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Accurate eigenvalue decomposition of real symmetric arrowhead matrices and applications

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ABSTRACT

We present a new algorithm for solving the eigenvalue problem for an $n \times n$ real symmetric arrowhead matrix. The algorithm computes all eigenvalues and all components of the corresponding eigenvectors with high relative accuracy in $O(n^2)$ operations under certain circumstances. The algorithm is based on a shift-and-invert approach. Only a single element of the inverse of the shifted matrix eventually needs to be computed with double the working precision. Each eigenvalue and the corresponding eigenvector can be computed separately, which makes the algorithm adaptable for parallel computing. Our results extend to Hermitian arrowhead matrices, real symmetric diagonal-plus-rank-one matrices and singular value decomposition of real triangular arrowhead matrices.

1. Introduction and preliminaries

In this paper, we consider the eigenvalue problem for a real symmetric matrix A which is zero except for its main diagonal and one row and column. Since eigenvalues are invariant under similarity transformations, we can symmetrically permute the rows and the columns of the given matrix.

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Therefore, we assume without loss of generality that the matrix A is an $n \times n$ real symmetric arrowhead matrix of the form

$$A = \begin{bmatrix} D & z \\ z^T & \alpha \end{bmatrix}, \tag{1}$$

where

$$D = \operatorname{diag}(d_1, d_2, \ldots, d_{n-1})$$

is diagonal matrix of order $n-1$,

$$z = [\,\zeta_1 \quad \zeta_2 \quad \cdots \quad \zeta_{n-1}\,]^T \tag{2}$$

is a vector and α is a scalar.

Such matrices arise in the description of radiationless transitions in isolated molecules [3], oscillators vibrationally coupled with a Fermi liquid [9], and quantum optics [17] (see Example 4 in Section 5). Such matrices also arise in solving symmetric real tridiagonal eigenvalue problems with the divide-and-conquer method (see [11] and Example 5 in Section 5) and in updating the symmetric eigenvalue problem.

In this paper, we present an algorithm which computes all eigenvalues and all components of the corresponding eigenvectors with high relative accuracy in $O(n^2)$ operations.

Without loss of generality, we may assume that A is irreducible, that is,

$$\zeta_i \neq 0, \quad \text{for all } i$$

and

$$d_i \neq d_j, \quad \text{for all } i \neq j,\ i, j = 1, \ldots, n-1.$$

If A has a zero in the last column, say $\zeta_i = 0$, then the diagonal element d_i is an eigenvalue whose corresponding eigenvector is the i-th unit vector, and we can reduce the size of the problem by deleting the i-th row and column of the matrix, eventually obtaining a matrix for which all elements ζ_j are non-zero. If $d_i = d_j$, then d_i is eigenvalue of matrix A (this follows from the interlacing property (7)), and we can reduce the size of the problem by annihilating ζ_j with a Givens rotation in the (i, j)-plane and proceeding as in the previous case.

Further, by symmetric row and column pivoting, we can order elements of D such that

$$d_1 > d_2 > \cdots > d_{n-1}. \tag{3}$$

Without loss of generality we can also assume that $\zeta_i > 0$ for all i, which can be attained by pre- and post-multiplication of the matrix A with the matrix $D_s = \operatorname{diag}(\operatorname{sign}(\zeta_1), \ldots, \operatorname{sign}(\zeta_{n-1}), 1)$.

To summarize, in the sequel, we assume that A is ordered and an irreducible arrowhead matrix of the form (1), where elements of the diagonal matrix D satisfy (3) and $\zeta_i > 0$ for all i.

Let

$$A = V \Lambda V^T \tag{4}$$

be the eigenvalue decomposition of A. Here

$$\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$$

is a diagonal matrix whose diagonal elements are the eigenvalues of A, and

$$V = [\,v_1 \quad \cdots \quad v_n\,]$$

is an orthonormal matrix whose columns are the corresponding eigenvectors.