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Evaluation of small elements of the eigenvectors of certain symmetric tridiagonal matrices with high relative accuracy

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ABSTRACT

Evaluation of the eigenvectors of symmetric tridiagonal matrices is one of the most basic tasks in numerical linear algebra. It is a widely known fact that, in the case of well separated eigenvalues, the eigenvectors can be evaluated with high relative accuracy. Nevertheless, in general, each coordinate of the eigenvector is evaluated with only high *absolute* accuracy. In particular, those coordinates whose magnitude is below the machine precision are not expected to be evaluated with any accuracy whatsoever.

It turns out that, under certain conditions, frequently encountered in applications, small (e.g. 10^{-50}) coordinates of eigenvectors of symmetric tridiagonal matrices can be evaluated with high *relative* accuracy. In this paper, we investigate such conditions, carry out the analysis, and describe the resulting numerical schemes. While our schemes can be viewed as a modification of already existing (and well known) numerical algorithms, the related error analysis appears to be new. Our results are illustrated via several numerical examples.

1. Introduction

The evaluation of eigenvectors of symmetric tridiagonal matrices is one of the most basic tasks in numerical linear algebra (see, for example, such classical texts as [2,5,8–10,13,14,24,26,27]). Several algorithms to perform this task have been developed; these include Power and Inverse Power methods, Jacobi Rotations, QR and QL algorithms, to mention just a few. Many of these algorithms have become standard and widely known tools.

In the case when the eigenvalues of the matrix in question are well separated, most of these algorithms will evaluate the corresponding eigenvectors to a high *relative* accuracy (see also Section 2 below). More specifically, suppose that $n > 0$ is an integer, that A is an n by n symmetric matrix, that λ is an eigenvalue of A,

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that $v \in \mathbb{R}^n$ is the corresponding unit-length eigenvector, and that $\hat{v} \in \mathbb{R}^n$ is its numerical approximation (produced by one of the standard algorithms). Then,

$$\|v - \hat{v}\| \leq M \cdot \varepsilon, \tag{1}$$

where $\| \cdot \|$ denotes the Euclidean norm, ε is the machine precision (e.g. $\varepsilon \approx 10^{-16}$ for double precision calculations), and M is proportional to the inverse of the distance between λ and the rest of the spectrum of A.

However, a closer look at (1) reveals that it only guarantees that the *coordinates* of v be evaluated to high *absolute* accuracy. This is due to the following trivial observation. Suppose that we add ε to the first coordinate $\hat{v}_1$ of $\hat{v}$. Then, the perturbed $\hat{v}$ will not violate (1). On the other hand, the relative accuracy of $\hat{v}_1$ can be as large as

$$\frac{|v_1 + \varepsilon - v_1|}{|v_1|} = \frac{\varepsilon}{|v_1|}. \tag{2}$$

In particular, if $|v_1| < \varepsilon$, then $\hat{v}_1$ is not guaranteed to approximate v_1 with any relative accuracy whatsoever.

Sometimes the poor relative accuracy of "small" coordinates is of no concern; for example, this is usually the case when v is only used to project other vectors onto it. Nevertheless, in several prominent problems, small coordinates of the eigenvector often need to be evaluated to high relative accuracy. Numerical evaluation of special functions provides a rich source of such problems; these include the evaluation of Bessel functions (see Sections 3.1, 3.2.2, 6.1), the evaluation of some quantities associated with prolate spheroidal wave functions (see Section 6.2, and also [23]), and the evaluation of singular values of the truncated Laplace transform (see [16]), among others.

In this paper, we describe a scheme for the evaluation of the coordinates of eigenvectors of certain symmetric tridiagonal matrices, to high relative accuracy. More specifically, we consider the matrices whose non-zero off-diagonal elements are constant (or approximately so), and whose diagonal elements constitute a monotonically increasing sequence (see, however, Remark 2 below). The connection of such matrices to Bessel functions and prolate spheroidal wave functions is discussed in Sections 3.2.2, 6.2, respectively. Also, we carry out detailed error analysis of our algorithm (see Sections 4.2, 4.3). While our scheme can be viewed as a modification of already existing (and well known) algorithms, such error analysis, perhaps surprisingly, appears to be new. In addition, we conduct several numerical experiments to illustrate the analysis, to demonstrate our scheme's accuracy, and to compare the latter to that of some classical algorithms (see Section 7).

The following is one of the principal analytical results of this paper (see Theorem 19 in Section 4.3 for a more precise statement, and Theorems 13, 14, 15, Corollary 6 in Section 4.2 below for the treatment of a more general case).

Theorem 1. *Suppose that $a \geq 1$ is a real number, and that, for any real $c \geq 1$, $n = n(c) > c$ is an integer, the real numbers $A_1(c), \dots, A_n(c)$ are defined via the formula*

$$A_j(c) = 2 + 2 \cdot \left(\frac{j}{c}\right)^a, \tag{3}$$

for every $j = 1, \dots, n$, and that the n by n symmetric tridiagonal matrix $A = A(c)$ is defined via the formula

$$A(c) = \begin{pmatrix} A_1 & 1 & & & & \\ 1 & A_2 & 1 & & & \\ & 1 & A_3 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & A_{n-1} & 1 \\ & & & & 1 & A_n \end{pmatrix}. \tag{4}$$

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