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The singular value expansion of the Volterra integral equation associated to a numerical differentiation problem

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ABSTRACT

We consider the Volterra integral equation of the first kind for the derivative of a given function with one-side boundary conditions. We give a method to obtain the singular value expansion for the corresponding integral kernel. This singular value expansion can be used to give algorithms for the solution of the numerical differentiation problem. A numerical experiment shows the results obtained by a simple version of such algorithms.

1. Introduction

We consider the numerical differentiation problem, where the derivatives of a function are approximated by using values of the function and eventually other knowledge about the function itself.

The direct use of numerical differentiation methods can support applications where functions are known only on discrete sets, such as in the context of sampling processes, or applications where the derivatives computation involves too complex formulas. A usual situation where such applications require the computation of numerical differentiation is the solution of optimization problems by derivative-free methods, see [4] for details.

A problem of slightly different nature is the solution of differential equations giving a relation between the unknown function and its derivatives. For such problems the approximation of derivatives plays a central role and allows the definition of algebraic equations for the corresponding numerical solution [6].

The simplest method for the numerical differentiation is given by the finite difference approximations. Despite their popularity, finite difference methods for the evaluation of the derivative have low accuracy and stability properties [7], [13]. Nevertheless, if the function is analytic on a neighborhood of the derivation point and it can be evaluated for each point of this neighborhood, the problem is well-conditioned [11] and it

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can be efficiently solved by numerical methods. So, in scientific literature, several numerical differentiation algorithms of arbitrary analytic function are present.

For example, methods to approximate derivatives of real functions using complex variables have been studied in [1], [2], [7], [15], [18]. In particular, the method proposed in [1] is based on numerical inversion of a complex Laplace transform; the one proposed in [7] uses the Fast Fourier Transform.

Differential quadrature [22] is another well-known method where derivatives are approximated by weighted sums of function values, and it has been applied extensively in various engineering problems [17]. The weighting coefficients of the polynomial based, Fourier expansion based and exponential based differential quadrature methods can be computed explicitly.

Numerical differentiation algorithms based on polynomial interpolation approximate the function derivative by the derivative of the interpolation polynomials. Some versions of this strategy have obtained good results in terms of accuracy and stability; for example, [3] uses low-order Chebyshev interpolation polynomials to compute the derivative of noisy functions, [10] and [12] use Neville algorithm for computing the interpolating polynomial in order to compute stable approximation of function derivative. We note that this algorithm is used in the routine D04AAF of the NAG Library [14] to approximate the derivatives up to order 14.

From standard arguments on Taylor series, the differentiation problem with one-side boundary conditions can be reformulated as a Volterra integral equation of the first kind. Several authors have discussed the use of such an integral equation for the numerical differentiation problem. For example, in [9] it is used to compute the stepsize in the finite-difference methods, in [21] has been proposed a sparse discretization of this integral equation, in [20] a fast multiscale solver has been proposed for the numerical solution of the Tikhonov regularization equation.

In this paper we consider the problem of numerical differentiation reformulated as this Volterra integral equation of the first kind. We present a method for the construction of the singular value expansion of the kernel of such an integral equation; so that, it allows the definition of simple algorithms to solve this integral equation and, in turn, to compute the numerical derivatives of a given function. A numerical experiment is used to test the proposed method by comparing the corresponding results with the ones obtained by a well-established scientific software.

In Section 2 the problem of numerical differentiation is described together with the corresponding Volterra integral equation of the first kind, as well as its solution obtained by using the singular value expansion of the corresponding integral kernel K. In Section 3, the characteristic equation for the singular values of K is given together with the analytic expressions of the corresponding left-singular functions and right-singular functions. In Section 4 some numerical examples are given. Section 5 describes some conclusions and future developments.

2. The integral equation for the derivation problem

Let $\nu \geq 1$ be a given integer number, and let $f : [0, 1] \to \mathbb{R}$ be a continuously differentiable function up to order ν, and suppose that $f^{(j)}(0)$, $j = 0, 1, \ldots, \nu-1$, are known or already calculated, where $f^{(j)}$ denotes the jth derivative of f. Hence, from standard arguments on Taylor formula, we have that the integral equation with unknown function $v : [0, 1] \to \mathbb{R}$

$$\mathcal{K}v(t) = f(t) - \sum_{j=0}^{\nu-1} \frac{f^{(j)}(0)}{j!} t^j, \quad t \in [0, 1],$$

where $\mathcal{K}$ is the integral operator having kernel $K : [0, 1] \times [0, 1] \to \mathbb{R}$ defined by

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