5	1.000000	1.031468	1.031468
6	1.200000	1.237762	1.237762
7	1.400000	1.444056	1.444056
8	1.600000	1.650349	1.650349
9	1.800000	1.856643	1.856643
S		0.037564	0.037564

Table 3. The comparison between exact and Tikhonov and SVD solutions for $T(0.7, j\delta t)$ with noiseless data when $\delta t = 0.002$.

j	Exact	SVD	Tikhonov 0
	$T(0.7, j\delta t)$	$\tilde{T}(0.7, j\delta t)$	$\tilde{T}(0.7, j\delta t)$
1	0.704000	0.704000	0.704000
2	0.708000	0.708000	0.708000
3	0.712000	0.712000	0.712000
4	0.716000	0.716000	0.716000
5	0.720000	0.720000	0.720000
S		$3.9e-018$	$6.8e-018$

Table 4. The comparison between exact and Tikhonov and SVD solutions for $T(x,t)$ with noisy data when $\delta t = 0.002$.

t	Exact	SVD	Tikhonov 0
	$T(0.7, j\delta t)$	$\tilde{T}(0.7, j\delta t)$	$\tilde{T}(0.7, j\delta t)$
1	0.704000	0.704126	0.704126
2	0.708000	0.708252	0.708252
3	0.712000	0.712378	0.712378
4	0.716000	0.716498	0.716498
5	0.720000	0.720613	0.720613
S		$1.4e-005$	$1.4e-005$

5. Conclusion

A numerical method, to estimate unknown boundary condition is proposed for these kinds of IHCPs and the following results are obtained.

1. The present study, successfully applies the numerical method to IHCPs.
2. Numerical results show that an excellent estimation can be obtained within a couple of minutes CPU time at pentium(R) 4 CPU 3.20 GHz.
3. The present method has been found stable with respect to small perturbation in the input data.

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