A NUMERICAL ALGORITHM FOR AN INVERSE PROBLEM OF A PARTIAL DIFFERENTIAL EQUATION WITH MULTI-PARAMETER TO BE DETERMINED*

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Abstract

A formulation of an inverse problem of a partial differential equation with multi-parameter to be determined is introduced. The numerical algorithm, pulse-spectrum technique, is extended to solve this type of inverse problem. An example for remote sensing of the thermal conductivity and specific heat of a nonhomogeneous material is demonstrated. Numerical simulations are carried out to test the feasibility and to study the general characteristics of this technique without real measurement data. It is found that the extended pulse-spectrum technique gives excellent results.

1. Introduction

In this paper, we consider an inverse problem of determining the coefficients of a partial differential operator with a known structure in terms of a governing equation, some initial conditions and boundary conditions, and some auxiliary information. We call this type of inverse problem "operator identification". It originates from various kinds of problems of mathematical physics, for example, heat transfer, structural dynamics, engineering synthesis, remote sensing, geophysical prospecting, medical diagnostics and so on.

In section 2, the inverse problem of a partial differential equation with multi-parameter to be determined is formulated and the pulse-spectrum technique (PST) is extended to solve this type of inverse problem. The PST was first introduced by Tsien and Chen[1] to solve an idealized one-dimensional velocity inversion problem in fluid dynamics. It was further developed to handle the noisy, poorly distributed and inadequately measured data by Chen and Tsien[10]. Later it was used to solve a one-dimensional inverse problem in electro-magnetic wave propagation by Tsien and Chen[11]. In a different direction, the PST was modified to solve an inverse problem of a one-dimensional diffusion equation[12]. The basic idea of the PST is to measure data in the time domain as functions which are Laplace transformable, and carry out numerically the synthesis of the unknown parameter in the complex frequency domain by a special iterative algorithm.

As an example, the remote sensing of the thermal conductivity and specific heat of a nonhomogeneous material is demonstrated. Numerical simulations are carried out to test the feasibility and to study the general characteristics of this

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technique without real measurement data. It is found that the extended PST does give excellent results for the inverse problem of multi-parameter to be determined.

2. Formulation of the Inverse Problem and Numerical Algorithm

Consider the following differential equation defined on the time-space domain

$$Lu(x, t)=\varphi(x, t), \quad (x, t)\in\Omega\times T, \tag{1}$$

where $x=(x_1, x_2, \cdots, x_p)$, Ω is a p-dimensional domain, $\partial\Omega$ is the boundary of Ω, $T=[t|0<t]$, $u(x, t)$ is a sufficiently smooth function defined on $\Omega\times T$, which is Laplace transformable with respect to time variable t. Furthermore we suppose that the differential operator has the following form (structure)

$$L=\sum_{k=1}^{m}[A_k(\alpha_k(x)C_k)+\beta_k(x)D_k], \tag{2}$$

where A_k, C_k and D_k are elementary linear operators (for example, differentiation, integration, or their various combinations). A_k and C_k are operators of variable x and D_k is an operator of variable t. The coefficient $\alpha_k(x)$ is a piecewise smooth function on Ω; $\beta_k(x)$ is a piecewise continuous function on Ω.

The inverse problem of the differential Eq. (1), i. e. operator identification, can be described as follows: The governing equation will be in the form

$$Lu(x, t)=\varphi(x, t), \quad (x, t)\in\Omega\times T \tag{3}$$

with initial condition as

$$Eu(x, 0)=0, \quad x\in\Omega \tag{4}$$

and boundary condition as

$$Bu(x, t)=f(x, t), \quad x\in\partial\Omega, \ 0<t \tag{5}$$

and auxiliary boundary conditions as

$$B_iu(x, t)=f_i(x, t), \quad x\in\partial\Omega_i, \ i=1, 2, \cdots, I, \tag{6}$$

where E, B and B_i are initial operator, boundary operator and auxiliary boundary operator respectively. In Eq. (6) I is the number of auxiliary boundary conditions, and $\partial\Omega_i$ is a part of boundary $\partial\Omega$.

The inverse problem is to determine the coefficients $\alpha_k(x)$, $\beta_k(x)$ $(k=1, 2, \cdots, m)$ of the unknown operator from known operators A_k, C_k, D_k, B, B_i, E and Eqs. (3)—(6).

Numerical Algorithm. The PST calls for the Laplace transformation of (3), (5), (6). So the problem is transformed from the time domain to the complex frequency domain and the corresponding problem is

$$\sum_{k=1}^{m}[A_k(\alpha_k(x)C_k)+\beta_k(x)P(s)]U(x, s)=\Phi(x, s), \tag{7}$$

$$\tilde{B}U(x, s)=F(x, s), \quad x\in\partial\Omega, \tag{8}$$

$$\tilde{B}_iU(x, s)=F_i(x, s), \quad x\in\partial\Omega_i, \ i=1, 2, \cdots I, \tag{9}$$

where $P(s)$ is the polynomial of frequency s, and $U(x, s)$, $\Phi(x, s)$, $F(x, s)$, $F_i(x, s)$, $\tilde{B}U(x, s)$ and $\tilde{B}_iU(x, s)$ are Laplace transformations of $u(x, t)$, $\varphi(x, t)$, $f(x, t)$, $f_i(x, t)$, $Bu(x, t)$ and $B_iu(x, t)$ respectively.

Now, the synthesis is carried out in the (x, s) domain, and the unknown

parameters will be determined by an iterative process. The iterative numerical algorithm begins with

$$\alpha_k^{n+1}(x)=\alpha_k^n(x)+\delta\alpha_k^n(x),\quad \beta_k^{n+1}(x)=\beta_k^n(x)+\delta\beta_k^n(x),$$
$$U^{n+1}(x,\ s)=U^n(x,\ s)+\delta U^n(x,\ s),\quad k=1,\ 2,\ \cdots,\ m,\ n=0,\ 1,\ 2,\ \cdots, \tag{10}$$

where the superscripts denote the cycles of iteration, $\alpha_k^0(x)$ and $\beta_k^0(x)$ are initial guess for the unknown coefficients $\alpha_k(x)$, $\beta_k(x)$ and $\|\delta\alpha_k^n\|<\|\alpha_k^n\|$; $\|\delta\beta_k^n\|<\|\beta_k^n\|$; $\|\delta U^n\|<\|U^n\|$. Substituting (10) into (7) and (8) we get

$$\hat{L}^n(U^n(x,\ s)+\delta U^n(x,\ s))=\Phi(x,\ s),$$
$$\tilde{B}(U^n(x,\ s)+\delta U^n(x,\ s))=F(x,\ s),\quad x\in\partial\Omega,$$

where operator

$$\hat{L}^n=\sum_{k=1}^{m}[A_k(\alpha_k^n(x)+\delta\alpha_k^n(x))c_k+(\beta_k^n(x)+\delta\beta_k^n(x))P(s)].$$

Splitting the above equation, according to the order of δ and neglecting the terms of $o(\delta^2)$, one obtains two equations: one is for $U^n(x,\ s)$:

$$L^nU^n(x,\ s)=\Phi(x,\ s),\quad x\in\Omega,$$
$$\tilde{B}U^n(x,\ s)=F(x,\ s),\quad x\in\partial\Omega, \tag{11}$$

where

$$L^n=\sum_{k=1}^{m}[A_k(\alpha_k^n(x)c_k)+\beta_k^n(x)P(s)], \tag{12}$$

and the other is for $\delta U^n(x,\ s)$:

$$L^n\delta U^n(x,\ s)=-\sum_{k=1}^{m}[A_k(\delta\alpha_k^n(x)c_k)+\delta\beta_k^n(x)P(s)]U^n(x,\ s),\quad x\in\Omega \tag{13}$$

$$\tilde{B}\delta U^n(x,\ s)=0,\quad x\in\partial\Omega. \tag{14}$$

By the method of Green's function, Eq. (13) can be changed to a Fredholm integral equation of first kind which relates to $\delta\alpha_k^n$, $\delta\beta_k^n$ and δU^n:

$$\delta U^n(x,\ s)=-\int_\Omega G^n(x,\ x',\ s)\sum_{k=1}^{m}[A_k(\delta\alpha_k^n(x')c_k)+\delta\beta_k^n(x')P(s)]U^n(x',\ s)dx', \tag{15}$$

where $G^n(x,\ x',\ s)$ is Green's function of the differential operator L^n with homogeneous boundary condition.

For the purpose of iteration and acceleration of the convergence, $U^{n+1}(x,\ s)$ on the left side of (15) can be replaced by $U(x,\ s)$. Then (15) becomes

$$U(x,\ s)-U^n(x,\ s)=-\int_\Omega G^n(x,\ x',\ s)\sum_{k=1}^{m}[A_k(\delta\alpha_k^n(x')c_k)$$
$$+\delta\beta_k^n(x')P(s)]U^n(x',\ s)dx'. \tag{16}$$

Applying operator $\tilde{B}_i$ to both sides of (16) yields, with the help of (9),

$$F_i(x,\ s)-\tilde{B}_iU^n(x,\ s)=-\int_\Omega \tilde{B}_iG^n(x,\ x',\ s)\sum_{k=1}^{m}[A_k(\delta\alpha_k^n(x')c_k)$$
$$+\delta\beta_k^n(x')P(s)]U^n(x',\ s)dx',\quad i=1,\ 2,\ \cdots,\ I. \tag{17}$$

If $U^n(x,\ s)$ is known, then (17) is a system of Fredholm integral equations of first kind for unknown $\delta\alpha_k^n(x)$ and $\delta\beta_k^n(x)$, $k=1,\ 2,\ \cdots,\ m$.

Eqs. (10), (11) and (17) form the basic structure for each iteration in the iterative numerical algorithm of PST. The procedure is

(a) Use a numerical integration subroutine to evaluate the Laplace transforms

$\varphi(x, t), f(x, t)$ and $f_i(x, t), i=1, 2, \cdots, I$, for different values of $s=s_j$, $j=1, 2, \cdots, J$.

(b) Give initial guess: $\alpha_k^0(x)$, $\beta_k^0(x)$, $k=1, 2, \cdots, m$.

(c) Solve (11) and calculate Green's function of operator L^0 for $s=s_j$, $j=1, 2, \cdots, J$, to obtain $U^0(x, s_j)$ and $G^0(x, x', s_j)$.

(d) Solve (17) to obtain $\delta\alpha_k^0(x)$, $\delta\beta_k^0(x)$; obtain from (10) $\alpha_k^1(x)$, $\beta_k^1(x)$, $k=1, 2, \cdots, m$.

This is the essence of the first cycle of itration. As for other cycles, just repeat the procedure (b)—(d), until the criterion of convergence is satisfied.

Example. "Remote sensing of thermal conductivity and specific heat". An example for an inverse problem of a differential equation with multi-parameter to be determined is given here. The inverse problems for linear and nonlinear diffusion equations have been studied by many researchers [5]–[9]. However, the techniques they employed require the knowledge of the heat flux at the boundary, which cannot be easily measured. Moreover, by using those techniques only one unknown parameter can be determined. In our example, the thermal conductivity and specific heat of a nonhomogeneous material can be inferred from a small number of experimental data obtained through remote sensing techniques on the boundary as opposed to *in situ* techniques in the interior. Experimentally, if a reliable experiment can be performed, the measured physical quantity should be as fundamental as possible; in this case, the temperature measurement is preferred to the heat flux measurement.

Consider a diffusion equation of one dimension

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial u(x, t)}{\partial x}\right)=\rho(x)c(x)\frac{\partial u(x, t)}{\partial t}, \quad 0\leqslant x\leqslant 1, \ 0<t.$$

Without loss of generality, suppose $\rho(x)=1$. The above equation becomes

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial u(x, t)}{\partial x}\right)=c(x)\frac{\partial u(x, t)}{\partial t}, \quad 0\leqslant x\leqslant 1, \ 0<t \tag{18}$$

with initial condition

$$u(x, 0)=0, \tag{19}$$

boundary conditions

$$u(0, t)=f(t), \quad u(1, t)=h(t), \quad 0\leqslant t \tag{20}$$

and auxiliary boundary conditions

$$\left.\frac{\partial u(x, t)}{\partial x}\right|_{x=0}=a(t), \quad \left.\frac{\partial u(x, t)}{\partial x}\right|_{x=1}=b(t), \quad 0\leqslant t, \tag{21}$$

Where $f(t), h(t), a(t)$ and $b(t)$ are given functions which are Laplace transformable, $k(x)$ and $c(x)$ are thermal conductivity and specific heat respectively, to be determined from Eqs. (18)—(21).

Obviously, Eq. (18) is a specific case of Eq. (3) with $m=1$, operators $A_1=\frac{\partial}{\partial x}$, $C_1=\frac{\partial}{\partial x}$, $D_1=\frac{\partial}{\partial t}$, unknown coefficients $\alpha_1(x)=k(x)$, $\beta_1(x)=c(x)$ and $\varphi(x, t)=0$.

Using the Laplace transform on the differential equation and boundary conditions (18), (20) and (21), with the help of (10), we get

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial U(x, s)}{\partial x}\right)-sc(x)U(x, s)=0, \tag{22}$$

$$U(0, s)=F(s), \quad U(1, s)=H(s), \tag{23}$$

$$\left.\frac{\partial U(x, s)}{\partial x}\right|_{x=0}=A(s), \quad \left.\frac{\partial U(x, s)}{\partial x}\right|_{x=1}=B(s). \tag{24}$$

Numerical Simulation. In order to test the feasibility and to study the general characteristics of the computational algorithm without real measurement data, the following numerical simulation procedure is carried out:

$k^*(x)$ and $c^*(x)$, which are supposed to represent the correct thermal conductivity and specific heat of an object, and also the boundary conditions $f(t)$ and $h(t)$, which are supposed to represent the measured data, should be chosen. Their Laplace transform $F(s)$ and $H(s)$ are numerically computed for a chosen discrete set of $s=s_j$, $j=1, 2, \cdots, J$.

The two-point boundary value problems (22), (23) with the chosen $k^*(x)$, $c^*(x)$, $F(s_j)$ and $G(s_j)$ are solved by means of the finite difference method (or other numerical methods). Thus one generates the rest of the supposedly measured data $A(s_j)$ and $B(s_j)$, $j=1, 2, \cdots, J$, by a simple finite difference approximation.

$k^0(x)$ and $c^0(x)$ are assumed. Then, according to the procedure described above, $k^1(x)$ and $c^1(x)$ are obtained. In a similar manner, $k^2(x)$ and $c^2(x)$ are obtained. This is continued until finally a numerical limit, $k^n(x)$ and $c^n(x)$, is reached.

The L_2-norms $\|k^*(x)-k^n(x)\|_2$ and $\|c^*(x)-c^n(x)\|_2$ can be used as a criterion for evaluating the performance of the computational algorithm.

To avoid the expenses in performing the numerical Laplace transformation, $f(t)=1-e^{-t}$ and $h(t)=0$ are chosen such that $F(s)=1/(s(s-1))$ and $H(s)=0$.

To make the solution $\delta k^n(x)$ unique to Eq. (17), we should add a boundary condition $\delta k^n(0)=0$. If we add another boundary condition for $\delta c^n(x)$, for example $\delta c^n(1)=0$, then the accuracy of the solution can be improved greatly. These conditions mean that the initial guess $k^0(x)$ and $c^0(x)$ should be identical with the exact solution at the boundary points, i. e. $k^0(0)=k^*(0)$, $c^0(1)=c^*(1)$.

The trapezoidal rule with 16 nodes on the interval [0, 1] is used to discretize the integrals for all the examples. The numerical simulation here is carried out for five examples. The numerical results are plotted in Figs. 1—5. The maximum norms of $\|k^*(x)-k^n(x)\|_\infty$ and $\|c^*(x)-c^n(x)\|_\infty$ for various cases can be estimated from the

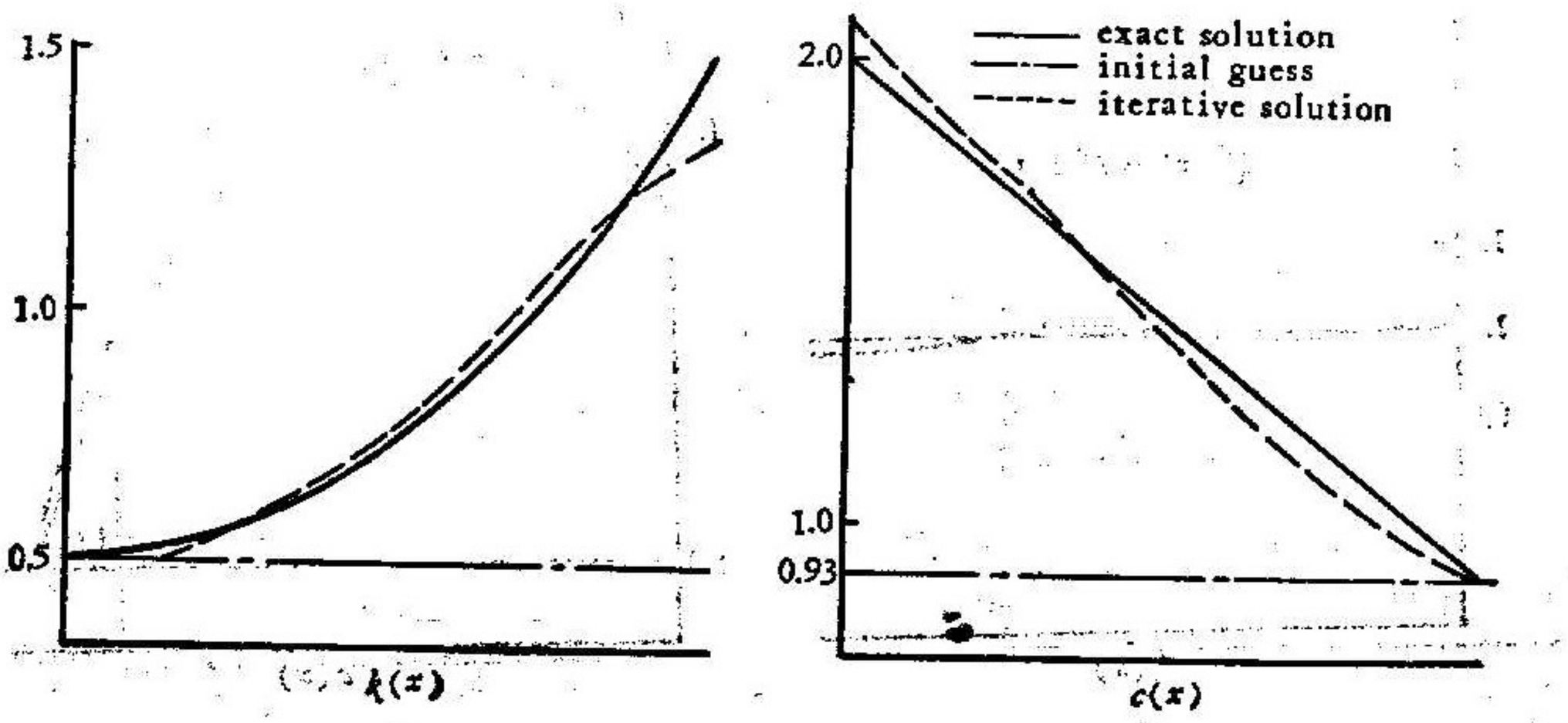

Fig. 1

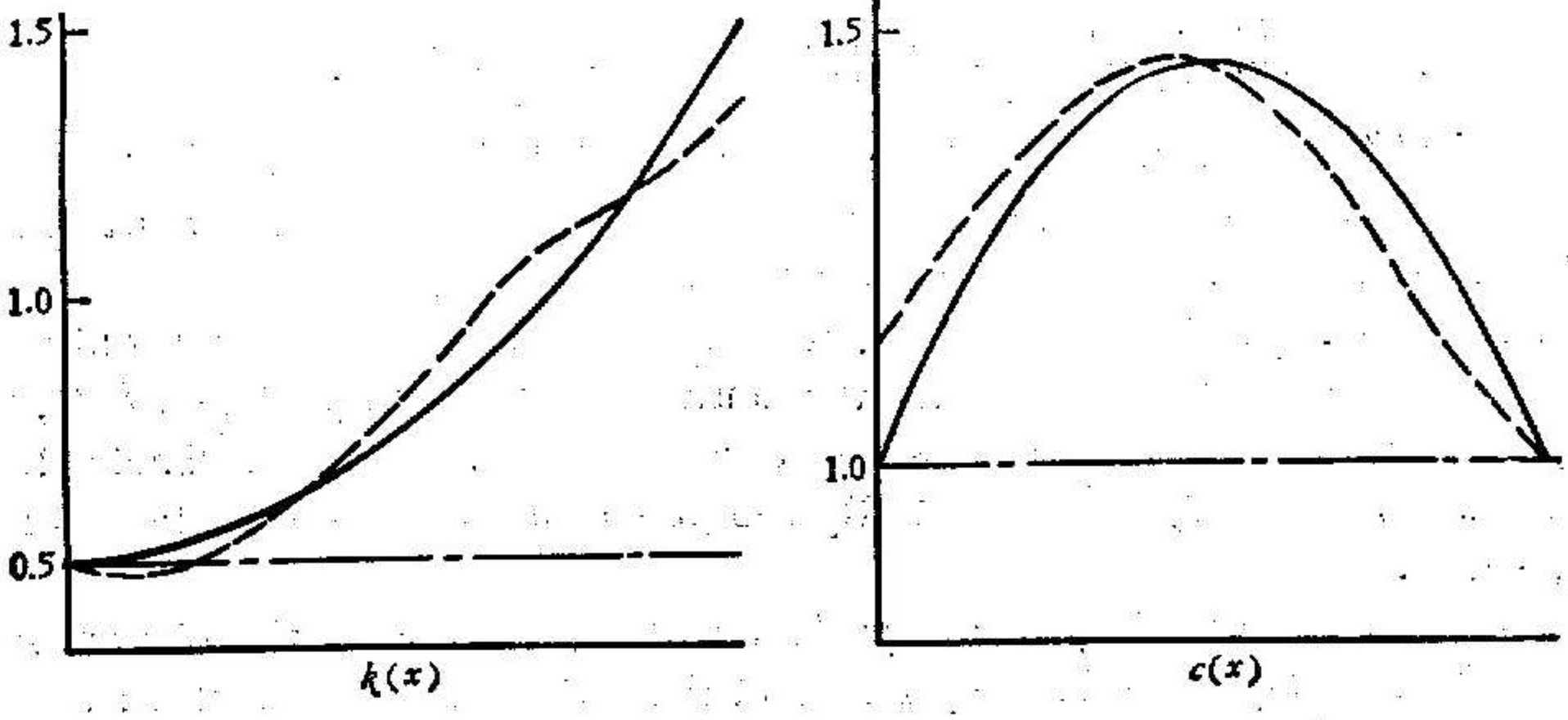

Fig. 2

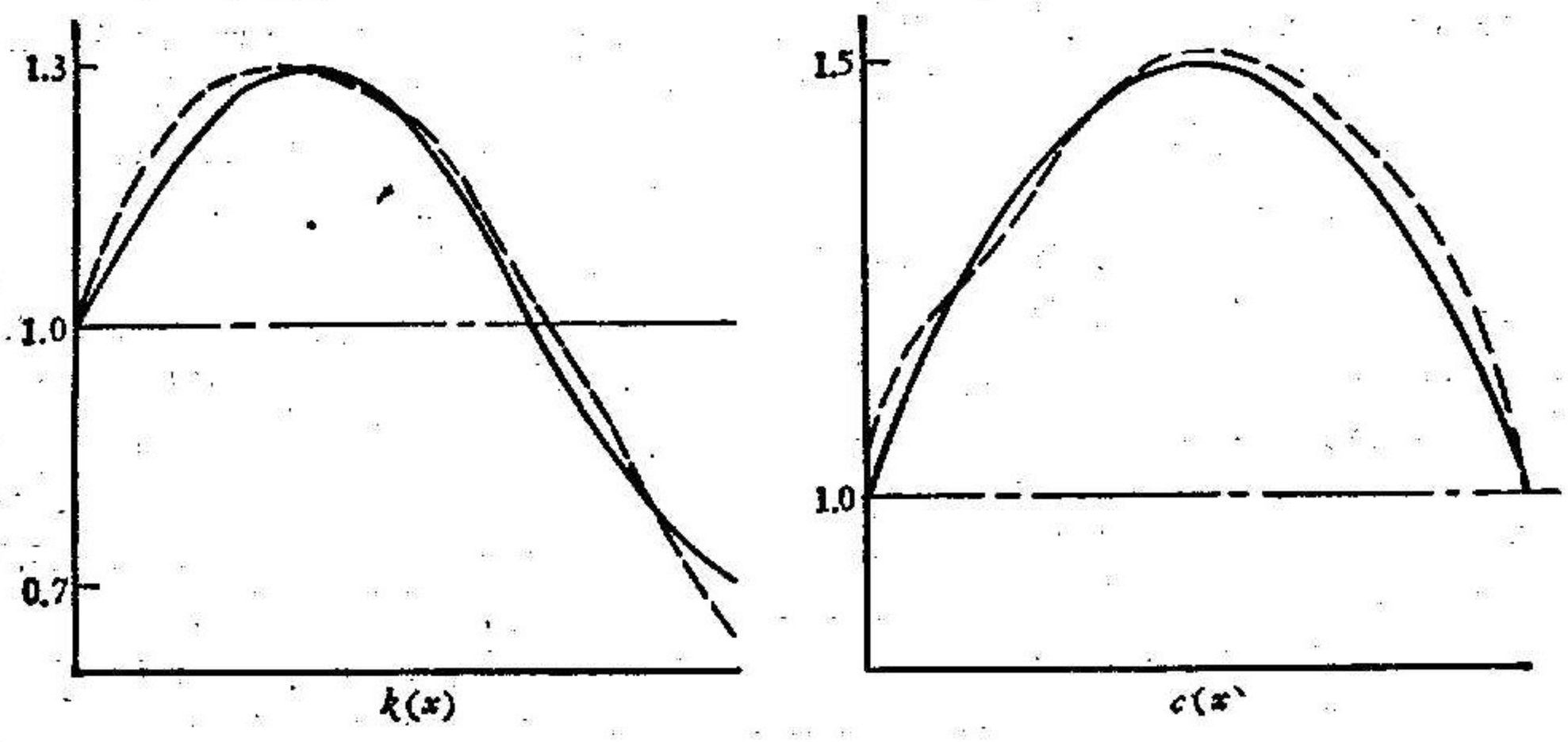

Fig. 3

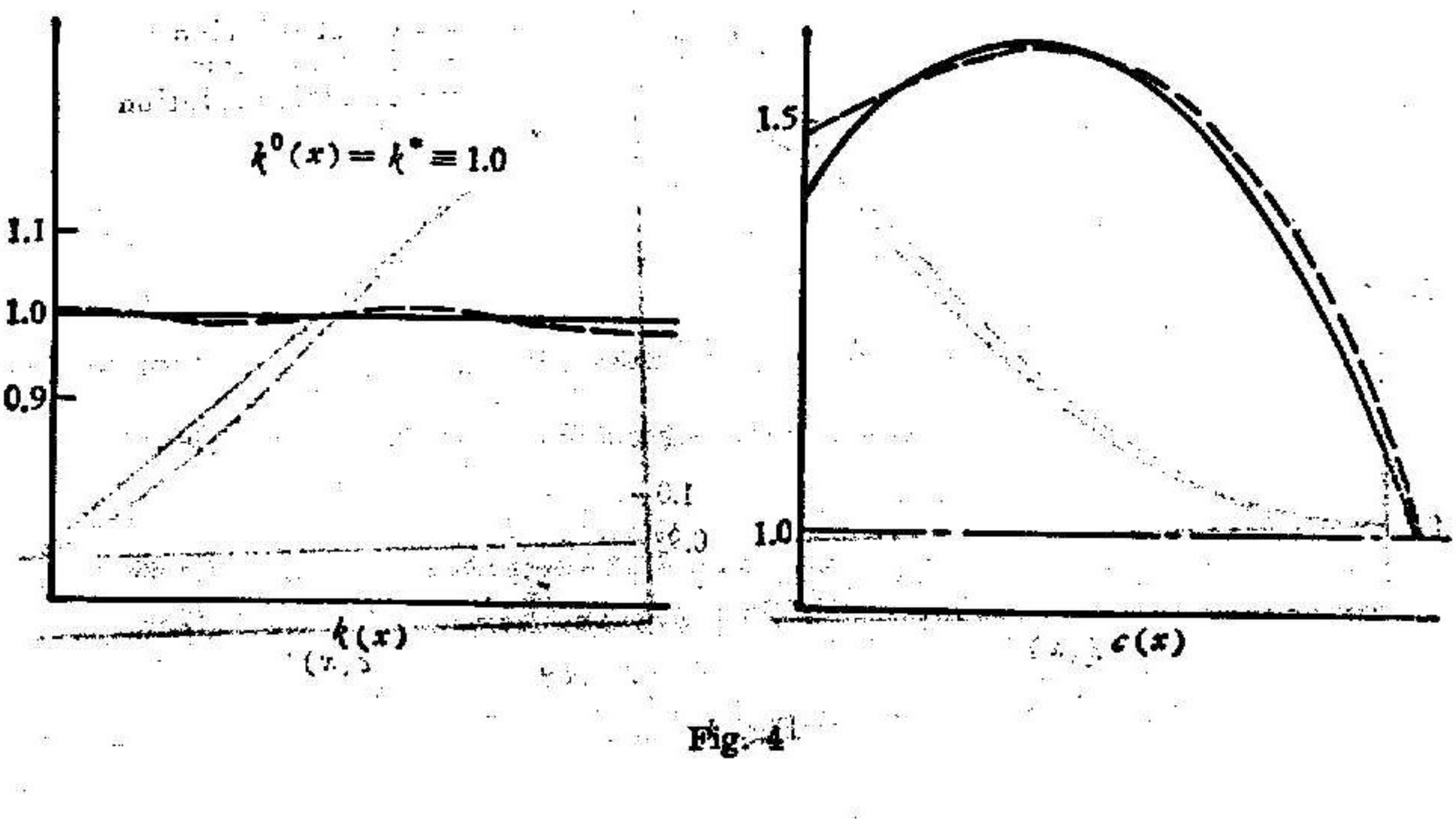

Fig. 4

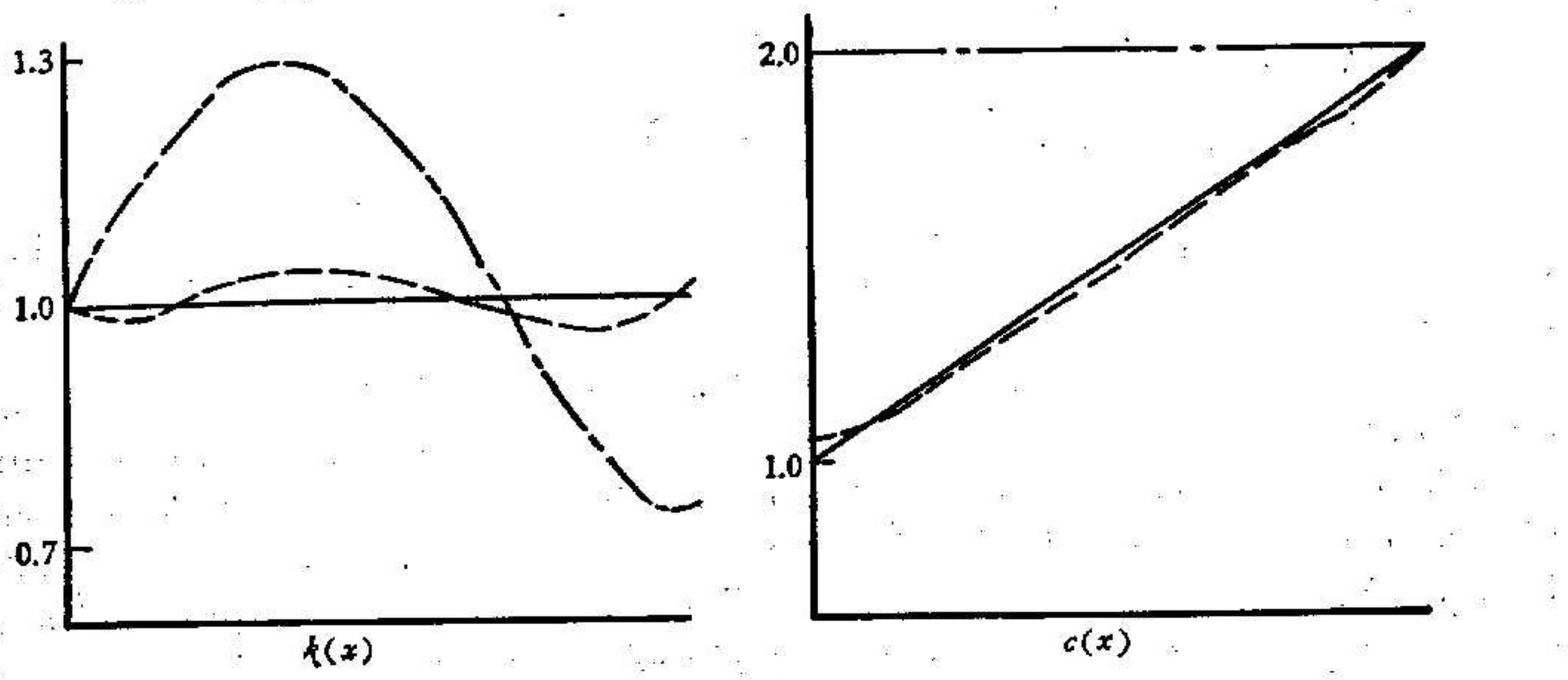

Fig. 5

graphs in these figures. The L_2-norms $e_k^n = \|k^*(x) - k^n(x)\|_2$ and $e_c^n = \|c^*(x) - c^n(x)\|_2$ for various cases are tabulated in Table 1. e_k^n and e_c^n as two functions of the number of iterative cycles for the numerical examples in Fig. 4 and Fig. 5 are shown in Fig. 6 and Fig. 7 respectively.

Table 1

Fig.	1	2	3	4	5
e_k^0	3.52	2.53	0.68	0	0.67
e_k^n	0.062	0.097	0.023	0.0016	0.016
e_c^0	6.33	1.06	2.02	3.50	5.51
e_c^n	0.094	0.069	0.026	0.021	0.015
n	10	13	15	7	19

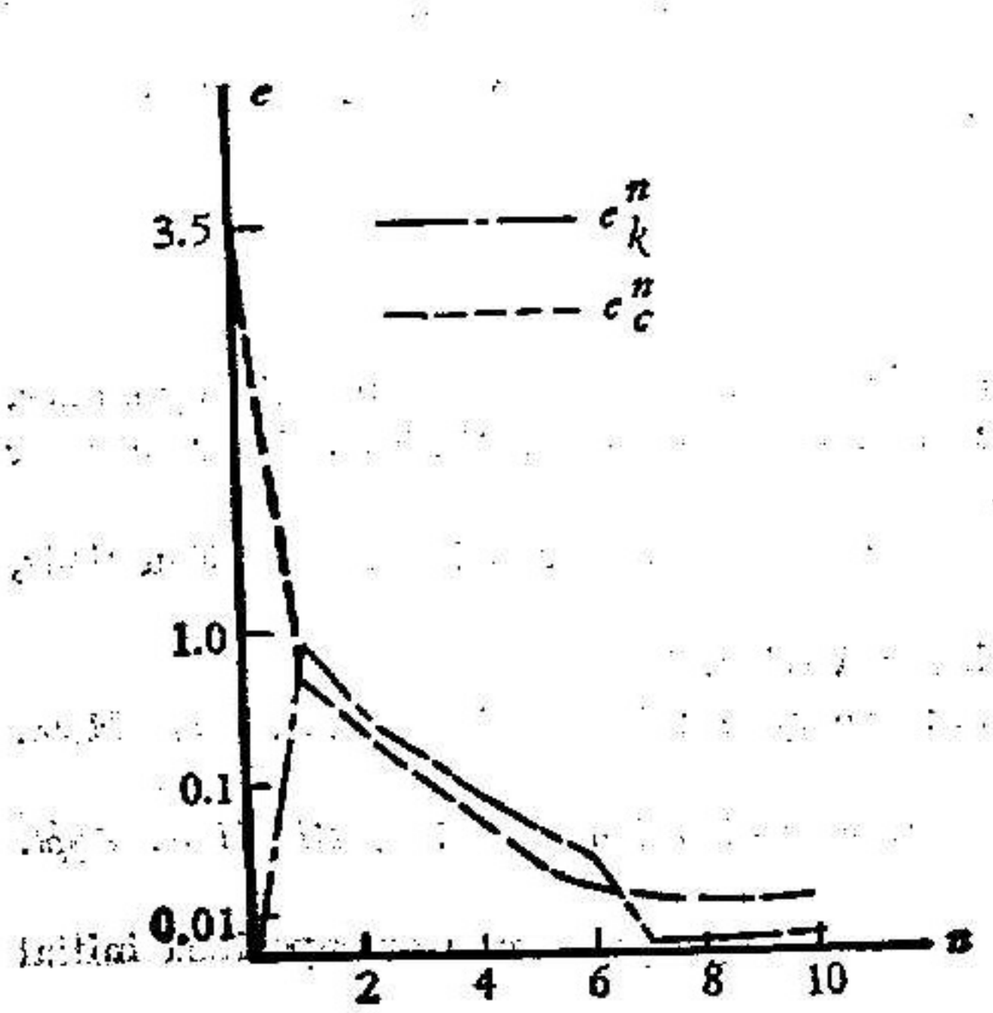

Fig. 6

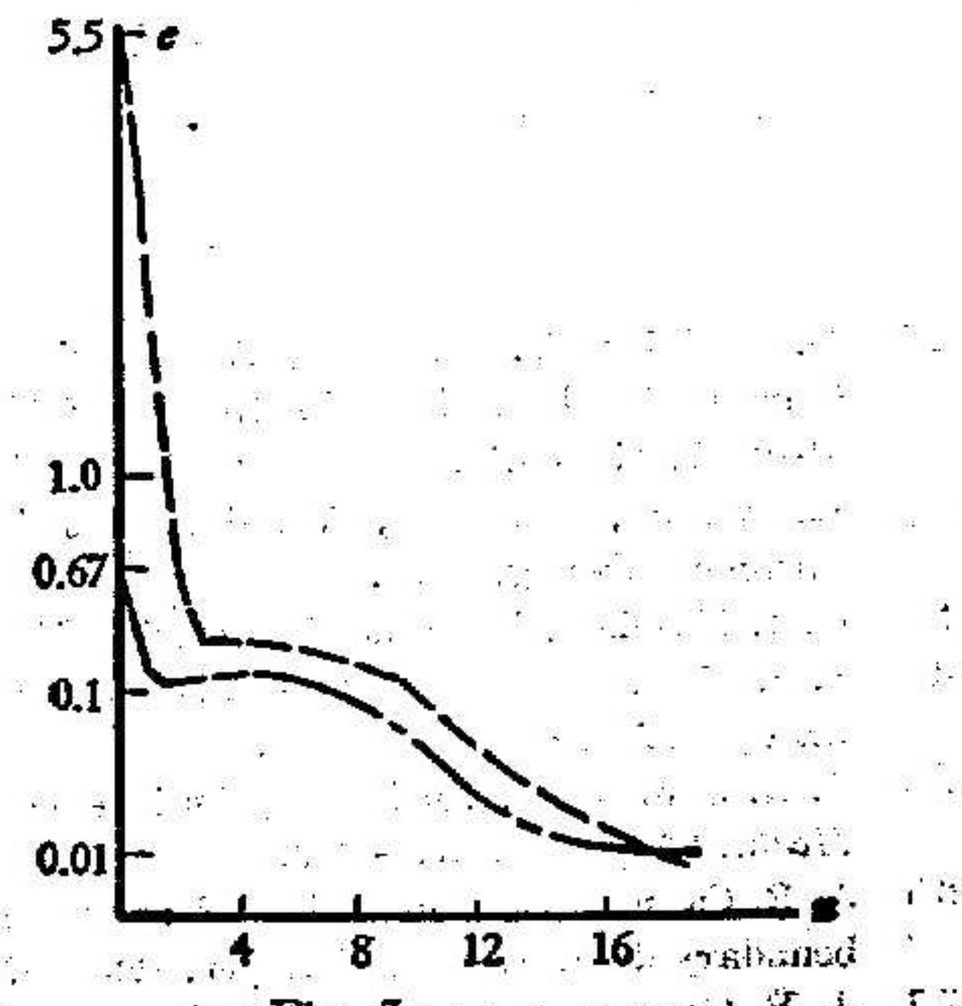

Fig. 7

3. Discussion

In the earlier paper[12], we studied the general characteristics of PST. It is still effective for the inverse problems with multi-parameter to be determined. In addition, it should be pointed out that:

Both the number of frequency set and their values $s_j's$ affect the accuracy of the solution. The fewer the $s_j's$, the rougher the solutions. However, if too large a number of $s_j's$ is accepted, the condition number of the linear systems of equations from the discrete Fredholm integration of first kind will be too large. So the proper choice of the set s_j is important for accurate and stable solutions. Hagin[14] proposed a well-conditioned matrix criterion for choosing s_j in solving the Fredholm integral equation of first kind with oscillatory kernel. It can be employed, but not always. Fortunately, when we solve the Fredholm integral equation of first kind by using the Phillips-Tikhonov regularization method, the smooth functional involves second-order stabilizers with constant coefficients[19]–[20], the regularization parameter was decreasing with the iteration; then the change of the set $s=s_j$ results in no significant differences in solutions. So in this paper, we set $s_j=j$; $j=1, 2, \cdots, 11$, in all the examples.

From the derivation of the iterative numerical algorithm in section 2, it is clear that there is no restriction on space dimension or the type of differential operator L for our algorithm, whether L is hyperbolic or parabolic.

The main problem of the numerical algorithm is the consumption of computer time. The direct problem (11), Green's function and Fredholm integral equation of first kind (17) should be solved in each iterative cycle. We can solve (11) and calculate Green's function with respect to the same differential operator L^* simultaneously. Actually, we can avoid calculating Green's function, if the algorithm is derived in a different way; but it is beyond this paper.

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