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A Note on the Computation of Eigenvalues and Vectors of Hermitean Matrices†

The matrix eigenvalue problem, so important in physics, chemistry and engineering, is straightforward in principle. In practice, considerations of numerical accuracy and speed put a severe restriction on the class and size of solvable matrices. Modern digital computers necessarily play a vital role in the solution for large matrices.

There are two popular machine methods for obtaining all the eigenvalues and eigenvectors of a real symmetric matrix of order N. The iterative procedure of Jacobi[1] is better known. The method of Givens[2] is more involved, but probably somewhat more accurate. Both schemes have been subjected to detailed error analysis.[2,3] The computing time required turns out to be roughly the same.

The Jacobi method is a highly convergent iterative process, which yields as its limit a diagonal eigenvalue matrix and a corresponding eigenvector matrix through a sequence of 2×2 plane rotations. The Givens method initially produces a triple-diagonal matrix by $\frac{1}{2}(N-1)(N-2)$ plane rotations. Each of these rotations produce two zeros symmetrically above and below the triple diagonal. An iterative root-finding technique based on the Sturm sequence property is then used. Back substitution produces the eigenvectors for the triple diagonal matrix and multiplication by the (combined) rotation matrix yields the desired eigenvectors.

The diagonalization of an $N \times N$ Hermitean matrix H by unitary matrices is, in many respects, similar to that of a real symmetric matrix because the eigenvalues are all real. The complex analog of Jacobi's method has been previously considered.[4] Since complex arithmetic is time consuming and prone to round-off errors, it would seem that the Hermitean character of H could be exploited to reduce the amount of complex arithmetic involved. This will be shown to be indeed the case.

Consider the Hermitean analog of Givens' method. The only change in the algorithm for obtaining the triple-diagonal matrix T is that orthogonal rotation matrices are replaced by corresponding unitary matrices. For a given Hermitean matrix A, the $(p-1,q)$th and $(q,p-1)$th elements can be simultaneously made zero by the 2×2 unitary transformation‡

$$A' = u^* A u, \quad u = u(p,q),$$

$$u_{pp} = u_{qq} = \cos\theta, \quad u_{pq} = -\bar{u}_{qp} = e^{i\mu}\sin\theta,$$

$$u_{rs} = \delta_{rs}, \quad r \neq p,q, \quad s \neq p,q,$$

with

$$\mu = (\text{phase of } A_{p-1,q}) - (\text{phase of } A_{p-1,p}),$$

$$\tan\theta = -(\text{modulus of } A_{p-1,q})/(\text{modulus of } A_{p-1,p}).$$

Only the elements in the pth and qth rows and columns are affected.

Starting from H, successive application of the above algorithm with (p,q) running through the ordered sequence of $\frac{1}{2}(N-1)(N-2)$ rotations

$$(2,3),(2,4)\cdots(2,N);(3,4),\cdots(3,N);$$

$$\cdots(N-2,N-1),(N-2,N);(N-1,N)$$

preserves the created zeros and yields a triple-diagonal Hermitean matrix T:

$$T = U^* H U; \quad U = \text{combined rotation matrix.}$$

$$T_{kk} = \alpha_k, \quad T_{k,k+1} = \beta_k e^{i\phi_k} = \bar{T}_{k+1,k}.$$

On expanding the characteristic determinant $|T-\lambda I|$ by minors it is seen that

$$\Delta_k = (T_{kk}-\lambda)\Delta_{k-1} - T_{k-1,k}T_{k,k-1}\Delta_{k-2}$$

where $\Delta_k \equiv$ determinant of the first k rows and columns of $T-\lambda I$, $\Delta_0 \equiv 1$, $\Delta_{-1} \equiv 0$. But, since T is Hermitean,

$$T_{k-1,k}T_{k,k-1} = |T_{k-1,k}|^2 = \beta_{k-1}^2.$$

Examination reveals that the real symmetric matrix R obtained by replacing $\beta_k e^{\pm i\phi_k}$ by the modulus β_k for all k has the same characteristic determinant and therefore the same eigenvalues as T. This is in fact true for all principal minors of R. The Givens root-finding scheme can then be applied directly to yield the eigenvalues by *real*

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‡For simplicity of expression the polar form is used here. In actual computations the rectangular form $z = x + iy$ is preferable.

arithmetic. The increase in speed and accuracy by this measure is believed significant.

One further observation leads to simplification of the problem of back substitution for finding the eigenvectors in Givens' method; moreover, it renders possible the use of the more straightforward Jacobi scheme for real symmetric matrices to obtain the eigenvectors as well as the eigenvalues. Namely, the replacement by moduli mentioned above can be achieved by the trivial diagonal unitary transformation

$$R=V^*TV=V^*(U^*HU)\,V=(UV)^*H(UV)$$

where

$$V=\mathrm{diag}\left\{\exp -i\sum_{j=1}^{k-1}\phi_j\right\}.$$

If the eigenvalue matrix of R is Λ and the corresponding (real) eigenvector matrix is W, we have simply

$$\Lambda=W^*RW=(VW)^*T(VW)=(UVW)^*H(UVW)$$

and $X=UVW$ is the corresponding unitary eigenvector matrix of H.

Λ and W can be found by either the Jacobi real symmetric method or the Givens scheme for treating the real triple-diagonal problem. The fullest use of the triple diagonal nature of R is realized via Givens' approach. However, the concentration of non-zero elements along the co-diagonal could be an asset towards the convergence and accuracy of the Jacobi method even though the successive rotations disperse the non-zero elements beyond the co-diagonals. This aspect of the problem deserves further investigation.

From a practical point of view, computer installations which possess the real Jacobi code or the Givens real symmetric code can now directly utilize a large portion of these programs for the solution of the Hermitean problem, thereby saving considerable programming and debugging effort. The two methods presented here are being programmed for the IBM 704 and will be compared with the Jacobi method for speed and accuracy.

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References

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4. A. S. Householder, *Principles of Numerical Analysis* (McGraw-Hill, New York 1953) pp. 160-162. (A 704 machine code has been written by E. Kineke of the Computing Center, IBM Research Center.)

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