Section 6

DIFFERENCES BETWEEN THE EISPACK SUBROUTINES AND THE HANDBOOK ALGOL PROCEDURES

This section describes, subroutine by subroutine, the major differences between the EISPACK subroutines and their Algol antecedents in the Handbook [1]. These differences fall into four categories: 1) correction of several errors, 2) minor algorithmic improvements, 3) changes based on consideration of Fortran language efficiency, and finally, 4) changes to better unify the individual programs into a package.

Some of the changes apply to EISPACK as a whole.

1) The base B of the floating point representation on the machine and the machine precision MACHEP have become internally set variables in the Fortran programs rather than parameters.

2) The orthogonality threshold parameter TOL has been removed from the Householder reduction subroutines by substituting the alternate scaling technique discussed in the "Organisational and Notational Details" section of the Handbook, Contribution II/2, p. 221.

3) The procedure CDIV called to perform complex division in the Handbook procedures has been replaced by ordinary division operations with complex-mode Fortran operands. The procedures CABS and CSQRT called to perform complex modulus and complex square-root operations have been replaced by references to corresponding members of the Fortran library which use complex-mode operands.

4) The Handbook procedure-calls for row interchange in the balancing process, for determination of Sturm counts in the bisection process, and for selection of new trial vectors in the inverse iteration process have been replaced by in-line Fortran coding.

Specific changes to individual members of EISPACK are as follows.

BALANC - IGH=1 rather than IGH=0 is returned when the matrix can be permuted to triangular form; IGH is used as an array declarator subscript in other subroutines and must not be "0".

TRED1 - Unnecessary operations in the last reduction step that can introduce roundoff error into the first diagonal element have been skipped, enabling the resultant tridiagonal form to more literally duplicate that from TRED2. Also see TRED2 below.

TRED2 - The arithmetic operation G*(Z/H) is computed instead as (G/H)*Z, enabling the resultant tridiagonal form to more literally duplicate that from TRED1. The tridiagonal forms from TRED1 and TRED2 are now identical (on most machines) except possibly for the sign of the first subdiagonal element. This property in turn ensures that TQL1 and TQL2, or IMTQL1 and IMTQL2, produce identical eigenvalues in most cases.

TRED3 - As for TRED1.

TRBAK1 - Instead of back transforming eigenvectors M1 through M2 as is done in the Handbook, TRBAK1 transforms eigenvectors 1 through M. (The M1, M2 form of specification would be more natural if subroutine BISECT were patterned after the Handbook BISECT rather than the Handbook TSTURM.)

TRBAK3 - As for TRBAK1.

HQR - Provision for recognition of balancing parameters LOW and IGH has been made. Also see HQR2 below.

HQR2 - Roots of a quadratic equation with discriminant zero are now classified as real rather than complex as in the Handbook. This change corrects an error which may otherwise be made in determining the corresponding eigenvectors. For consistency the change has been made to HQR also.

- The last component of complex vectors of the reduced form is initialized to (0,1) rather than (1,0), rendering the vector matrix of the reduced form strictly triangular and thereby simplifying the final transformation to the eigenvectors of the original matrix.

INVIT - The complex eigenvector corresponding to either member of a pair of conjugate complex eigenvalues may be obtained, not just the one corresponding to the value with positive imaginary part. However, if both are requested, only the eigenvector corresponding to the eigenvalue with positive imaginary part is computed.

- The eigenvector growth requirement has been relaxed by a factor of 10, reducing the number of convergence failures.

TSTURM - Small subdiagonal entries of the tridiagonal form are treated as zeros in the computation but are not replaced by zeros in storage. The subdiagonal array is required in TRBAK1 and modification of any of its elements by TSTURM introduces errors in the back transformation.

- The input interval (RLB,RUB) is refined making use of Gerschgorin bounds, thereby reducing the computation time of the bisection process.

- The logical array INT has been eliminated by making use instead of information present in the reduced triangular form and input subdiagonal array.

BISECT - The bisection process of TSTURM is used instead of that in the Handbook BISECT procedure. They differ primarily in the specification of the subset of the eigenvalues to be computed.

- The eigenvalues are strictly ordered, rather than locally ordered within submatrices as in TSTURM; they are tagged with their submatrix associations by use of the array IND.

TRIDIB - As for BISECT except that the bisection process of the Handbook BISECT procedure is used.

COMLR - Provision for recognition of balancing parameters LOW and IGH has been made.

CINVIT - The vector growth requirement has been relaxed by a factor of 10, reducing the number of convergence failures.

RATQR - The largest as well as the smallest eigenvalues can be requested. The specification of "NEGATIVE DEFINITE" (when proper) improves the determination of the largest values in the same way as "POSITIVE DEFINITE" does the smallest.

- An error return has been provided for an incorrectly specified definiteness parameter.

- The incidence of underflow has been markedly reduced by replacement of tiny squared subdiagonal elements by zeros at each iteration.

- The eigenvalues are tagged with their submatrix associations by use of the array IND. A further modification that saves the input matrix makes it possible to link RATQR with TINVIT to compute the corresponding eigenvectors.

A number of the EISPACK subroutines which have no Handbook antecedents are patterned closely after existing Handbook procedures.

CBAL is a complex analogue of BALANC,

CBABK2 is a complex analogue of BALBAK,

CORTH is a complex analogue of ORTHES,

CORTB is a complex analogue of ORTBAK,

COMQR is a unitary analogue of COMLR,

COMQR2 is a unitary analogue of COMLR2,

HTRIDI is a complex analogue of TRED1,

HTRIBK is a complex analogue of TRBAK1,

HTRID3 is a complex analogue of TRED3,

HTRIB3 is a complex analogue of TRBAK3,

IMTQLV is an extension of IMTQL1 that tags the eigenvalues with their submatrix associations as in BISECT,

TQLRAT is a rational variant of TQL1, and

TINVIT is that part of TSTURM which determines the eigenvectors after the eigenvalues have been found.

Subroutines FIGI, FIGI2, and BAKVEC provide the EISPACK capability for special nonsymmetric tridiagonal matrices not present in the Handbook procedures. They may be considered analogous to TRED1, TRED2, and TRBAK1 respectively.

Finally, various minor textual changes have been made to render the first of each of the following pairs of subroutines a virtual subset of the second: (COMLR,COMLR2), (HQR,HQR2), (TQL1,TQL2), (IMTQL1,IMTQL2), and (BISECT,TSTURM).