The Eigenvalue Problem for Hermitian Matrices with Time Reversal Symmetry

J. J. Dongarra,* J. R. Gabriel,* D. D. Koelling,* and J. H. Wilkinson†
Mathematics and Computer Science
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439
and
Stanford University
Stanford, California 94305

Submitted by Gene H. Golub

ABSTRACT

This paper describes a computational method for dealing with a class of matrices which arise in quantum mechanics involving time reversal and inversion symmetry. The algorithms presented here have greatly reduced the computational effort required to solve this problem and also produce a stable, more accurate solution.

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1. INTRODUCTION

An important problem in quantum mechanics involving time reversal and inversion symmetry is the computation of the eigensystem of a $2n \times 2n$ complex Hermitian matrix. This problem arises from the use of relativistic kinematics in the calculation of electronic structure for molecules and solids containing heavy atoms [4, 5]. The complex Hermitian matrix H is expressible

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in the form

$$H=\begin{bmatrix} A & B \\ -\bar{B} & \bar{A} \end{bmatrix}; \tag{1.1}$$

here and elsewhere the bar denotes the complex conjugate. From the Hermitian property of H we have

$$A = A^H, \qquad B = -\bar{B}^H = -B^T. \tag{1.2}$$

The first of these implies that A is Hermitian; the second implies that B is *complex skew symmetric*. Notice that B is not skew Hermitian and in general will not even be normal.

If λ is an eigenvalue of H (necessarily real) and

$$\begin{bmatrix} A & B \\ -\bar{B} & \bar{A} \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix}, \tag{1.3}$$

then

$$Ax + By = \lambda x \quad \text{and} \quad -\bar{B}x + \bar{A}y = \lambda y. \tag{1.4}$$

Hence,

$$\bar{A}\bar{x} + \bar{B}\bar{y} = \lambda \bar{x} \quad \text{and} \quad -B\bar{x} + A\bar{y} = \lambda \bar{y}. \tag{1.5}$$

and

$$\begin{bmatrix} A & B \\ -\bar{B} & \bar{A} \end{bmatrix}\begin{bmatrix} \bar{y} \\ -\bar{x} \end{bmatrix} = \lambda \begin{bmatrix} \bar{y} \\ -\bar{x} \end{bmatrix}, \tag{1.6}$$

showing that if $[x, y]^T$ is an eigenvector corresponding to λ, then $[\bar{y}, -\bar{x}]^T$ is also an eigenvector corresponding to λ. It is clear that the two vectors are orthogonal. Hence, the $2n$ eigenvalues of H consist of n pairs of equal eigenvalues.

In what follows it is assumed that the reader is familiar with the Givens and Householder algorithms for the reduction of a Hermitian matrix to a real symmetric tridiagonal matrix via elementary similarity transformations based on plane rotations and elementary Hermitians respectively.

The eigenvalues of H may be found simply by treating it as a complex $2n \times 2n$ Hermitian matrix, ignoring its structure. If this is done by reducing it to tridiagonal form with the Householder algorithm, then the structure of H is immediately destroyed by the first transformation. Since every eigenvalue of H appears twice, there is a similarity transformation by a unitary matrix of eigenvectors which reduces H to

$$H' = \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}, \tag{1.7}$$

where D is a diagonal matrix containing in general distinct elements.

It follows that there are also unitary transformations of possibly simpler form which reduce H to

$$H' = \begin{bmatrix} K & 0 \\ 0 & K \end{bmatrix} \quad \text{or} \quad H'' = \begin{bmatrix} T & 0 \\ 0 & T \end{bmatrix}, \tag{1.8}$$

where K is Hermitian and T is real tridiagonal.

The transformations which reduce H to diagonal form must have elements from the Galois field of the characteristic equation, since they solve that equation. The questicn for us is whether reduction to the K or T form can be done without access to that Galois field.

Usually in cases where symmetry leads to multiple eigenvalues there are unitary matrices U which are elements of a finite group and commute with H. In these cases the Galois field of each U is easily accessible, and reduction to the K form is straightforward from Schur's lemma. But in the case of time reversal these techniques cannot be used. From a group theoretical point of view, this paper shows that the T form with T real can be reached from H in Equation (1.1) by the standard numerical techniques of linear algebra.

2. MOTIVATION

The motivation for the algorithm we shall describe sprang from a consideration of the eigenvalue problem for a simple $n \times n$ complex Hermitian matrix X. We may write $X = Y + iZ$, where Y and iZ are the real and imaginary parts. The Hermitian property of X implies that

$$Y = Y^T \quad \text{and} \quad Z = -Z^T, \tag{2.1}$$

i.e., Y is real and symmetric and Z is real and skew symmetric. The matrix X may be reduced to real tridiagonal form in $n-2$ major steps. Each major step consists of two minor steps. (We emphasize that we are not recommending this as an efficient method of solving the standard Hermitian problem.) If we write

$$X = X^{(1)}, \tag{2.2}$$

then the rth major step may be expressed in the form

$$X^{(r+1)} = P^{(r)}D^{(r)}X^{(r)}(D^{(r)})^H P^{(r)}, \tag{2.3}$$

where $D^{(r)}$ is a complex unitary diagonal matrix and $P^{(r)}$ is a real elementary Hermitian matrix of the form $I - 2u^{(r)}(u^{(r)})^T$. The first step is wholly typical and is adequately illustrated by considering a matrix of order 4. We have then

$$X^{(1)} = \begin{bmatrix} y_{11} & y_{12}+iz_{12} & y_{13}+iz_{13} & y_{14}+iz_{14} \\ y_{12}-iz_{12} & y_{22} & y_{23}+iz_{23} & y_{24}+iz_{24} \\ y_{13}-iz_{13} & y_{23}-iz_{23} & y_{23} & y_{34}+iz_{34} \\ y_{14}-iz_{14} & y_{24}-iz_{24} & y_{34}-iz_{34} & y_{44} \end{bmatrix}. \tag{2.4}$$

where we have suppressed the upper suffix in the elements of $X^{(1)}$. The diagonal matrix $D^{(1)}$ is chosen so as to make the first column of $D^{(1)}X^{(1)}(D^{(1)})^H$ real and hence also the first row real, since the Hermitian property is obviously preserved. Clearly the diagonal elements of $D^{(1)}$ must be

$$1, \quad \frac{y_{12}+iz_{12}}{r_{12}}, \quad \frac{y_{13}+iz_{13}}{r_{13}}, \quad \frac{y_{14}+iz_{14}}{r_{14}}, \tag{2.5}$$

where

$$r_{1i} = \left(y_{1i}^2 + z_{1i}^2\right)^{1/2} \tag{2.6}$$

and we have

$$D^{(1)}X^{(1)}(D^{(1)})^H = \begin{bmatrix} y_{11} & r_{12} & r_{13} & r_{14} \\ r_{12} & y_{22} & y_{23}+iz_{23} & y_{24}+iz_{24} \\ r_{13} & y_{23}-iz_{23} & y_{33} & y_{34}+iz_{34} \\ r_{14} & y_{24}-iz_{24} & y_{34}-iz_{34} & y_{44} \end{bmatrix}, \tag{2.7}$$

where we use y_{ij}, z_{ij} to denote the new values. This is the first minor step.

The real elementary Hermitian matrix $P^{(1)}$ may now be chosen so that $P^{(1)}D^{(1)}X^{(1)}(D^{(1)})^H P^{(1)}$ is tridiagonal as far as its first row and first columns are concerned, exactly as in the standard Householder reduction of a real matrix. This is the second minor step. At the end of the rth step, $X^{(r+1)}$ is of the form illustrated when $n = 7$, $r = 3$:

$$X^{(4)} = \begin{bmatrix} x & x & & & & & \\ x & x & x & & & & \\ & x & x & x & & & \\ & & x & x & x & x & x \\ & & & x & x & x & x \\ & & & x & x & x & x \\ & & & x & x & x & x \end{bmatrix}, \tag{2.8}$$

where the matrix in the bottom right hand corner is a Hermitian matrix of order $n - r$. The $r + 1$st major step is determined by this matrix of order $n - r$ in exactly the same way as the first step was determined by the original matrix of order n. At the end of the $n - 2$nd major step $X^{(n-1)}$ will be a real symmetric tridiagonal matrix apart from the last pair of off-diagonal elements, which will in general be complex. These can be made real by doing the first minor step of the $n - 1$st major step. The second minor step is not required.

Let us now relate this somewhat more closely to the problem of Section 1. The eigenvalues of X may be found via those of the $2n \times 2n$ *real* symmetric matrix

$$\tilde{H} = \begin{bmatrix} Y & Z \\ -Z & Y \end{bmatrix}. \tag{2.9}$$

[The symmetry of this matrix follows from the relations (2.1).] Notice that the matrix H of (1.1) would reduce to this form if the matrices A and B were real. If the eigenvalues (real) of X are $\lambda_1, \lambda_2, \ldots, \lambda_n$, then those of $\tilde{H}$ are $\lambda_1, \lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_n, \lambda_n$. Let P be a permutation matrix such that in $P\tilde{H}P^T$ rows $1, 2, 3, \ldots, 2n$ of $\tilde{H}$ have become rows $1, n+1, 2, n+2, \ldots, n, 2n$, and similarly for the columns. We have then typically, when $n = 4$,

$$\tilde{H}^{(1)} \equiv P\tilde{H}P$$

$$\equiv \left[\begin{array}{cc|cc|cc|cc} y_{11} & 0 & y_{12} & z_{12} & y_{13} & z_{13} & y_{14} & z_{14} \\ 0 & y_{11} & -z_{12} & y_{12} & -z_{13} & y_{13} & -z_{14} & y_{14} \\ \hline y_{12} & -z_{12} & y_{22} & 0 & y_{23} & z_{23} & y_{24} & z_{24} \\ z_{12} & y_{12} & 0 & y_{22} & -z_{23} & y_{23} & -z_{24} & y_{24} \\ \hline y_{13} & -z_{13} & y_{23} & -z_{23} & y_{33} & 0 & y_{34} & z_{34} \\ z_{13} & y_{13} & z_{23} & y_{23} & 0 & y_{33} & -z_{34} & y_{34} \\ \hline y_{14} & -z_{14} & y_{24} & -z_{24} & y_{34} & -z_{34} & y_{44} & 0 \\ z_{14} & y_{14} & z_{24} & y_{24} & z_{34} & y_{34} & 0 & y_{44} \end{array}\right]. \tag{2.10}$$

If we compare this with (2.4), then we see that each element $a + ib$ in (2.4) is represented by the real 2×2 matrix

$$\begin{bmatrix} a & b \\ -b & a \end{bmatrix}. \tag{2.11}$$

When b is zero (i.e. for a real entry) we have

$$\begin{bmatrix} a & 0 \\ 0 & a \end{bmatrix} = aI_2. \tag{2.12}$$

We observe that

$$\begin{bmatrix} a/r & -b/r \\ b/r & a/r \end{bmatrix}\begin{bmatrix} a & b \\ -b & a \end{bmatrix} = \begin{bmatrix} r & 0 \\ 0 & r \end{bmatrix}, \tag{2.13}$$

where $r = (a^2 + b^2)^{1/2}$ and the first 2×2 matrix in (2.13) is clearly a real orthogonal matrix.

If corresponding to the first minor step in connection with $X^{(1)}$ we form $\tilde{D}^{(1)}\tilde{H}^{(1)}(\tilde{D}^{(1)})^T$, where $\tilde{D}^{(1)}$ is a block diagonal matrix with diagonal blocks

$$I_2, \quad \frac{1}{r_{12}}\begin{bmatrix} y_{12} & z_{12} \\ -z_{12} & y_{12} \end{bmatrix}, \quad \frac{1}{r_{13}}\begin{bmatrix} y_{13} & z_{13} \\ -z_{13} & y_{13} \end{bmatrix}, \quad \frac{1}{r_{14}}\begin{bmatrix} y_{14} & z_{14} \\ -z_{14} & y_{14} \end{bmatrix}. \tag{2.14}$$

we have

$$\tilde{D}^{(1)}\tilde{H}^{(1)}[\tilde{D}^{(1)}]^T = \left[\begin{array}{cc|cc|cc|cc} y_{11} & 0 & r_{12} & 0 & r_{13} & 0 & r_{14} & 0 \\ 0 & y_{11} & 0 & r_{12} & 0 & r_{13} & 0 & r_{14} \\ \hline r_{12} & 0 & y_{22} & 0 & y_{23} & z_{23} & y_{24} & z_{24} \\ 0 & r_{12} & 0 & y_{22} & -z_{23} & y_{23} & -z_{24} & y_{24} \\ \hline r_{13} & 0 & y_{23} & -z_{23} & y_{33} & 0 & y_{34} & z_{34} \\ 0 & r_{13} & z_{23} & y_{23} & 0 & y_{33} & -z_{34} & y_{34} \\ \hline r_{14} & 0 & y_{24} & -z_{24} & y_{34} & -z_{34} & y_{44} & 0 \\ 0 & r_{14} & z_{24} & y_{24} & z_{34} & y_{34} & 0 & y_{44} \end{array}\right] \tag{2.15}$$

(where we use y_{ij}, z_{ij} to denote the current values). Obviously (2.15) is related to (2.7) in the same way as (2.10) is related to (2.4), and elements denoted by y_{ij} and z_{ij} in (2.15) are the same as those in (2.7). The permutation of the rows served only as motivation; if we revert to original ordering we have

$$\left[\begin{array}{cccc|cccc} y_{11} & r_{12} & r_{13} & r_{14} & 0 & 0 & 0 & 0 \\ r_{12} & y_{22} & y_{23} & y_{24} & 0 & 0 & z_{23} & z_{24} \\ r_{13} & y_{23} & y_{33} & y_{34} & 0 & -z_{23} & 0 & z_{34} \\ r_{14} & y_{24} & y_{34} & y_{44} & 0 & -z_{24} & -z_{34} & 0 \\ \hline 0 & 0 & 0 & 0 & y_{11} & r_{12} & r_{13} & r_{14} \\ 0 & 0 & -z_{23} & -z_{24} & r_{12} & y_{22} & y_{23} & y_{24} \\ 0 & z_{23} & 0 & -z_{34} & r_{13} & y_{23} & y_{33} & y_{34} \\ 0 & z_{24} & z_{34} & 0 & r_{14} & y_{24} & y_{34} & y_{44} \end{array}\right]. \tag{2.16}$$

This has the same structure as $\tilde{H}$, but the skew symmetric matrix now has a null first row and column. If we now premultiply and postmultiply (2.16) with the real orthogonal matrix

$$\begin{bmatrix} P^{(1)} & 0 \\ 0 & P^{(1)} \end{bmatrix}, \tag{2.17}$$

we are left with

$$\left[\begin{array}{c|c|c|c} x & x \; 0 \; \cdots \; 0 & 0 & 0 \; 0 \; \cdots \; 0 \\ \begin{matrix} x \\ 0 \\ \vdots \\ 0 \end{matrix} & Y^{(2)} & \begin{matrix} 0 \\ 0 \\ \vdots \\ 0 \end{matrix} & Z^{(2)} \\ \hline 0 & 0 \; 0 \; \cdots \; 0 & x & x \; 0 \; \cdots \; 0 \\ \begin{matrix} 0 \\ 0 \\ \vdots \\ 0 \end{matrix} & -Z^{(2)} & \begin{matrix} x \\ 0 \\ \vdots \\ 0 \end{matrix} & Y^{(2)} \end{array}\right]. \tag{2.18}$$

Obviously the reduction of the $2n \times 2n$ real matrix proceeds exactly as did that of the $n \times n$ complex matrix, and in fact the same arithmetic is involved in the two methods. The $2n \times 2n$ matrix retains the same structure throughout and is finally of the double tridiagonal form

$$\begin{bmatrix} x & x & & & & & & \\ x & x & x & & & & & \\ & x & x & x & & & & \\ & & x & x & & & & \\ & & & & x & x & & \\ & & & & x & x & x & \\ & & & & & x & x & x \\ & & & & & & x & x \end{bmatrix}, \tag{2.19}$$

the two tridiagonal matrices being the same. At the beginning of the rth stage, the Y and Z matrices are of the forms illustrated when $n = 7$, $r = 4$ by

$$Y^{(r)} = \begin{bmatrix} x & x & & & & & \\ x & x & x & & & & \\ & x & x & x & & & \\ & & x & x & x & x & x \\ & & & x & x & x & x \\ & & & x & x & x & x \\ & & & x & x & x & x \end{bmatrix} \tag{2.20}$$

and

$$Z^{(r)} = \begin{bmatrix} 0 & & & & & & \\ & 0 & & & & & \\ & & 0 & & & & \\ & & & 0 & x & x & x \\ & & & x & 0 & x & x \\ & & & x & x & 0 & x \\ & & & x & x & x & 0 \end{bmatrix}.$$

The current $Y^{(r)}$ still is real and symmetric, and the $Z^{(r)}$ is real and skew symmetric. The rth minor step effectively operates on the matrices of order $n - r + 1$ in the bottom right hand corner of $Y^{(r)}$ and $Z^{(r)}$. In the first minor step of this rth step the elements of the first row and column of the remaining matrix in $Z^{(r)}$ are annihilated; in the second minor step $Y^{(r)}$ is reduced to tridiagonal form as far as its rth row and column are concerned via a similarity transformation with a real elementary Hermitian matrix. This step is exactly the same as the rth minor step in the classical Householder tridiagonalization of a real symmetric matrix. When this real similarity transformation is applied to $Z^{(r)}$, none of the previously induced zeros are affected.

The elementary similarity transformations in the Householder tridiagonalization of a real symmetric matrix Y are usually coded via the relations

$$\begin{aligned}(I-2uu^T)Y(I-2uu^T) &= Y-2u(u^TY)-2(Yu)u^T+4u(u^TYu)u^T\\ &= Y-2up^T-2pu^T+4\alpha uu^T\\ &= Y-2uq^T-2qu^T,\end{aligned} \tag{2.21}$$

where

$$p=Yu,\qquad \alpha=u^Tp,\qquad q=p-\alpha u. \tag{2.22}$$

The analogous relations for a real skew symmetric matrix Z are

$$\begin{aligned}(I-2uu^T)Z(I-2uu^T) &= Z-2u(u^TZ)-2(Zu)u^T+4u(u^TZu)u^T\\ &= Z+2up^T-2pu^T,\end{aligned} \tag{2.23}$$

where

$$p=Zu,\qquad u^TZ=-u^TZ^T=-p^T,\qquad u^TZu=0, \tag{2.24}$$

the last two results following from the skew symmetry of Z. Equation (2.21) shows the obvious symmetry of the transformed Y, while Equation (2.23) shows the obvious skew symmetry of the transformed Z. These results are of great importance in connection with the problem defined in (1.3).

The volume of computation involved in processing the $2n\times 2n$ real matrix is identical with that in the processing of the $n\times n$ complex matrix described earlier; even the rounding errors are the same.

We emphasize once again that we are not recommending that the standard eigenvalue problem for a complex Hermitian matrix should be solved in this way; it is most efficiently done by tridiagonalization of X using the complex equivalent of the usual Householder tridiagonalization.

3. THE $2n\times 2n$ COMPLEX PROBLEM

We turn now to the problem defined by Equation (1.3) and shall show that the matrix can be reduced to the form

$$\begin{bmatrix} T & 0\\ 0 & T\end{bmatrix}, \tag{3.1}$$

where T is a real symmetric $n \times n$ tridiagonal matrix. There are $n - 2$ major steps, each of which consists of two minor steps. These steps have a great deal in common with those for the real $2n \times 2n$ matrix, as can be seen from the following description of the first major step. If we reorder the rows and columns of the $2n \times 2n$ matrix as in the previous section, we obtain a matrix of the form

$$\left[\begin{array}{cc|cc|cc|cc} a_{11} & 0 & a_{12} & b_{12} & a_{13} & b_{13} & a_{14} & b_{14} \\ 0 & a_{11} & -\bar{b}_{12} & \bar{a}_{12} & -\bar{b}_{13} & \bar{a}_{13} & -\bar{b}_{14} & \bar{a}_{14} \\ \hline \bar{a}_{12} & -b_{12} & a_{22} & 0 & a_{23} & b_{23} & a_{24} & b_{24} \\ \bar{b}_{12} & a_{12} & 0 & a_{22} & -\bar{b}_{23} & \bar{a}_{23} & -\bar{b}_{24} & \bar{a}_{24} \\ \hline \bar{a}_{13} & -b_{13} & \bar{a}_{23} & -b_{23} & a_{33} & 0 & a_{34} & b_{34} \\ \bar{b}_{13} & a_{13} & \bar{b}_{23} & a_{23} & 0 & a_{33} & -\bar{b}_{34} & \bar{a}_{34} \\ \hline \bar{a}_{14} & -b_{14} & \bar{a}_{24} & -b_{24} & \bar{a}_{34} & -b_{34} & a_{44} & 0 \\ \bar{b}_{14} & a_{14} & \bar{b}_{24} & a_{24} & \bar{b}_{34} & a_{34} & 0 & a_{44} \end{array}\right], \tag{3.2}$$

where the a_{ij} and b_{ij} are complex and the a_{ii} are real. We observe that

$$\begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix} \begin{bmatrix} x & y \\ -\bar{y} & \bar{x} \end{bmatrix} = \begin{bmatrix} ax - b\bar{y} & b\bar{x} + ay \\ -\bar{b}x - \bar{a}\bar{y} & \bar{a}\bar{x} - \bar{b}y \end{bmatrix} = \begin{bmatrix} u & v \\ -\bar{v} & \bar{u} \end{bmatrix}, \tag{3.3}$$

where

$$u = ax - b\bar{y}, \qquad v = b\bar{x} + ay, \tag{3.4}$$

so that the product of matrices of the form

$$\begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix} \tag{3.5}$$

is a matrix of the same form. Matrices of this type do not, in general, commute, though they do so if all of the elements are real. Fortunately we do not need this property. Applications of the above show that

$$\begin{bmatrix} \bar{a}/r & -b/r \\ \bar{b}/r & a/r \end{bmatrix} \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix} = \begin{bmatrix} r & 0 \\ 0 & r \end{bmatrix}, \tag{3.6}$$

where

$$r = \left(|a|^2 + |b|^2\right)^{1/2}, \tag{3.7}$$

while

$$\begin{bmatrix} \bar{a}/r & -b/r \\ \bar{b}/r & a/r \end{bmatrix} \begin{bmatrix} a/r & b/r \\ -\bar{b}/r & \bar{a}/r \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I_2, \tag{3.8}$$

so that the first matrix in (3.6) is unitary. In the first minor step we perform a unitary similarity transformation on (3.2) with the 2×2 block diagonal matrix defined by

$$\operatorname{diag}\left(I_2, \frac{1}{r_{12}} \begin{bmatrix} a_{12} & b_{12} \\ -\bar{b}_{12} & \bar{a}_{12} \end{bmatrix}, \frac{1}{r_{13}} \begin{bmatrix} a_{13} & b_{13} \\ -\bar{b}_{13} & \bar{a}_{13} \end{bmatrix}, \frac{1}{r_{14}} \begin{bmatrix} a_{14} & b_{14} \\ -\bar{b}_{14} & \bar{a}_{14} \end{bmatrix} \right). \tag{3.9}$$

From (3.3), (3.6), and (3.8) the transformed matrix is of the form

$$\left[\begin{array}{cc|cc|cc|cc} a_{11} & 0 & r_{12} & 0 & r_{13} & 0 & r_{14} & 0 \\ 0 & a_{11} & 0 & r_{12} & 0 & r_{13} & 0 & r_{14} \\ \hline r_{12} & 0 & a_{22} & 0 & a_{23} & b_{23} & a_{24} & b_{24} \\ 0 & r_{12} & 0 & a_{22} & -\bar{b}_{23} & \bar{a}_{23} & -\bar{b}_{24} & \bar{a}_{24} \\ \hline r_{13} & 0 & \bar{a}_{23} & -b_{23} & a_{33} & 0 & a_{34} & b_{34} \\ 0 & r_{13} & \bar{b}_{23} & a_{23} & 0 & a_{33} & -\bar{b}_{34} & \bar{a}_{24} \\ \hline r_{14} & 0 & \bar{a}_{24} & -b_{24} & \bar{a}_{34} & -b_{34} & a_{44} & 0 \\ 0 & r_{14} & \bar{b}_{24} & a_{24} & \bar{b}_{34} & a_{34} & 0 & a_{44} \end{array}\right], \tag{3.10}$$

where as usual a_{ij}, b_{ij} now denote values after the transformations. These new values are derived via relations of the type exemplified in Equation (3.3). The reordering was performed only for convenience; returning to the original ordering, we have

$$\left[\begin{array}{cccc|cccc} a_{11} & r_{12} & r_{13} & r_{14} & 0 & 0 & 0 & 0 \\ r_{12} & a_{22} & a_{23} & a_{24} & 0 & 0 & b_{23} & b_{24} \\ r_{13} & \bar{a}_{23} & a_{33} & a_{34} & 0 & -b_{23} & 0 & b_{34} \\ r_{14} & \bar{a}_{24} & \bar{a}_{34} & a_{44} & 0 & -b_{24} & -b_{34} & 0 \\ \hline 0 & 0 & 0 & 0 & a_{11} & r_{12} & r_{13} & r_{14} \\ 0 & 0 & -\bar{b}_{23} & -\bar{b}_{24} & r_{12} & a_{22} & \bar{a}_{23} & \bar{a}_{24} \\ 0 & \bar{b}_{23} & 0 & -\bar{b}_{34} & r_{13} & a_{23} & a_{33} & \bar{a}_{34} \\ 0 & \bar{b}_{24} & \bar{b}_{34} & 0 & r_{14} & a_{24} & a_{34} & a_{44} \end{array}\right]. \tag{3.11}$$

This matrix has the same structure as the original, but the first row and column of the A part are now real, and the first row and column of the B part are null. We have now completed the first minor step of the first major step. In the second minor step we perform a real orthogonal similarity with the matrix

$$\begin{bmatrix} P^{(1)} & 0 \\ 0 & P^{(1)} \end{bmatrix}, \tag{3.12}$$

where $P^{(1)}$ is the real elementary Hermitian (i.e. a matrix of the form $I - 2uu^T$) which annihiliates elements $(1,3),(1,4),\ldots,(1,n)$ and $(3,1),(4,1),\ldots,(n,1)$ of the A matrix. This is determined from the r_{1i} exactly as in the first major step of the classical Householder tridiagonalization algorithm. The null first row and column in the B part are obviously preserved. After r steps the configuration is of the form illustrated when $n = 5$, $r = 2$ by

$$\left[\begin{array}{cc|ccc|cc|ccc}
\alpha_1 & \beta_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\beta_2 & \alpha_2 & \beta_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & \beta_3 & a_{33} & a_{34} & a_{34} & 0 & 0 & 0 & b_{34} & b_{35} \\
0 & 0 & \bar{a}_{34} & a_{44} & a_{45} & 0 & 0 & -b_{34} & 0 & b_{45} \\
0 & 0 & \bar{a}_{35} & \bar{a}_{45} & a_{55} & 0 & 0 & -b_{35} & -b_{45} & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & \alpha_1 & \beta_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \beta_2 & \alpha_2 & \beta_3 & 0 & 0 \\
\hline
0 & 0 & 0 & -\bar{b}_{34} & -\bar{b}_{35} & 0 & \beta_3 & a_{33} & \bar{a}_{34} & \bar{a}_{35} \\
0 & 0 & \bar{b}_{34} & 0 & -\bar{b}_{45} & 0 & 0 & a_{34} & a_{44} & \bar{a}_{45} \\
0 & 0 & \bar{b}_{35} & \bar{b}_{45} & 0 & 0 & 0 & a_{35} & a_{45} & a_{55}
\end{array}\right]. \tag{3.13}$$

The Hermitian form of the A part is still preserved, and so is the complex skew symmetric form of the B part. The A part is already tridiagonal in the first r rows and columns, while the B part is null in its first r rows and columns.

The first major step is wholly typical. In major step $r+1$ we first make the elements in rows and columns $r+1$ of the A part real, and the elements in rows and columns $r+1$ of the B part are annihilated. We then construct a real elementary Hermitian $P^{(r+1)}$ which will annihilate elements $(r+1, r+2)$, $(r+1, r+3), \cdots, (r+1, n)$, and $(r+2, r+1), (r+3, r+1), \cdots, (n, r+1)$ of the A part and apply the real orthogonal similarlity based on the matrix

$$\begin{bmatrix} P^{(r+1)} & 0 \\ 0 & P^{(r+1)} \end{bmatrix} \tag{3.14}$$

to the full $2n\times 2n$ array. On completion of the $n-2$nd major step, the A parts will be tridiagonal and the B parts will be completely null. A will be real except for elements $(n-1,n)$ and $(n,n-1)$, but they can be made real by doing what is in effect the first minor step of an $n-1$st major step.

Obviously we do not need to have the full $2n\times 2n$ array; we need store only the current A array and the current B array, and in storing them we can take advantage of the symmetry and skew symmetry respectively. It is even more convenient to think of the A and B matrices as separated into their real and imaginary parts. Thus we write

$$A^{(r)} = U^{(r)} + iV^{(r)}, \qquad B^{(r)} = X^{(r)} + iY^{(r)} \tag{3.15}$$

for each stage, where $U^{(r)}$, $V^{(r)}$, $X^{(r)}$, and $Y^{(r)}$ are real, $U^{(r)}$ being symmetric and $V^{(r)}$, $X^{(r)}$, and $Y^{(r)}$ being skew symmetric. In the first minor step of each major step the formula for the elements of the transformed U, V, X, and Y matrices are derived from their original values by thinking in terms of the complex $A^{(r)}$ and $B^{(r)}$. The transformation $P^{(r)}$ is then determined entirely from rows r (or columns r) of $U^{(r)}$, and we compute $P^{(r)}U^{(r)}P^{(r)}$, $P^{(r)}V^{(r)}P^{(r)}$, $P^{(r)}X^{(r)}P^{(r)}$, and $P^{(r)}Y^{(r)}P^{(r)}$. Notice that three of the four transformations are of skew symmetric matrices and involve rather less work then the transformation of the real symmetric matrix. On completion, V, X, and Y are completely annihilated and U is a real symmetric tridiagonal matrix.

4. THE GENERALIZED PROBLEM

The standard problem (1.3) has been presented first for convenience, but in practice the problem commonly arises in the form

$$H_1 z = \lambda H_2 z, \tag{4.1}$$

where both H_1 and H_2 have the same structure as H in (1.1) and H_2 is positive definite. The generalized problem can be reduced to the standard problem if we can determine the matrix S such that

$$SH_2S^H = I. \tag{4.2}$$

We have then

$$SH_1S^H(S^{-H}z) = \lambda SH_2S^H(S^{-H}z). \tag{4.3}$$

Obviously for economy of computation it is desirable to determine S in a factorized form

$$S = S_k \cdots S_2 S_1 \tag{4.4}$$

and in such a way that

$$\begin{aligned} &S_1 H_1 S_1^H, \quad S_1 H_2 S_1^H, \\ &S_2 S_1 H_1 S_1^H S_2^H, \quad S_2 S_1 H_2 S_1^H S_2^H, \\ &\cdots \end{aligned} \tag{4.5}$$

have the same structure as H at every stage.

This can be done in $n-1$ major steps, each step being determined by the current H_2 matrix. The first major step is wholly typical. It consists of two minor steps. The first minor step is exactly that applied to H as described in Section 3 and is best motivated by thinking in terms of the permuted form of H_2. This reduces H_2 to the form illustrated in (3.11) (with the original ordering). In the second minor step we premultiply by the real matrix

$$\begin{bmatrix} L_1 & 0 \\ 0 & L_1 \end{bmatrix} \tag{4.6}$$

and postmultiply by the transpose of this, where L_1 is typically of the form

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -r_{12}/a_{11} & 1 & 0 & 0 \\ -r_{13}/a_{11} & 0 & 1 & 0 \\ -r_{14}/a_{11} & 0 & 0 & 1 \end{bmatrix} \tag{4.7}$$

when $n=4$. This annihilates the off-diagonal elements in the first rows and columns of the A part. The B part is unaffected, since its first row and column are null. The structure of H_2 is obviously preserved. If we think in terms of the real and the imaginary parts of the A and B matrices of H_2, the second minor step obviously affects only the real part of A.

After $n-1$ steps of this kind, H_2 is reduced to the form

$$\begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} \tag{4.8}$$

where D is a real positive diagonal matrix. This can be reduced to the identity matrix by premultication and postmultication with

$$\begin{bmatrix} D^{-1/2} & 0 \\ 0 & D^{-1/2} \end{bmatrix} \tag{4.9}$$

All transformations applied to H_2 must also be applied to H_1. The structure of H_1 is obviously presrved, though, of course, it remains a full matrix (i.e. no zeros are induced). More work is involved in the transformation of H_1 than of H_2, both for this reason and also because all off-diagonal elements of H_1 remain complex throughout.

5. RELATIVE PERFORMANCE

The performance of the algorithms presented in this paper is best described by comparing them against standard methods as implemented in the EISPACK [3] collection of software. In EISPACK there are routines for dealing with Hermitian matrices, which is the closest we can get to the matrix described in Equation (1.1). The routine in EISPACK to handle this case is CH. This uses a sequence of Householder transformations to reduce the full $2n \times 2n$ complex Hermitian matrix to real tridiagonal form; then the QR algorithm is used on this $2n \times 2n$ tridiagonal matrix to find the eigenvalues. For the generalized problem, the matrix H_2 can be decomposed using a Cholesky decomposition, say from LINPACK [1]. This would then be applied to the matrix H_1, transforming the generalized problem into a standard one. The table below gives the ratios of execution time for the two approaches:

	λ	λ and z
Standard problem $Hz = \lambda z$ EISPACK: ours	2.5	3
Generalized problem $H_1 z = \lambda H_2 z$ LINPACK and EISPACK: ours	2.25	2.75

Thus, the procedures developed here are over twice as fast as standard available techniques. These ratios hold true for large order problems as well as small problems.

For the standard problem, if just the eigenvalues are desired, the requirement for storage using the EISPACK routines is the same as our approach. For the case where the eigenvalues and eigenvectors are required, our approach needs an additional $n^2/2$ real locations to save information of the transformations. In the generalized problem, if just the eigenvalues are computed, the storage requirements are the same. For computing both the eigenvalues and eigenvectors an additional n^2 real locations are necessary for our procedure.

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