Journal of Computational and Applied Mathematics 232 (2009) 227–239

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

A new approach to numerical differentiation

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ARTICLE INFO

Article history:
Received 27 July 2007
Received in revised form 31 May 2009

Keywords:
Numerical differentiation
Ill-posed problem
TSVD method
Singular system
Discrete sine transform

ABSTRACT

In this paper we consider the numerical differentiation of functions specified by noisy data. A new approach, which is based on an integral equation of the first kind with a suitable compact operator, is presented and discussed. Since the singular system of the compact operator can be obtained easily, TSVD is chosen as the needed regularization technique and we show that the method calls for a discrete sine transform, so the method can be implemented easily and fast. Numerical examples are also given to show the efficiency of the method.

1. Introduction

Numerical differentiation is a problem to determine the derivative of a function from the values on an interval or some scattered points. It arises from many scientific researches and applications, e.g., the identification of the discontinuous points in an image process [1]; the problem of solving the Abel integral equation [2]; the problem of determining the peaks in chemical spectroscopy [3] and some inverse problems in mathematical physical equations [4]. The main difficulty is that it is an ill-posed problem, which means that small errors in the measurement of a function may lead to large errors in its computed derivatives [5,4]. A number of techniques have been developed for numerical differentiation [6–8,4,9]. One type of method is to transform the differentiation problem into an operator equation of the first kind. In fact, for given $g(t) \in H^1[0, 1]$, to find $f = Dg = g'$ is equivalent to solve the Volterra integral equation of the first kind

$$(K_1 f)(s) = \int_0^s f(t)\mathrm{d}t = g(s) - g(0), \quad s \in [0, 1]. \tag{1.1}$$

In this paper we will point out the disadvantage of operator K_1 and a new operator which is a modified form of K_1 will be presented. Since a singular system of the new operator can be obtained easily, it seems natural to use the TSVD method for this problem and good results may be expected. A convergence result, analogous to the literature [4], will be obtained by our method. Comparing with the Tikhonov regularization method used in [4], the regularization parameter can be obtained easily by TSVD method. Moreover, it is well known that the Tikhonov method has a finite saturation index, which means that it is impossible to improve the convergence rates of the regularization solution with increasing smoothness assumption of exact solutions. But for TSVD method this disadvantage will be overcome. Moreover, we will point out that our method calls for a discrete sine transform when the noisy values of the function to be differentiated at the nodes are given, so the method can be implemented easily and fast.

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doi:10.1016/j.cam.2009.06.001

The paper is organized as follows. The disadvantage of operator K_1 will be pointed out in Section 2, and in Section 3 an improved operator will be presented and its properties will be discussed. In Section 4, algorithms based on TSVD method for numerical differentiation are proposed and analyzed. The numerical implement of the method will be discussed in Section 5, some numerical examples are also given to show the efficiency of the new method.

2. A classical operator and its disadvantage

In some papers, numerical differentiation is considered as a Volterra integral equation of the first kind: [5,9]

$$(K_1 f)(s) = \int_0^s f(t)\mathrm{d}t = g(s) - g(0) =: \overline{g}(s), \quad s \in [0, 1] \tag{2.1}$$

where $K_1 : L^2[0, 1] \to H^1[0, 1] \subset L^2[0, 1]$ is a compact operator. Instead of g, in practice we usually only have perturbed data g^δ. And the conditions

$$\|g^\delta - g\| \le \delta \tag{2.2}$$

$$g^\delta(0) - g(0) = \epsilon, \qquad |\epsilon| \le C_1\delta \tag{2.3}$$

are assumed with δ being a known error level and C_1 a constant. The perturbed form of Eq. (2.1) is

$$(K_1 f)(s) = \overline{g}^\delta(s), \tag{2.4}$$

where

$$\overline{g}^\delta(s) = g^\delta(s) - g^\delta(0). \tag{2.5}$$

The self-adjoint operator $K_1^* K_1$ can be given as

$$(K_1^* K_1 f)(r) = \int_r^1 \int_0^s f(t)\mathrm{d}t\mathrm{d}s, \quad r \in [0, 1]. \tag{2.6}$$

It can be verified that the eigen problem $K_1^* K_1 e = \lambda e$ is equivalent to

$$\begin{cases} \lambda e'' + e = 0 \\ e(1) = e'(0) = 0 \end{cases} \tag{2.7}$$

and the solution is

$$\lambda_j = \frac{4}{(2j-1)^2\pi^2}, \qquad e_j = e_j(t) = \sqrt{2}\cos\lambda_j^{-1/2}t, \quad j \in N.$$

Therefore the singular values and the corresponding singular functions of the operator K_1 can be taken as [5]

$$\begin{aligned} &\sigma_j = \lambda_j^{1/2} = \frac{2}{(2j-1)\pi}, \\ &v_j = e_j, = \sqrt{2}\cos\sigma_j^{-1}t, \qquad u_j = \sigma_j^{-1}K v_j = \sqrt{2}\sin\sigma_j^{-1}s, \quad j \in N. \end{aligned} \tag{2.8}$$

In the following we discuss the generalized smooth scale of a function with respect to the operator K_1, which is a key index concerning convergence rates of a regularization method [5]. We need some results of Fourier series. For a periodic function $\phi(t)$ with period $2l$, its Fourier series has the form

$$\phi(t) \sim \frac{a_0}{2} + \sum_{j=1}^{\infty}\left(a_j\cos\frac{j\pi t}{l} + b_j\sin\frac{j\pi t}{l}\right),$$

or

$$\phi(t) \sim \sum_{j=-\infty}^{\infty} c_j \mathrm{e}^{j\pi \mathrm{i}t/l},$$

where

$$a_j = \frac{1}{l}\int_{-l}^{l}\varphi(t)\cos\frac{j\pi t}{l}, \quad j = 0, 1, 2, \ldots$$

$$b_j = \frac{1}{l}\int_{-l}^{l}\varphi(t)\sin\frac{j\pi t}{l}, \quad j = 1, 2, \ldots$$

$$c_j = \frac{1}{2}(a_j - \mathrm{i}b_j), \qquad b_0 = 0, \qquad a_{-j} = a_j, \qquad b_{-j} = -b_j.$$