Smith, B.T., et al. 1976, Matrix Eigensystem Routines — EISPACK Guide, 2nd ed., vol. 6 of Lecture Notes in Computer Science (New York: Springer-Verlag). [3]

Stoer, J., and Bulirsch, R. 1980, *Introduction to Numerical Analysis* (New York: Springer-Verlag), §6.6.6. [4]

11.4 Hermitian Matrices

The complex analog of a real, symmetric matrix is a Hermitian matrix, satisfying equation (11.0.4). Jacobi transformations can be used to find eigenvalues and eigenvectors, as also can Householder reduction to tridiagonal form followed by QL iteration. Complex versions of the previous routines jacobi, tred2, and tqli are quite analogous to their real counterparts. For working routines, consult [1,2].

An alternative, using the routines in this book, is to convert the Hermitian problem to a real, symmetric one: If $\mathbf{C} = \mathbf{A} + i\mathbf{B}$ is a Hermitian matrix, then the $n \times n$ complex eigenvalue problem

$$(\mathbf{A} + i\mathbf{B}) \cdot (\mathbf{u} + i\mathbf{v}) = \lambda(\mathbf{u} + i\mathbf{v})$$
(11.4.1)

is equivalent to the $2n \times 2n$ real problem

$$\begin{bmatrix} \mathbf{A} & -\mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}$$
(11.4.2)

Note that the $2n \times 2n$ matrix in (11.4.2) is symmetric: $\mathbf{A}^T = \mathbf{A}$ and $\mathbf{B}^T = -\mathbf{B}$ if **C** is Hermitian.

Corresponding to a given eigenvalue λ , the vector

$$\begin{bmatrix} -\mathbf{v} \\ \mathbf{u} \end{bmatrix}$$
(11.4.3)

is also an eigenvector, as you can verify by writing out the two matrix equations implied by (11.4.2). Thus if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of **C**, then the 2n eigenvalues of the augmented problem (11.4.2) are $\lambda_1, \lambda_1, \lambda_2, \lambda_2, \ldots$, λ_n, λ_n ; each, in other words, is repeated twice. The eigenvectors are pairs of the form $\mathbf{u} + i\mathbf{v}$ and $i(\mathbf{u} + i\mathbf{v})$; that is, they are the same up to an inessential phase. Thus we solve the augmented problem (11.4.2), and choose one eigenvalue and eigenvector from each pair. These give the eigenvalues and eigenvectors of the original matrix **C**.

Working with the augmented matrix requires a factor of 2 more storage than the original complex matrix. In principle, a complex algorithm is also a factor of 2 more efficient in computer time than is the solution of the augmented problem. In practice, most complex implementations do not achieve this factor unless they are written entirely in real arithmetic. (Good library routines always do this.)

CITED REFERENCES AND FURTHER READING:

Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one) to any server computer, is strictly prohibited. To order Numerical Recipes books, diskettes, or CDROMs visit website http://www.nr.com or call 1-800-872-7423 (North America only), or send email to trade@cup.cam.ac.uk (outside North America). World Wide Web sample page from NUMERICAL RECIPES IN FORTRAN 77: Copyright (C) 1988-1992 by Cambridge University Press. Programs Copyright Programs Copyright (C) THE E ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X) 1988-1992 by Numerical Recipes Software.

Wilkinson, J.H., and Reinsch, C. 1971, *Linear Algebra*, vol. II of *Handbook for Automatic Computation* (New York: Springer-Verlag). [1]

Smith, B.T., et al. 1976, Matrix Eigensystem Routines — EISPACK Guide, 2nd ed., vol. 6 of Lecture Notes in Computer Science (New York: Springer-Verlag). [2]

11.5 Reduction of a General Matrix to Hessenberg Form

The algorithms for symmetric matrices, given in the preceding sections, are highly satisfactory in practice. By contrast, it is impossible to design equally satisfactory algorithms for the nonsymmetric case. There are two reasons for this. First, the eigenvalues of a nonsymmetric matrix can be very sensitive to small changes in the matrix elements. Second, the matrix itself can be defective, so that there is no complete set of eigenvectors. We emphasize that these difficulties are intrinsic properties of certain nonsymmetric matrices, and no numerical procedure can "cure" them. The best we can hope for are procedures that don't exacerbate such problems.

The presence of rounding error can only make the situation worse. With finiteprecision arithmetic, one cannot even design a foolproof algorithm to determine whether a given matrix is defective or not. Thus current algorithms generally *try* to find a *complete* set of eigenvectors, and rely on the user to inspect the results. If any eigenvectors are almost parallel, the matrix is probably defective.

Apart from referring you to the literature, and to the collected routines in [1,2], we are going to sidestep the problem of eigenvectors, giving algorithms for eigenvalues only. If you require just a few eigenvectors, you can read $\S11.7$ and consider finding them by inverse iteration. We consider the problem of finding *all* eigenvectors of a nonsymmetric matrix as lying beyond the scope of this book.

Balancing

The sensitivity of eigenvalues to rounding errors during the execution of some algorithms can be reduced by the procedure of *balancing*. The errors in the eigensystem found by a numerical procedure are generally proportional to the Euclidean norm of the matrix, that is, to the square root of the sum of the squares of the elements. The idea of balancing is to use similarity transformations to make corresponding rows and columns of the matrix have comparable norms, thus reducing the overall norm of the matrix while leaving the eigenvalues unchanged. A symmetric matrix is already balanced.

Balancing is a procedure with of order N^2 operations. Thus, the time taken by the procedure balanc, given below, should never be more than a few percent of the total time required to find the eigenvalues. It is therefore recommended that you *always* balance nonsymmetric matrices. It never hurts, and it can substantially improve the accuracy of the eigenvalues computed for a badly balanced matrix.

The actual algorithm used is due to Osborne, as discussed in [1]. It consists of a sequence of similarity transformations by diagonal matrices **D**. To avoid introducing rounding errors during the balancing process, the elements of **D** are restricted to be exact powers of the radix base employed for floating-point arithmetic (i.e., 2 for most machines, but 16 for IBM mainframe architectures). The output is a matrix that is balanced in the norm given by summing the absolute magnitudes of the matrix elements. This is more efficient than using the Euclidean norm, and equally effective: A large reduction in one norm implies a large reduction in the other.

Note that if the off-diagonal elements of any row or column of a matrix are all zero, then the diagonal element is an eigenvalue. If the eigenvalue happens to Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine readable files (including this one) to any server computer, is strictly prohibited. To order Numerical Recipes books, diskettes, or CDROMs visit website http://www.nr.com or call 1-800-872-7423 (North America only), or send email to trade@cup.cam.ac.uk (outside North America) World Wide Web sample page from NUMERICAL RECIPES IN FORTRAN 77: Copyright (C) 1988-1992 by Cambridge University Press. Programs Copyright University Press. Programs Copyright (C) THE , IE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X) 1988-1992 by Numerical Recipes Software. use. Further reproduction, or any copying of machine-