

Mathematics Notes

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SEVER: A Routine for Computing Symmetric Matrix Eigenvalues and Eigenvectors with Error Bounds

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Abstract

Subroutine SEVER computes a complete eigensystem with error bounds for a real symmetric matrix. Householder's method is used to reduce the matrix to tridiagonal form. The eigenvalues and eigenvectors of the tridiagonal matrix are computed by the QR algorithm. The computed eigenvalues are subjected to one Rayleigh quotient correction using the computed eigenvectors. Upper bounds on the absolute errors of the computed eigensystem are calculated.

Key word: mathematics

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FOREWORD

The Sandia Laboratories Mathematical Program Library consists of a number of dependable, high-quality, general-purpose, mathematical computing routines. The standards established for the library require that these routines be mathematically sound, effectively implemented, extensively tested, and thoroughly documented. This report documents one such routine.

The library emphasizes the effective coverage of various distinct mathematical areas with a minimum number of routines. Nevertheless, it may contain other routines similar in nature but complementary to the one described here. Additional information on the mathematical program library, a description of the standard format for documenting these routines, and a guide to other routines in the library are contained in SC-M-69-337.

This report is also identified within Sandia Laboratories as Computing Publication ML0005/ALL. This report and its corresponding library routine are expected to be available from COSMIC shortly after publication.

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SEVER: A ROUTINE FOR COMPUTING SYMMETRIC MATRIX
EIGENVALUES AND EIGENVECTORS WITH ERROR BOUNDS

1. Introduction

1.1 Background

SEVER was written to provide the Sandia Mathematical Program Library with a quality routine for computing an eigensystem with error bounds of a real symmetric matrix. The methods used in SEVER were chosen and the routine was constructed to avoid some of the more common deficiencies in existing routines for symmetric matrix eigensystem calculation. Among such deficiencies are the lack of precision in the calculation of clustered or multiple eigenvalues, inability to handle eigenvalues which differ only in sign, nonorthogonality of eigenvectors corresponding to eigenvalues of multiplicity greater than one, and lack of any measure of the precision or reliability of the results.

The ALGOL routine of Martin et al⁸ was converted to FORTRAN and constitutes that segment of SEVER which reduces the input matrix to tridiagonal form.

The ALGOL routine of Bowdler et al³ was converted to FORTRAN and is a subroutine called by SEVER to compute the eigenvalues and eigenvectors of the tridiagonal matrix.

1.2 Applicable Programming Languages and Computer Systems

SEVER is written in a subset of Control Data 6600 FORTRAN. Except for two DATA statements containing error messages and two replacement statements involving octal literals, it is believed that the program conforms to American National Standard FORTRAN. However, complete portability of the routine is not implied and, because of machine-dependent

constants (e.g., the smallest positive floating point number which when added to 1.0 yields a floating point sum not 1.0), modified versions of SEVER may be required for machines other than the CDC 6600.

SEVER has executed successfully and has been tested thoroughly under the Control Data 6600 SCOPE operating system with the FUN and RUN compilers.

This routine is maintained for the convenience of the user on a library file on the CDC 6600 and is accessible by means of one control card described in Appendix C.

1.3 Considerations Regarding Use

SEVER computes all of the eigenvalues of a real symmetric matrix and a set of orthonormal eigenvectors. An upper bound on the absolute error of each computed eigenvalue is returned as well as an upper bound on the absolute error of the computed eigenvector. Lengths of residual vectors are also returned. Double precision eigenvalues are computed and returned but these values should be used in conjunction with the eigenvalue absolute error bounds. Both the single and double precision eigenvalues are returned in nonincreasing algebraic order.

SEVER may be used to compute an eigensystem for a complex Hermitian matrix. See Section 7 for details on how this may be done.

The nature of arithmetic and format conversion may cause zero eigenvalues and zero components of eigenvectors to look as if they were nonzero numbers which are very small in absolute value. In these cases the user must determine whether a small eigenvalue or a small eigenvector component is actually zero (see Section 2.7).

2. Usage

2.1 Entry

The calling sequence is:

```
CALL SEVER(A,EV,VEC,ERVAL,DPA,N,NDIM,KER)
```

2.2 Description of Arguments

In the following description an argument which must be preset by the calling program before a call to SEVER is referred to as an input argument. An argument which will return with a value determined in SEVER is referred to as an output argument. SEVER has no arguments which are both input and output. An example of a calling sequence is given in Section 2.4.

- A A real input array which must be dimensioned with exactly NDIM rows and at least NDIM columns. Normally, A should be dimensioned (NDIM, NDIM). The leading N by N subarray of A must contain the real symmetric matrix whose eigensystem is to be computed. A is returned unchanged.
- EV A real output array which, upon return from SEVER, contains the computed eigenvalues in nonincreasing algebraic order. EV must be dimensioned at least N in the calling program, and normally would be dimensioned NDIM.
- VEC The real output array which, upon return from SEVER, contains the computed eigenvectors. The eigenvectors are stored in the columns of VEC corresponding to the eigenvalues in EV. That is, the k-th column of VEC contains a computed eigenvector of length one corresponding to the computed eigenvalue in the k-th element of array EV. VEC must be dimensioned with exactly NDIM rows and at least NDIM columns. Normally, VEC would be dimensioned (NDIM, NDIM).

ERVAL The real output array containing upper bounds on the absolute errors of the computed double precision eigenvalues (see Section 2.7). In case it is not possible to bound the error on some eigenvalue, a -1.0 is returned in the element of ERVAL corresponding to that eigenvalue. ERVAL must be dimensioned at least N and normally would be dimensioned NDIM in the calling program.

DPA A double precision output array which must be dimensioned (NDIM, 3) and declared type double in the calling program. DPA must be supplied by the user in order that certain inner products in the Rayleigh quotient eigenvalue correction and error calculations may be accumulated in double precision. Upon return, the first column of DPA contains the Rayleigh quotient eigenvalues in double precision. The second column contains an upper bound on the absolute error (= relative error) of the computed eigenvector as measured in the two norm. If such a bound cannot be computed, i.e., ERVAL(K) = -1, the length of the k-th residual vector (Section 4) is returned. The third column of DPA contains the length of the residual vector in every case.

N The integer order of the matrix to be resolved. N must not be smaller than 3. (The distinction between N and NDIM facilitates the solution of different size problems in successive calls in the same execution of the calling program.) N is an input argument.

NDIM The integer number of rows and usually the number of columns allocated to A in the calling program. NDIM must not be smaller than N. NDIM is an input argument.

KER An output error indicator. Its value upon return is 1 for normal execution, 2 if the dimensions and size of the matrix are inconsistent, and 3 if more than 30 QR iterations are required for some eigenvalue.

2.3 Restrictions Between Arguments

- A and VEC Treated as square arrays, and each must be dimensioned with exactly NDIM rows and at least N columns. Normally each of these arrays should be dimensioned (NDIM, NDIM).
- EV and ERVAL Arrays, each of which must be dimensioned at least N. Normally each array should be dimensioned NDIM.
- A, EV, ERVAL, VEC, and DPA Must be distinct arrays. If KER is returned as 2, no values are assigned to EV, VEC, ERVAL or DPA. If KER is returned as 3, the values assigned to EV, VEC, ERVAL, and DPA may not be meaningful.
- N and NDIM Must satisfy $3 \leq N \leq \text{NDIM}$.

2.4 Principal Uses with Example

The following is a segment of a possible calling program for computing the eigensystem of a 4 x 4 real symmetric matrix A for which up to 25 rows and columns are allocated:

```
PROGRAM EIGVAL(INPUT,OUTPUT)
  DIMENSION A(25,25),EV(25),ERVAL(25),VEC(25,25)
  DOUBLE PRECISION DPA(25,3)
  DO 1 I = 1,4
1  READ 101, (A(I,J),J=1,4)
101 FORMAT(4E10.3)
  CALL SEVER(A,EV,VEC,ERVAL,DPA,4,25,KER)
  ..
  Print results of calculation
  ..
END
```

Note that N and NDIM are the only arguments which may appear as constants in the calling statements.

2.5 Library Routines Explicitly Required

SEVER requires the standard routines SQRT, DSQRT, DBLE, IABS, and ABS, and the Sandia Mathematical Program Library routine ERRCHK.¹

SEVER also references QRVEC which is a subordinate routine contained in the Sandia library. QRVEC is used only by SEVER and is conceptually a part of SEVER.

2.6 User-Supplied Routines Required

SEVER requires no user-supplied routines.

2.7 Cautions and Restrictions

Even though a symmetric matrix is determined by either its upper or lower triangle, the whole matrix must be supplied to the routine. No symmetry check is made. If a nonsymmetric matrix is supplied to the routine, the results will be spurious.

It is extremely likely that zero eigenvalues and zero components of eigenvectors will be returned as very small nonzero numbers. If the absolute value of a computed eigenvalue is smaller than the corresponding value in ERVAL a necessary condition for a zero has been satisfied. The true value of such an eigenvalue may indeed be zero but it is not possible for the routine to make such a determination.

A value of -1.0 for the computed error of an eigenvalue does not necessarily mean that that eigenvalue and its eigenvector are of poor quality. It merely means that it was not possible to compute an upper bound on the absolute error of the computed eigenvalue and computed eigenvector. (See Section 4 for full details on the error calculation.) Furthermore, if some eigenvalue error is returned as -1.0, so must at least one of its adjacent neighbors in the ERVAL array. The error calculation cannot fail for a single eigenvalue.

The computed absolute error bound applies to the computed double precision eigenvalue. The computed single precision eigenvalue may have

a truncation error induced in its last bit. In particular, on the CDC 6600 the single precision eigenvalue may have a truncation-induced error of $2^{\beta-48}$ where the computed eigenvalue is represented by $\alpha 2^{\beta}$ with $1/2 \leq \alpha < 1$.

The second and third columns of the array DPA, which contain vector errors and residual vector lengths, respectively, are not meaningful to full double precision. In fact, only the first significant digit and exponent are usually of any interest.

The routine makes no checks for fault conditions such as underflow or overflow and, if these fault conditions occur, the results may be invalidated.

The routine will not handle a matrix smaller than 3×3 .

2.8 Error Conditions, Messages, and Codes

The subroutine SEVER contains two error messages. If the input variables N and NDIM do not satisfy $3 \leq N \leq NDIM$, the message

INPUT DIMENSIONS ARE INCONSISTENT

is printed and KER is returned as 2.

If more than thirty QR iterations are required for some eigenvalue, the message

NO CONVERGENCE IN 30 QR ITERATIONS

is printed and KER is returned as 3.

The error messages are processed by the Sandia Mathematical Program Library routine ERRCHK; the occurrence of either error message results in a fatal error unless the user has previously made an appropriate call to ERRSET.¹ To make error conditions nonfatal, ERRSET must be called before SEVER is called. For example, to make the errors

nonfatal and set a maximum of 10 messages to be printed the following call must be made:

CALL ERRSET(10,0).

If ERRSET has been called in order to make the error conditions nonfatal and the input dimensions are inconsistent, then KER is set to 2, a return to the calling program is made, and no computations are done. If ERRSET has been called and more than 30 QR iterations are required for some eigenvalue, then KER is set to 3 and a return is made to the calling program. In this case the results may be spurious.

3. Mathematical Method

3.1 Statement of the Problem

Let A, the machine representation of a real symmetric matrix, have eigenvalues $\{\lambda_i\}$ and orthonormal eigenvectors $\{x_i\}$ so that $Ax_i = \lambda_i x_i$. The problem then is to compute scalars $\{\bar{\lambda}_i\}$, vectors $\{\bar{x}_i\}$, with error bounds $\{\epsilon_i\}$ and $\{\eta_i\}$ so that $|\lambda_i - \bar{\lambda}_i| \leq \epsilon_i$ and $\|x_i - \bar{x}_i\| \leq \eta_i$. Hopefully, $|\lambda_i - \bar{\lambda}_i|$ and $\|x_i - \bar{x}_i\|$ are small and "close" to the ϵ_i and η_i . That is, it is desirable for the error bounds to be small and sharp.

3.2 Methods Used

The $n \times n$ matrix A is reduced to tridiagonal form by a sequence of $n-2$ orthogonal similarity transformations each of which makes one row and one column of the off tridiagonal zero. The eigenvalues and eigenvectors of the tridiagonal matrix are computed by a version of the QR algorithm especially modified for symmetric tridiagonal matrices.³ The Rayleigh quotient corrected eigenvalue is calculated using the computed eigenvectors. Each error bound is computed as a function of the length of the residual vector and of the separation of the eigenvalue from its nearest neighbor.

3.3 Mathematical Range and Domain

SEVER computes an eigensystem for a real symmetric matrix. The eigenvalue range is the real line, and the eigenvector range is the unit n -sphere.

The precise range and domain of the subroutine would require a very difficult and pedantic description.

3.4 Equations and Discussion

The real symmetric matrix A is reduced to tridiagonal form by a sequence of orthogonal similarity transformations generated by matrices of the form $I - 2uu^T$, where I is the identity matrix and u is a column vector of length one. That is, let $A_1 = A$ and $A_{i+1} = P_i^{-1}A_iP_i$ where $P_i = I - 2u_iu_i^T$. A_i is tridiagonal in its first $i-1$ rows and columns, and A_{n-1} is the desired tridiagonal form. The matrices P_i are called elementary Hermitians and the method of tridiagonalization is called Householder's method (Reference 11, p. 342).

Each similarity transformation can be conveniently carried out as follows:

$$\begin{aligned}A_2 &= (I - 2uu^T)A_1(I - 2uu^T) \\ &= A_1 - 2uu^TA_1 - 2A_1uu^T + 4(u^TA_1u)uu^T \\ &= A_1 - (uq^T + qu^T)\end{aligned}\tag{1}$$

where $q = p - \alpha u$, $p = 2Au$ and $\alpha = u^Tp$.

Thus no matrix multiplications are required to perform each similarity transformation.

For the first transformation, the vector u is given by $u = \frac{a - c}{\|a - c\|}$ where a is the first column (or row) of A , $c = (a_{11}, \pm s, 0, \dots, 0)^T$ and s^2 is the sum of the squares of the off diagonal elements of the

first row. Succeeding transformations are carried out by considering a matrix of one smaller order each time.

The QR algorithm for an arbitrary real matrix A consists of forming a sequence $\{A_k\}$ as follows: let $A_1 = A$ and for each k factor $A_k = Q_k R_k$ where Q_k is orthogonal and R_k is upper triangular and define $A_{k+1} = R_k Q_k$. Note that $A_{k+1} = R_k Q_k = Q_k^{-1} A_k Q_k$; thus A_{k+1} is orthogonally similar to A_k and, therefore, to A_1 . The factorization $A_k = R_k Q_k$ can always be carried out,⁸ and if A_k is nonsingular it is equivalent to a Gram-Schmidt orthogonalization of the linearly independent column of A_k .

The convergence of the QR algorithm for arbitrary matrices is somewhat too detailed for discussion here (see Reference 4, p. 269). For real symmetric matrices, however, convergence of the QR algorithm to a diagonal matrix is guaranteed, and for real symmetric tridiagonal matrices the implementation of this algorithm assumes a rather simple form (see Section 4).

The algorithm may be modified to increase its rate of convergence by redefining R_k at each stage by $R_k = Q_k^T (A_k - \alpha_k I)$ and choose $A_{k+1} = R_k Q_k$. In this case A_{k+1} is not similar to A_1 but is similar to $A_1 - \sum \alpha_k I$. The choice of α_k is discussed in Section 4.

Let the eigenvalues and eigenvectors computed by the QR algorithm be $\bar{\lambda}_1, \dots, \bar{\lambda}_n$ and $\bar{x}_1, \dots, \bar{x}_n$. Define the Rayleigh quotient

$$\rho_i = \frac{\bar{x}_i^T A \bar{x}_i}{\bar{x}_i^T \bar{x}_i} \text{ where } A \text{ is the original matrix. Let } \epsilon_i \text{ be the length of the}$$

residual vector, $\epsilon_i = \|A \bar{x}_i - \rho_i \bar{x}_i\|$ and let a_i be the distance from the true eigenvalue λ_i to its nearest neighbor. Then the results which allow calculation of the error bounds of the computed eigensystem are

$$|\lambda_i - \rho_i| \leq \epsilon, \tag{2}$$

$$|\lambda_i - \rho_i| \leq \frac{\epsilon^2/a_i}{1 - \epsilon^2/a_i^2}, \text{ and} \tag{3}$$

$$\|x_i - \bar{x}_i\|^2 \leq \frac{\epsilon^2}{a_i^2} \left(1 + \frac{\epsilon^2}{a_i^2}\right), \tag{4}$$

where the vectors x_i and \bar{x}_i have length one. For proofs of these results, see Reference 12. Note that these inequalities yield upper bounds on the absolute errors of the computed eigensystem. Furthermore, since $\|x_i\| = 1$ the eigenvector inequality bounds both the relative and absolute errors.

3.5 Error Analysis, Bounds, and Estimates

The following three matrix norms are used:

$$\|A\|_2 = \max \{ \|Ax\| : \|x\| = 1 \} \quad (5)$$

where $\|x\|$ is the ordinary length of x , or $\|x\|^2 = x^T x$. Note that, for symmetric matrices, $\|A\|_2$ is the largest eigenvalue in absolute value of A .

$$\|A\|_\infty = \max_i \sum_{j=1}^n |a_{ij}|, \quad (6)$$

the maximum absolute value row sum of A .

$$\|A\|_E^2 = \sum_{ij} |a_{ij}|^2 = \sum_i |\lambda_i|^2, \quad (7)$$

where the λ_i are the eigenvalues of A .

It is true for all matrices that $\|A\|_2 \leq \|A\|_E$ and if λ is any eigenvalue of A , then $|\lambda| \leq \|A\|_t$ for $t = 2, \infty$, or E . If A is real symmetric then $\|A\|_2 \leq \|A\|_\infty$. While $\|A\|_E$ and $\|A\|_\infty$ do not bound the eigenvalues as sharply as $\|A\|_2$, they have the advantage of ease of computation.

The significant results concerning a posteriori error analysis of real symmetric matrix eigenvalue calculations are as follows: Let A , B , and $A+B$ be real symmetric matrices with eigenvalues $\{\lambda_i\}$, $\{\mu_i\}$, and $\{\nu_i\}$,

respectively, subscripted in nonincreasing order. Then

$$|\lambda_i - \nu_i| \leq \|B\|_2 = \max_i |\mu_i| \leq \|B\|_E \quad (8)$$

(Reference 9, p. 100) and

$$\sum (\lambda_i - \nu_i)^2 \leq \|B\|_E^2 = \sum |\mu_i|^2 \quad (9)$$

(Reference 11, p. 104). Thus, unlike the matrix inversion problem or the nonsymmetric eigenvalue problem, the eigenvalue problem for real symmetric matrices is not ill conditioned. In fact, it is Lipschitz continuous.

Suppose the real symmetric matrix A, whose elements are represented as decimal fractions, is presented to a digital computer algorithm for eigenvalue calculation. The algorithm computes not the eigenvalues of A but those of a slightly perturbed matrix A+D. The perturbation D arises from inexact machine representation of A and from errors induced in the diagonalization of A.

Equation 8 can be used to bound the errors arising from inexact machine representation of A. Suppose δ is the maximum relative error in the floating point representation of a real number. For most machines δ is bounded above by $1/2$ raised to one less than the mantissa length in bits. The matrix A in the machine is A+ Δ where the (i,j) element of Δ is δ_{ij} and $|\delta_{ij}| \leq |a_{ij}| \delta$. Thus, using Equation 8 and the fact that $\|\Delta\|_2 \leq \|\Delta\|_\infty$, the result is that $n \max_{i,j} |a_{ij}| \delta$ is the largest possible error in any computed eigenvalue due to imprecise machine representation of the initial data.

While analytical expressions for upper bounds of the error induced in the diagonalization exist, they are cumbersome to compute and are usually quite pessimistic (Reference 11, p. 297). At any rate, these errors are part of the a posteriori errors described in Sections 3.4 and 4.

Unfortunately, the eigenvector problem for real symmetric matrices is not as well conditioned as in the eigenvalue problem. In fact, the

eigenvectors of a real symmetric matrix may not even depend continuously on the matrix elements. However, if an eigenvalue is sufficiently well separated from its nearest neighbor, then the following shows that its corresponding eigenvector calculation is well conditioned: Let A and $A+B$ be real symmetric matrices with eigenvalues $\{\lambda_i\}$ and $\{\nu_i\}$ and corresponding eigenvectors $\{u_i\}$ and $\{v_i\}$ of length one. Let α_k be the distance from λ_k to its nearest neighbor. If $\alpha_k > \|B\|_2$ then

$$\|u_k - v_k\| \leq \gamma(1 + \gamma^2)^{1/2} \quad (10)$$

where $\gamma = \|B\|_2/(\alpha_k - \|B\|_2)$, see Reference 9.

To use this result, suppose B is the perturbation matrix resulting from inexact machine representation of the elements of A , $\|B\|_2 \leq n\delta$ and, if α is sufficiently larger than $\|B\|_2$, then $\|u_k - v_k\|$ is approximately $n\delta/\alpha$. A satisfactory qualitative statement of this result is that if the separation of an eigenvalue is significantly greater than the norm of the perturbation matrix then the corresponding eigenvector problem is well conditioned.

The eigenvector error induced by inexact diagonalization is accounted for in the a posteriori error bound of Equation 4.

Another source of error in the eigensystem calculation is inexact knowledge of the input matrix A . Upper bounds in the perturbations thus caused may be accounted for exactly as those caused by inexact machine representation of the matrices. For example, consider the realistic physical situation in which each element of a 200×200 matrix has an absolute error bounded by 5×10^{-3} , i.e., each element is correctly rounded to the nearest hundredth. In this case the norm of the error matrix $\|\Delta\|_\infty$ is bounded by $(200)(5)(10^{-3}) = 1$. Thus, the best possible bound on the absolute error of the computed eigenvalues is one. This rather pessimistic result is not dependent upon the method of eigenvalue calculation but is simply a property of the matrix. However, the absolute error bound can be reduced somewhat in the case of sparse or bandwidth-limited matrices.

4. Programming Method

The program divides naturally into four parts: the tridiagonalization, the calculation of eigenvalues and eigenvectors, the Rayleigh quotient correction, and the calculation of error bounds.

Before tridiagonalization the matrix A is copied into the array VEC , and the tridiagonalization and QR algorithm are carried out entirely within VEC . The tridiagonalization is carried out as described in Section 3.4. If, at the i -th stage, the sum of the squares of the off tridiagonal elements is sufficiently small no transformation is necessary. Indeed if this sum is small but not exactly zero then the corresponding transformation is in danger of not being orthogonal. Such a transformation is skipped if the sum of the squares of the off tridiagonal elements is less than the quotient of the smallest positive floating point number and the smallest positive floating point number which when added to 1.0 yields a sum not 1.0.

The off tridiagonal places of VEC are used to store the tridiagonalizing transformations for later use in calculating eigenvectors. In particular if $P^{-1}AP$ is tridiagonal and x is an eigenvector of $P^{-1}AP$ then Px is an eigenvector of A .

The tridiagonalization is carried out in single precision.

For convenience in programming, the QR algorithm is restated as a QL algorithm (i.e., the triangular factor is lower rather than upper). The algorithm is then stated:

$$Q_k (A_k - \alpha_k I) = L_k ,$$
$$A_{k+1} = L_k Q_k^T .$$
(11)

Note that the Q_k here are the transposes of the Q_k in Section 3.4.

for $i = n-1, n-2, \dots, 1$ and

$$e_1^{(k+1)} = s_1 p_1 \quad d_1^{(k+1)} = c_1 p_1 \quad (18)$$

Suppose the $(k-1)$ st eigenvalue has been found and is stored in d_{k-1} . At this stage the diagonal of the iterated matrix has eigenvalues in the first $k-1$ places and zeros in the first $k-1$ subdiagonal elements e_1, \dots, e_{k-1} . To find the k -th eigenvalue the QL iterations are continued until e_k is negligible or until 30 iterations are carried out. Furthermore, suppose some $e_j, j = k+1, \dots, n$ is negligible, then the QL iterations are carried out only on the submatrix with diagonal d_k, \dots, d_j . That is, the matrix is considered to be the direct sum of two matrices of smaller order.

The criterion for negligibility is as follows: Just before iterating for the k -th eigenvalue set $h_k = \epsilon(|d_k| + |e_k|)$ then any off diagonal element e_i for which $|e_i| \leq \max h_j, j = 1, \dots, k$ is regarded as negligible, where ϵ is the smallest positive floating point number which when added to 1.0 yields a sum not 1.0. On the CDC 6600 ϵ is taken to be 2^{-47} .

At the start of the iteration to find the k -th eigenvalue the shift α_k is taken to be the eigenvalue of the matrix

$$\begin{vmatrix} d_k & e_k \\ e_k & d_{k+1} \end{vmatrix}$$

which is nearer to d_k . This eigenvalue can be expressed as

$$d_k - \frac{e_k}{p + \text{sign}(p) \sqrt{p^2 + 1}},$$

$$\text{where } p = \frac{d_{k+1} - d_k}{2 e_k}.$$

The QR algorithm for symmetric tridiagonal matrices is known to converge (Reference 11, p. 548), and in testing it converged very rapidly. The routine allows up to thirty iterations per eigenvalue but this number is quite high. In testing on the CDC 6600 no more than seven were ever required.

The QR algorithm is carried out in single precision. For a quite detailed discussion of the computer implementation of this algorithm, see Reference 3.

The Rayleigh quotient ρ_i is computed using the relationship

$$\rho_i = \bar{x}_i^T A \bar{x}_i = \bar{x}_i^T (\bar{\lambda}_i \bar{x}_i + \eta_i) = \bar{\lambda}_i + \bar{x}_i^T \eta_i \quad (19)$$

where $\bar{\lambda}_i$ and \bar{x}_i are the computed eigenvalue and eigenvector respectively, A is the original matrix, and η_i is the residual vector $A\bar{x}_i - \bar{\lambda}_i\bar{x}_i$. The calculation of ρ_i is carried out in double precision. The $\bar{\lambda}_i$ is then changed from its QR computed eigenvalue to ρ_i which is then converted to single precision. Thus, upon return, EV contains the single precision versions of the members of the first column of DPA. Equation 2 of Section 3.4 shows that there is a true eigenvalue λ in the interval $[\rho_i - \epsilon_i, \rho_i + \epsilon_i]$. Thus a safe lower bound a_i on the distance between λ_i and its nearest neighbor may be computed:

$$a_1 = \rho_1 - \epsilon_1 - \rho_2 - \epsilon_2, \quad (20)$$

$$a_i = \min[\rho_i - \epsilon_i - \rho_{i+1} - \epsilon_{i+1}, \rho_{i-1} - \epsilon_{i-1} - \rho_i - \epsilon_i] \quad (21)$$

for $i = 2, \dots, n-1$, and

$$a_n = \rho_{n-1} - \epsilon_{n-1} - \rho_n - \epsilon_n. \quad (22)$$

The expressions for the eigenvalue and eigenvector errors, Equations 3 and 4, are useful only if $\epsilon \ll a$. Accordingly, if $10 \cdot \epsilon \geq a$ then no error calculation is attempted and the corresponding value of ERVAL is returned as -1.0. If $10\epsilon < a$ then the eigenvalue and eigenvector errors are computed as ϵ^2/a and ϵ/a respectively and the factors $(1 - \epsilon^2/a^2)^{-1}$ and $(1 + \epsilon^2/a^2)$ of Equations 3 and 4 are ignored.

5. Space, Time, and Accuracy Considerations

The size of SEVER is about 1200_{10} words on the CDC 6600. In addition, at least $2n^2 + 8n$ words for the matrix, eigenvalues, eigenvectors, and error bounds are required and are supplied by the user's calling program. On the CDC 6600 it is possible to resolve a 200 x 200 matrix.

For n larger than about 15, the time required for a complete eigen-system calculation is very nearly proportional to n^3 . For n smaller than 15, time required for subroutine linkage and initialization dominate and no simple relationship between time and n seems to exist. See Appendix B for machine-dependent details.

Accuracy is discussed in Section 3.5 and is not subject to user control. For machine-dependent details see Appendix B.

6. Testing Methods

6.1 General Discussion

There are many ways to test a routine which computes the eigen-system of a real symmetric matrix. A list of possible tests includes:

- (1) $\det (A - \lambda I) = 0$
- (2) $\text{trace} (A) = \sum \lambda_i$
- (3) $Ax = \lambda x$ or $\|Ax - \lambda x\| = 0$
- (4) Sum of idempotents, i.e., $A = \sum \lambda_i x_i x_i^T$, where $\|x\| = 1$
- (5) Computed solution compared to known exact solution
- (6) Orthogonality of computed eigenvectors

- (7) The eigenvalues of $A + I$ are 1 plus those of A , and the eigenvectors the same for each. Similarly the eigenvalues of αA are α times those of A .
- (8) Extensive running of the routine for "shakedown" purposes and timing determinations
- (9) Plausible results.

Items (1) and (4) are considered inconclusive and unnecessarily difficult to compute. Item (2) offers no additional information or assurance that is not given by other tests used to authenticate SEVER.

From a logical point of view, successful testing, no matter how extensive, is a necessary but not a sufficient condition for a routine to be valid.

6.2 Kinds of Tests Used

Item (3) is an internal check in SEVER. The value of $\|AX_i - \bar{\lambda}_i \bar{x}_i\|$ is returned in DPA(I,3) for the I-th eigenvalue-eigenvector pair. Of course one must test for a small value, since a zero will occur rarely. This test is quite inconclusive.

Item (5) is probably the most important test. Assurance of authenticity, a measure of precision of the routine, and a check on the sharpness of the error bounds are obtained by comparing true and computed solutions to nontrivial problems whose solutions are known.

Item (6) is checked by computing the Gram matrix of the matrix whose columns are the computed eigenvectors. The (i,j) element of the Gram matrix may be thought of as the cosine of the angle between eigenvectors i and j. This test measures the orthogonality of the eigenvectors but not their quality.

Item (7) is useful for checking the scale independence of the routine and offers a further check on the error bounds.

Items (8) and (9) are, of course, present in all tests and may be examined further by resolution of matrices whose elements are numbers chosen from a sequence of random numbers.

6.3 Normal Cases Tested

It is easy to construct small matrices with known eigensystems using Test (4) of Section 6.1. Such matrices usually present no difficulty and do not constitute a significant test. It is relatively easy to construct matrices whose elements are pseudo-random numbers and this was done to test in the sense of Items (8) and (9). It is extremely unlikely that a matrix of random numbers would exhibit clustered or multiple eigenvalues or any other difficulties.

6.4 Difficult Cases Tested

Possible difficulties arise with closely spaced eigenvalues and eigenvalues of multiplicity greater than one. In the latter case an eigenvalue admits linearly independent but nonorthogonal eigenvectors. For example, the matrix

$$\begin{bmatrix} 7 & 2 & 0 \\ 2 & 4 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

has eigenvalues 8, 3, and 3. The vectors $(-1, 2, -1)^T$ and $(-2, 4, 3)^T$ are a pair of linearly independent nonorthogonal eigenvectors corresponding to eigenvalue 3. The eigenvalue 3 does, however, admit a pair of orthogonal eigenvectors. In fact, infinitely many such pairs exist.

A difficulty, in some methods, occurs when the largest and smallest eigenvalues are equal in absolute value. This situation is no problem to the methods used in SEVER and is not considered a difficult case for this routine.

The example of Rosser et al¹⁰ is about as pathological as an eight by eight with small integer elements can get:

$$R_8 = \begin{bmatrix} 611 & 196 & -192 & 407 & -8 & -52 & -49 & 29 \\ 196 & 899 & 113 & -192 & -71 & -43 & -8 & -44 \\ -192 & 113 & 899 & 196 & 61 & 49 & 8 & 52 \\ 407 & -192 & 196 & 611 & 8 & 44 & 59 & -23 \\ -8 & -71 & 61 & 8 & 411 & -599 & 208 & 208 \\ -52 & -43 & 49 & 44 & -599 & 411 & 208 & 208 \\ -49 & -8 & 8 & 59 & 208 & 208 & 99 & -911 \\ 29 & -44 & 52 & -23 & 208 & 208 & -911 & 99 \end{bmatrix}$$

R_8 has eigenvalues:

$$\begin{aligned} 10 \sqrt{10405} &= 1020.0490184299968238 \\ &1020 \\ 510+100\sqrt{26} &= 1019.9019513592784830 \\ &1000 \\ &1000 \\ 510-100\sqrt{26} &= 0.0980486407215169971776 \\ &0 \\ -10 \sqrt{10405} &= -1020.0490184299968238 \end{aligned}$$

See Appendix B for machine-dependent results of SEVER with R_8 .

A large class of useful test matrices may be constructed using the Kronecker product $A \otimes B$. Let A be m by m and B be n by n . Then $A \otimes B$ is the nm by nm matrix:

$$A \otimes B = \begin{bmatrix} a_{11} B & a_{12} B & \dots & a_{1m} B \\ a_{21} B & a_{22} B & \dots & a_{2m} B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} B & a_{m2} B & \dots & a_{mm} B \end{bmatrix} \quad (23)$$

The eigenvalues of $A \otimes B$ are the nm products of an eigenvalue of A times one of B . Let x and y be eigenvectors of A and B with eigenvalues α and β respectively, then $x \otimes y$ is an eigenvector of $A \otimes B$ corresponding to $\alpha\beta$ where $x \otimes y$ is the mn component vector:

$$(x_1y_1, x_1y_2, \dots, x_1y_n, x_2y_1, \dots, x_2y_n, \dots, x_my_1, \dots, x_my_n)^T.$$

For details and proofs see Reference 6 or Reference 2.

A 32 x 32 test matrix $A (A = B \otimes R_8)$ was constructed where

$$B = \begin{bmatrix} 15/16 & 5/8 & 5/16 & -1/8 \\ 5/8 & 15/16 & 1/8 & 5/16 \\ 5/16 & 1/8 & 15/16 & 5/8 \\ -1/8 & 5/16 & 5/8 & 15/16 \end{bmatrix} \quad (24)$$

The eigenvalues of B are 2, 1.125, 0.5, and 0.125 exactly.

The matrix $A = B \otimes R_8$ is large enough to be nontrivial, is singular (in fact, $\text{rank}(A) = 28$), has multiple and clustered eigenvalues, and its nonzero eigenvalues span five orders of magnitude.

It is thought that matrices A , $A + I$, αA , and $\alpha A + I$ where $\alpha = 2^{-11}$ form a fairly significant test collection. Furthermore, each of these matrices admits an exact machine representation so that errors in the computed eigensystem are totally due to errors in the diagonalization. See Appendix B for machine-dependent results of SEVER with these matrices.

A nontrivial test matrix with predetermined eigenvalues d_1, \dots, d_n can be constructed as the product $U^T D U$ where U is a nontrivial orthogonal matrix and $D = \text{diag}(d_1, \dots, d_n)$. An extremely convenient choice for U is $1/\sqrt{n} H_n$ where H_n is an $n \times n$ symmetric Hadamard matrix of plus ones and minus ones and n is a power of two. A Hadamard matrix is one in which any two rows (or columns) agree in exactly half their places and disagree in half.⁵ H_n for $n = 2^k$ can be constructed as the k -fold Kronecker product of the matrix

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

with itself.⁷

The product $P = 1/n H_n D H_n$, called a Hadamard product, has eigenvalues d_1, \dots, d_n and the columns (or rows) of $1/\sqrt{n} H_n$ form an orthogonal set of eigenvectors. Furthermore, if n is a power of two then each element of p is exactly representable in a binary computer for a large class of D .

It is thought the Hadamard products $1/8 H_8 D_8 H_8$ and $1/16 H_{16} D_{16} H_{16}$ form a significant pair of tests where D_8 has diagonal elements 1.0 and $1.0 + 2^{-k}$ for $k = 38$ to 44 and D_{16} has diagonal elements 1.0 and $1.0 + 2^{-k}$ for $k = 24$ to 38 .

An example which further illustrates the difficulty in distinguishing between multiple and clustered eigenvalues is W_{21}^+ , see Reference 11, p. 309. W_{21}^+ is a tridiagonal matrix whose main diagonal is 10, 9, 8, ..., 1, 0, 1, ..., 8, 9, 10, and whose sub and super diagonals are all 1's. W_{21}^+ has pairs of extremely clustered eigenvalues. In fact the pair of largest eigenvalues agrees to 15 decimal places. See Appendix B for machine-dependent results of calculations with this matrix.

An example which illustrates the sharpness of the error bounds is W_{21}^- , again Reference 11, p. 309. W_{21}^- is identical with W_{21}^+ except the elements on the lower half of the main diagonal of W_{21}^- are the negatives of those on the lower half of the main diagonal of W_{21}^+ . W_{21}^- is singular and its nonzero eigenvalues occur in pairs differing only in sign.

6.5 Range, Error, and Fault Checks Tested

Both of the diagnostics in SEVER were checked. The diagnostics for the consistency of the input dimensions were checked by calling the routine with faulty parameters. The author was able to find no matrix with an eigenvalue which required more than thirty QR iterations. However, the viability of the related error check was tested by arbitrary lowering the limit on QR iterations to 5 in order to simulate an occurrence of the error condition.

7. Remarks

Suppose $C = A + iB$ is an $n \times n$ complex Hermitian matrix. Equating real and imaginary parts of

$$(A + iB)(x + iy) = \lambda(x + iy)$$

yields the $2n \times 2n$ symmetric problem $DZ = \lambda Z$ where, in blocks,

$$D = \begin{pmatrix} A & -B \\ B & A \end{pmatrix} \quad \text{and} \quad Z = \begin{pmatrix} x \\ y \end{pmatrix} .$$

Each eigenvalue of C occurs as an eigenvalue of D of multiplicity two. The first n components of an eigenvector of D from the real part of an eigenvector of C and the remaining n components form the imaginary part. That is, let x be a $2n$ component eigenvector of D corresponding to eigenvalue λ and let the first n components of x be an n vector x_1 and the remaining n components be an n vector x_2 . Then $x_1 + ix_2$ is an eigenvector of C corresponding to eigenvalue λ . Furthermore, the eigenvectors of C computed in this way are of length one and those corresponding to distinct eigenvalues are orthogonal.

There will be two real orthogonal eigenvectors of D corresponding to each one of C . However, when these two real $2n$ component vectors are each converted to n component complex eigenvectors of C it is easily seen that one is a scalar multiple of the other and that the scalar is a complex number of absolute value one.

In case D has some eigenvalue of multiplicity $2k$, $k > 1$, care must be used in choosing eigenvectors of C in order to guarantee orthogonality.

8. Certification

This routine was subjected to a wide variety of tests. The performance of the routine throughout the tests was checked carefully.

The nature of the tests, the reliability of the routine, the error analyses conducted, and the observed variation in accuracy are reported in this document. While it is believed that the facts recorded and the judgments expressed regarding accuracy and reliability are strong indications of the general quality and validity of the routine, the tests should not be considered to be exhaustive. The use of this routine outside of the stated range of application or in violation of stated restrictions may produce unspecified results. The statements made in this document are intended to apply only to those versions of the indicated routine which are released by the Sandia Laboratories Mathematical Program Library project.

The author wrote SEVER and converted to FORTRAN the ALGOL routine in Reference 8 for tridiagonalization; converted the ALGOL routine in Reference 3 for eigenvalues and eigenvectors; added the Rayleigh quotient correction and error bound calculation; and performed the tests described above.

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APPENDIX A

The SEVER Listing

The changes which may have to be made for use of SEVER on machines other than the CDC 6600 are the DATA statements in lines SEV 480 and SEV 490 and the octal constants in lines SEV 640 and SEV 2370. ERRCHK is called in SEV 530 and SEV 1580.

C	SUBROUTINE SEVER(A, EV, VEC, ERVAL, DPA, N, NDIM, KER)	SEV	10
C		SEV	20
C	SANDIA MATHEMATICAL PROGRAM LIBRARY	SEV	30
C	MATHEMATICAL COMPUTING SERVICES DIVISION 9422	SEV	40
C	SANDIA LABORATORIFS	SEV	50
C	P. O. BOX 5800	SEV	60
C	ALBUQUERQUE, NEW MEXICO 87115	SEV	70
C		SEV	80
C	WRITTEN BY WILLIAM R. GAVIN	SEV	90
C		SEV	100
C	CONTROL DATA 6600 VERSION	SEV	110
C		SEV	120
C	ABSTRACT	SEV	130
C		SEV	140
C	THIS ROUTINE COMPUTES ALL THE EIGENVALUES OF A REAL SYMMETRIC	SEV	150
C	MATRIX AND AN EIGENVECTOR OF LENGTH ONE CORRESPONDING TO EACH	SEV	160
C	EIGENVALUE. THE COMPUTED EIGENVALUES ARE SUBJECTED TO A	SEV	170
C	RAYLEIGH QUOTIENT CORRECTION. UPPER BOUNDS ON THE ABSOLUTE	SEV	180
C	ERRORS OF THE COMPUTED EIGENSYSTEM ARE CALCULATED.	SEV	190
C		SEV	200
C	DESCRIPTION OF PARAMETERS	SEV	210
C		SEV	220
C	A THE SYMMETRIC MATRIX WHOSE EIGENSYSTEM IS TO BE COMPUTED	SEV	230
C	EV CONTAINS THE EIGENVALUES OF A IN NON-INCREASING	SEV	240
C	ALGEBRAIC ORDER	SEV	250
C	VEC CONTAINS THE EIGENVECTORS. COLUMN J OF VEC CONTAINS THE	SEV	260
C	EIGENVECTOR CORRESPONDING TO THE EIGENVALUE IN EV(J).	SEV	270
C	THE EIGENVECTOR IS OF LENGTH UNITY.	SEV	280
C	ERVAL CONTAINS UPPER BOUNDS ON THE ABSOLUTE ERRORS OF THE	SEV	290
C	COMPUTED EIGENVALUES	SEV	300
C	DPA IS AN NDIM BY 3 DOUBLE PRECISION ARRAY	SEV	310
C	COL. 1 CONTAINS RAYLEIGH CORRECTED EIGENVALUES.	SEV	320
C	COL. 2 CONTAINS THE LENGTHS OF THE RESIDUAL VECTORS	SEV	330
C	COL. 3 CONTAINS UPPER BOUNDS ON THE ABSOLUTE ERRORS	SEV	340
C	OF THE COMPUTED EIGENVECTORS AS MEASURED IN	SEV	350
C	THE TWO NORM	SEV	360
C	N ORDER OF THE MATRIX WHOSE EIGENSYSTEM IS COMPUTED	SEV	370
C	NDIM DIMENSION OF ARRAYS PASSED INTO SUBROUTINE	SEV	380
C	KER OUTPUT ERROR CODE	SEV	390
C	1 NORMAL (NO ERROR)	SEV	400
C	2 N LESS THAN 3 OR GREATER THAN NDIM	SEV	410
C	3 MORE THAN 30 QR ITERATIONS REQUIRED	SEV	420
C		SEV	430
C		SEV	440
C	DIMENSION A(NDIM,ND...),EV(NDIM),VEC(NDIM,NDIM),ERVAL(NDIM)	SEV	450
C	DIMENSION DPA(NDIM,3),MSG(7),MSG2(7)	SEV	460
C	DOUBLE PRECISION DPA,DS,DP,DTV	SEV	470
C	DATA(MSG= 2 ,43H INPUT DIMENSIONS ARE INCONSISTANT) SEV	480
C	DATA(MSG2= 3 ,43H NO CONVERGENCE IN 30 QR ITERATIONS) SEV	490
C	KER=1	SEV	500
C	IF(N.LE.2.OR. N.GT.NDIM) KER=2	SEV	510
C	IF(KER.EQ.1) GOTO 1	SEV	520
C	CALL FRRCHK(43,MSG)	SEV	530
C	RETURN	SEV	540

C		SEV 550
C	COPY A INTO VECTOR ARRAY	SEV 560
C		SEV 570
	1 DO 2 I=1,N	SEV 580
	DO 2 J=1,N	SEV 590
	2 VEC(I,J)=A(I,J)	SEV 600
	NM1=N-1	SEV 610
	NM2=N-2	SEV 620
C*****		SEV 630
	EPS=00061400000000000000	SEV 640
C	EPS IS THE QUOTIENT OF THE SMALLEST POSITIVE FLOATING POINT	SEV 650
C	NUMBER AND THE SMALLEST POSITIVE FLOATING POINT NUMBER WHICH	SEV 660
C	WHEN ADDED TO 1.0 YIELDS A SUM NOT 1.0 . THIS IS A MACHINE	SEV 670
C	DEPENDENT CONSTANT AND MUST BE CHANGED FOR USE OF THIS	SEV 680
C	ROUTINE ON COMPUTERS OTHER THAN THE CDC 6600.	SEV 690
C*****		SEV 700
	NP2=N+2	SEV 710
C		SEV 720
C	BFGIN TRIDIAGONALIZATION	SEV 730
C		SEV 740
C-----		SEV 750
C	THE TRIDIAGONALIZATION IS A FORTRAN VERSION OF THE ALGOL	SEV 760
C	ROUTINE OF MARTIN, REINSCH, AND WILKINSON. NUMER MATH 11,	SEV 770
C	181-195(1968).	SEV 780
C-----		SEV 790
	DO 15 IB=2,N	SEV 800
	I=NP2-IB	SEV 810
	L=I-2	SEV 820
	FACT=VEC(I,I-1)	SEV 830
	GSTO=0.0	SEV 840
	IF(L.EQ.0) GOTO 4	SEV 850
	DO 3 K=1,L	SEV 860
	3 GSTO=GSTO+VEC(I,K)**2	SEV 870
	4 HOLD=GSTO+FACT*FACT	SEV 880
C-----		SEV 890
C	OMIT THIS TRANSFORMATION IF GSTO IS TOO SMALL TO MAKE	SEV 900
C	IT ORTHOGONAL	SEV 910
C-----		SEV 920
	IF(GSTO.GT.EPS) GOTO 5	SEV 930
	ERVAL(I)=FACT	SEV 940
	HOLD=0.0	SEV 950
	GOTO 14	SEV 960
	5 L=L+1	SEV 970
	TEMP=SORT(HOLD)	SEV 980
	IF(FACT.GT.0.0) TEMP=-TEMP	SEV 990
	ERVAL(I)=TEMP	SEV 1000
	GSTO=TEMP	SEV 1010
	HOLD=HOLD-FACT*GSTO	SEV 1020
	VEC(I,I-1)=FACT-GSTO	SEV 1030
	FACT=0.0	SEV 1040
	DO 9 J=1,L	SEV 1050
	VEC(J,I)=VEC(I,J)/HOLD	SEV 1060
	GSTO=0.0	SEV 1070
	DO 6 K=1,J	SEV 1080

6	GSTO=GSTO+VEC(J,K)*VEC(I,K)	SEV 1090
	JP1=J+1	SEV 1100
	IF(JP1.GT.L) GOTO 8	SEV 1110
	DO 7 K=JP1,L	SEV 1120
7	GSTO=GSTO+VEC(K,J)*VEC(I,K)	SEV 1130
8	ERVAL(J)=GSTO/HOLD	SEV 1140
	FACT=FACT+GSTO*VEC(J,I)	SEV 1150
9	CONTINUE	SEV 1160
10	HH=FACT/(HOLD+HOLD)	SEV 1170
	DO 13 J=1,L	SEV 1180
	FACT=VEC(I,J)	SEV 1190
	ERVAL(J)=ERVAL(J)-HH*FACT	SEV 1200
	GSTO=FRVAL(J)	SEV 1210
	DO 12 K=1,J	SEV 1220
12	VEC(J,K)=VEC(J,K)-FACT*ERVAL(K)-GSTO*VEC(I,K)	SEV 1230
13	CONTINUE	SEV 1240
14	EV(I)=HOLD	SEV 1250
15	CONTINUE	SEV 1260
	EV(1)=0.0	SEV 1270
	ERVAL(1)=0.0	SEV 1280
C		SEV 1290
C	ACCUMULATE TRANSFORMATION MATRIX	SEV 1300
C		SEV 1310
	EV(1)=VEC(1,1)	SEV 1320
	VEC(1,1)=1.0	SEV 1330
	DO 25 I=2,N	SEV 1340
	L=I-1	SEV 1350
	IF(EV(I).EQ.0.0) GOTO 23	SEV 1360
	DO 22 J=1,L	SEV 1370
	GSTO=0.0	SEV 1380
	DO 19 K=1,L	SEV 1390
19	GSTO=GSTO+VEC(I,K)*VEC(K,J)	SEV 1400
	DO 21 K=1,L	SEV 1410
21	VEC(K,J)=VEC(K,J)-GSTO*VEC(K,I)	SEV 1420
22	CONTINUE	SEV 1430
23	EV(I)=VEC(I,I)	SEV 1440
	VEC(I,I)=1.0	SEV 1450
	DO 24 J=1,L	SEV 1460
	VEC(I,J)=0.0	SEV 1470
24	VEC(J,I)=0.0	SEV 1480
25	CONTINUE	SEV 1490
C-----		SEV 1500
C	THE TRIDIAGONALIZATION IS NOW COMPLETE	SEV 1510
C	DIAGONAL ELEMENTS ARE IN EV	SEV 1520
C	OFF DIAGONAL ELEMENTS ARE IN ERVAL	SEV 1530
C	COMPUTE THE EIGENVALUES AND EIGENVECTORS OF THE TRIDIAGONAL	SEV 1540
C	MATRIX	SEV 1550
C-----		SEV 1560
	CALL QRVFC(EV,ERVAL,VEC,N,NDIM,KER)	SEV 1570
	IF(KER.NE.1) CALL ERRCHK(43,MESG2)	SEV 1580
C-----		SEV 1590
C	COMPUTE RAYLEIGH CORRECTED EIGENVALUES	SEV 1600
C-----		SEV 1610
	DO 49 IV=1,N	SEV 1620

DO 45 J=1,N	SEV 1630
DS=0.0D+00	SEV 1640
DO 43 K=1,N	SEV 1650
DP=DBLE(A(J,K))*DBLE(VEC(K,IV))	SEV 1660
43 DS=DS+DP	SEV 1670
DS=DS-DBLE(EV(IV))*DBLE(VEC(J,IV))	SEV 1680
45 DPA(J,3)=DS	SEV 1690
DS=0.0D+00	SEV 1700
DP=0.0D+00	SEV 1710
DO 47 K=1,N	SEV 1720
DP=DP+DPA(K,3)**2	SEV 1730
47 DS=DS+DBLE(VEC(K,IV))*DPA(K,3)	SEV 1740
DPA(IV,2)=DSQRT(DP)	SEV 1750
DPA(IV,1)=DBLE(EV(IV))+DS	SEV 1760
EV(IV)=DPA(IV,1)	SEV 1770
49 CONTINUE	SEV 1780
C-----	SEV 1790
C A TRUE EIGENVALUE IS IN THE INTERVAL	SEV 1800
C * DPA(IV,1)-DPA(IV,2) , DPA(IV,1)+DPA(IV,2) *	SEV 1810
C-----	SEV 1820
C COMPUTE UPPER BOUNDS ON THE ABSOLUTE ERRORS IN THE	SEV 1830
C COMPUTED EIGENSYSTEM	SEV 1840
C-----	SEV 1850
DS = DPA(1,1)-DPA(1,2)-DPA(2,1)-DPA(2,2)	SEV 1860
IF(DPA(1,2).LT.1.0D+01*DS) GOTO 51	SEV 1870
ERVAL(1)=-1.0	SEV 1880
DPA(1,3)=DPA(1,2)	SEV 1890
ERVAL(2)=-1.0	SEV 1900
DPA(2,3)=DPA(2,2)	SEV 1910
NUP=3	SEV 1920
GOTO 52	SEV 1930
51 DPA(1,3)=DPA(1,2)/DS	SEV 1940
ERVAL(1)=DPA(1,3)*DPA(1,2)	SEV 1950
NUP=2	SEV 1960
52 IF(NUP.GT.NM1) GOTO 57	SEV 1970
DO 54 K=NUP,NM1	SEV 1980
DP=DPA(K-1,1)-DPA(K,1)-DPA(K-1,2)-DPA(K,2)	SEV 1990
DS=DPA(K,1)-DPA(K,2)-DPA(K+1,1)-DPA(K+1,2)	SEV 2000
IF(DS.LT.DP) DP=DS	SEV 2010
IF(DPA(K,2).LT.1.0D+01*DP) GOTO 53	SEV 2020
DPA(K,3)=DPA(K,2)	SEV 2030
ERVAL(K)=-1.0	SEV 2040
GOTO 54	SEV 2050
53 DPA(K,3)=DPA(K,2)/DP	SEV 2060
ERVAL(K)=DPA(K,3)*DPA(K,2)	SEV 2070
54 CONTINUE	SEV 2080
57 CONTINUE	SEV 2090
DS = DPA(NM1,1)-DPA(NM1,2)-DPA(N,1)-DPA(N,2)	SEV 2100
IF(DPA(N,2).LT.1.0D+01*DS)GOTO 56	SEV 2110
ERVAL(N) = -1.0	SEV 2120
DPA(N,3)=DPA(N,2)	SEV 2130
RETURN	SEV 2140
56 DPA(N,3)=DPA(N,2)/DS	SEV 2150
ERVAL(N)=DPA(N,2)*DPA(N,3)	SEV 2160
RETURN	SEV 2170
END	SEV 2180

SUBROUTINE QRVEC(DG,EG,VEC,N,NDIM,KER)	SEV 2190
C-----	SEV 2200
C QRVEC COMPUTES EIGENVALUES AND EIGENVECTORS OF A SYMMETRIC	SEV 2210
C TRIDIAGONAL MATRIX	SEV 2220
C	SFV 2230
C DG ARRAY OF DIAGONAL ELEMENTS	SEV 2240
C	SEV 2250
C EG ARRAY OF SUB(SUPER) DIAGONAL ELEMENTS	SEV 2260
C	SFV 2270
C VEC VECTOR ARRAY. THE VECTORS ARE TRANSFORMED INTO VECTORS	SEV 2280
C OF THE ORIGINAL MATRIX AS THEY ARE COMPUTED.	SEV 2290
C-----	SEV 2300
C-----	SEV 2310
C THIS SUBROUTINE IS A FORTRAN VERSION OF THE ALGOL ROUTINE	SEV 2320
C OF BOWDLER, MARTIN, REINSCH, AND WILKINSON. NUMER. MATH. 11,	SEV 2330
C 293-306(1968)	SEV 2340
C-----	SEV 2350
C DIMENSION DG(NDIM),EG(NDIM),VEC(NDIM,NDIM)	SEV 2360
C EPS=016414000000000000000000	SEV 2370
C*****	SEV 2380
C EPS IS THE SMALLEST POSITIVE FLOATING POINT NUMBER WHICH WHEN	SEV 2390
C ADDED TO 1.0 YIELDS A FLOATING POINT SUM NOT 1.0 . THIS IS A	SEV 2400
C MACHINE DEPENDENT CONSTANT AND MUST BE CHANGED FOR USE OF	SEV 2410
C THIS PROGRAM ON COMPUTERS OTHER THAN THE CDC 6600.	SEV 2420
C*****	SEV 2430
C NM1=N-1	SEV 2440
C DO 1 I=2,N	SEV 2450
C 1 FG(I-1)=FG(I)	SFV 2460
C FG(N)=0.0	SFV 2470
C R=0.0	SEV 2480
C F=0.0	SFV 2490
C	SEV 2500
C DIAGONALIZATION LOOP.	SEV 2510
C	SEV 2520
C DO 14 L=1,N	SEV 2530
C J=0	SEV 2540
C H=EPS*(ABS(DG(L))+ABS(EG(L)))	SEV 2550
C IF(R.LT.H) B=H	SEV 2560
C	SEV 2570
C LOOK FOR SMALL SUB-DIAGONAL ELEMENT	SEV 2580
C	SFV 2590
C DO 2 M=L,N	SFV 2600
C KM=M	SFV 2610
C IF(ABS(EG(M)).LT.R) GOTO 3	SEV 2620
C 2 CONTINUE	SEV 2630
C 3 IF(KM.EG.L) GOTO 13	SEV 2640
C	SFV 2650
C CHECK ITERATION COUNT	SEV 2660
C	SEV 2670
C 4 IF(J.GT.30) GOTO 18	SEV 2680
C J=J+1	SEV 2690
C	SFV 2700
C FORM THE SHIFT FOR THIS ITERATION	SEV 2710
C	SEV 2720

	P=(DG(L+1)-DG(L))/(EG(L)+EG(L))	SEV 2730
	R=SQRT(P*P+1.0)	SEV 2740
	IF(P) 5,6,6	SEV 2750
5	DENOM=P-R	SEV 2760
	GOTO 7	SEV 2770
6	DENOM=P+R	SEV 2780
7	H=DG(L)-EG(L)/DENOM	SEV 2790
	DO 8 I=L,N	SEV 2800
8	DG(I)=DG(I)-H	SEV 2810
	F=F+H	SEV 2820
C		SEV 2830
C	ONE QL TRANSFORMATION	SEV 2840
C		SEV 2850
	P=DG(KM)	SEV 2860
	C=1.0	SEV 2870
	S=0.0	SEV 2880
	KM1=KM-1	SEV 2890
	KL=KM1+L	SEV 2900
	DO 12 IX=L,KM1	SEV 2910
	I=KL-IX	SEV 2920
	G=C*EG(I)	SEV 2930
	H=C*P	SEV 2940
	IF(ABS(P).LT.ABS(EG(I)))GOTO 9	SEV 2950
	C=EG(I)/P	SEV 2960
	R=SQRT(C*C+1.0)	SEV 2970
	EG(I+1)=S*P*R	SEV 2980
	S=C/R	SEV 2990
	C=1.0/R	SEV 3000
	GOTO 10	SEV 3010
9	C=P/EG(I)	SEV 3020
	R=SQRT(C*C+1.0)	SEV 3030
	FG(I+1)=S*EG(I)*R	SEV 3040
	S=1.0/R	SEV 3050
	C=C*S	SEV 3060
10	P=C*DG(I)-S*G	SEV 3070
	DG(I+1)=H+S*(C*G+S*D G(I))	SEV 3080
C		SEV 3090
C	END OF QL STEP FORM THE VECTOR	SEV 3100
C		SEV 3110
	DO 11 K=1,N	SEV 3120
	H=VEC(K,I+1)	SEV 3130
	VEC(K,I+1)=S*VEC(K,I)+C*H	SEV 3140
	VEC(K,I)=C*VEC(K,I)-S*H	SEV 3150
11	CONTINUE	SEV 3160
12	CONTINUE	SEV 3170
	FG(L)=S*P	SEV 3180
	DG(L)=C*P	SEV 3190
	IF(ABS(EG(L)).GT.R) GOTO 4	SEV 3200
C		SEV 3210
C	AN EIGENVALUE HAS BEEN FOUND UNDO THE SHIFT	SEV 3220
C		SEV 3230
	13 DG(L)=DG(L)+F	SEV 3240
	14 CONTINUE	SEV 3250
C		SEV 3260

C	END OF DIAGONALIZATION LOOP	SEV 3270
C		SEV 3280
C	SORT EIGENVALUES IN DESCENDING ORDER AND PLACE VECTORS	SEV 3290
C	ACCORDINGLY	SEV 3300
C		SEV 3310
	DO 17 J=1,NM1	SEV 3320
	IX=J	SEV 3330
	JP1=J+1	SEV 3340
	TP=DG(J)	SEV 3350
	DO 15 K=JP1,N	SEV 3360
	IF(DG(K).LE.TP) GOTO 15	SEV 3370
	TP=DG(K)	SEV 3380
	IX=K	SEV 3390
15	CONTINUE	SEV 3400
	IF(IX.EQ.J) GOTO 17	SEV 3410
	TP=DG(IX)	SEV 3420
	DG(IX)=DG(J)	SEV 3430
	DG(J)=TP	SEV 3440
C		SEV 3450
C	INTERCHANGE COLUMNS OF VECTOR MATRIX	SEV 3460
C		SEV 3470
	DO 16 L=1,N	SEV 3480
	TP=VEC(L,J)	SEV 3490
	VEC(L,J)=VEC(L,IX)	SEV 3500
16	VEC(L,IX)=TP	SEV 3510
17	CONTINUE	SEV 3520
	RETURN	SEV 3530
C		SEV 3540
C	ERROR RETURN (MORE THAN 30 ITERATIONS)	SEV 3550
C		SEV 3560
18	KFR=3	SEV 3570
	RETURN	SEV 3580
	FND	SEV 3590

APPENDIX B

Test Results of SEVER on the CDC 6600

APPENDIX B

Test Results of SEVER on the CDC 6600

The table of execution times for SEVER was constructed using matrices whose elements were taken from a sequence of random numbers uniformly distributed between -1 and +1. The sequence was computed using the CDC 6600 library function RANF. Two separate executions of each order from 10 through 100 in increments of 5 were done and the table reflects the average of these two times. One 150 x 150 randomly constructed matrix was resolved. In no case were any of the eigenvalues of the randomly constructed matrices clustered or multiple. Thus it was possible for SEVER to compute an error bound for each eigenvalue of each matrix.

Table of Execution Times in Seconds

<u>n</u>	<u>Time</u>	<u>n</u>	<u>Time</u>	<u>n</u>	<u>Time</u>
10	0.110	45	7.014	80	37.242
15	0.315	50	9.459	85	44.460
20	0.709	55	12.463	90	52.662
25	1.298	60	16.173	95	61.651
30	2.191	65	20.338	100	72.216
35	3.402	70	25.235	150	235.104
40	4.966	75	30.825		

For the larger values of n , the time in seconds is nearly kn^3 where k is approximately 7×10^{-5} .

One 200 x 200 matrix was loaded to verify that SEVER was indeed capable of handling such a matrix on a CDC 6600 with 3×2^{15} available core locations. In this case the required arrays and subroutine SEVER as compiled by the FUN compiler required approximately 86,000 locations. Subroutine SEVER requires about 1200 decimal locations.

The examples which follow, with the exception of the last one, are as described in Section 6.4. In all examples except the four 32×32 Kronecker products and the 16×16 Hadamard product, the upper triangle of the test matrix is displayed. In all cases the single precision eigenvalues, eigenvalue errors, and residual lengths are displayed followed by the double precision eigenvalues with 28 significant figures printed out. The eigenvectors and Gram matrices are displayed where space allows. Only the first eight components of the eighth, sixteenth, twenty-fourth, and thirty-second eigenvectors of the Kronecker products are displayed. These components constitute all of the distinct elements of the eigenvectors of these matrices. Only the first eight components of the first eight eigenvectors of the 16×16 Hadamard product are displayed.

The Hadamard products H_{16} and H_8 illustrate the inevitable deterioration in the quality of the computed eigenvectors in the case of extremely clustered eigenvalues. The computed eigensystems of these matrices also point out the inconclusiveness of small residual vectors as measures of the quality of computed eigenvectors. The computed eigenvalues of both matrices are correct to at least the first 48 bits of their floating point representations.

In cases where the exact eigenvalues and eigenvector components are known the decimal position of the first significant digit of the actual absolute error is underlined. The reader can compare this error with the computed error bound.

The last example is Rosser's matrix, R_8 , with the last two bits of each element randomly perturbed. This example is meant to show that the error induced by inexact knowledge of the input matrix can be greater than the error induced by inexact diagonalization.

PREVIOUS KRONECKER PRODUCT + IDENTITY

	EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH		EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH
1	2.041098036860E+03	8.22E-18	9.160-09	8.980-10	2	2.041000000000E+03	8.21E-18	9.150-09	8.970-10
3	2.040803902719E+03	2.27E-18	3.400-09	6.670-10	4	2.001000000000E+03	-1.00E+00	8.290-10	8.290-10
5	2.001000000000E+03	-1.00E+00	8.820-10	8.820-10	6	1.148555145734E+03	4.02E-18	8.540-09	4.710-10
7	1.148500000000E+03	4.10E-18	8.630-09	4.760-10	8	1.148389695279E+03	2.23E-18	4.500-09	4.960-10
9	1.126000000000E+03	-1.00E+00	4.190-10	4.190-10	10	1.126000000000E+03	-1.00E+00	4.600-10	4.600-10
11	5.110245092150E+02	1.12E-18	6.770-09	1.660-10	12	5.110000000000E+02	1.17E-18	6.910-09	1.690-10
13	5.109509756796E+02	6.01E-19	3.500-09	1.720-10	14	5.010000000000E+02	-1.00E+00	1.510-10	1.510-10
15	5.010000000000E+02	-1.00E+00	1.630-10	1.630-10	16	1.285061273037E+02	5.09E-19	9.120-09	5.590-11
17	1.285000000000E+02	6.74E-19	1.050-08	6.430-11	18	1.284877439199E+02	3.28E-19	5.170-09	6.340-11
19	1.260000000000E+02	-1.00E+00	3.590-11	3.590-11	20	1.260000000000E+02	-1.00E+00	4.180-11	4.180-11
21	1.196097281443E+00	6.22E-21	2.690-10	2.310-11	22	1.110304720812E+00	1.12E-20	4.270-10	2.620-11
23	1.049024320361E+00	1.37E-20	6.100-10	2.240-11	24	1.012256080090E+00	4.33E-20	1.880-09	2.300-11
25	1.000000000000E+00	-1.00E+00	4.530-11	4.530-11	26	1.000000000000E+00	-1.00E+00	2.240-11	2.240-11
27	1.000000000000E+00	-1.00E+00	1.720-11	1.720-11	28	1.000000000000E+00	-1.00E+00	2.210-11	2.210-11
29	-1.265061273037E+02	2.10E-22	1.280-12	1.630-10	30	-5.090245092150E+02	7.23E-22	1.370-12	5.260-10
31	-1.146555145734E+03	1.32E-21	1.440-12	9.160-10	32	-2.039098036860E+03	3.40E-22	6.170-13	5.510-10

1	2.0410980368599936476926265910+03	2	2.04099999999999999999999999999999475380+03	3	2.0408039027185569660056959050+03
4	2.0009999999999999999999999999999995060+03	5	2.000999999999999999999999999999994470+03	6	1.1485551457337464268271023410+03
7	1.148499999999999999999999999999998830+03	8	1.1483896952791882933781750320+03	9	1.1259999999999999999999999999997480+03
10	1.125999999999999999999999999999994460+03	11	5.1102450921499841192315620120+02	12	5.11000000000000000000000000005650+02
13	5.1095097567963924150141117810+02	14	5.0099999999999999999999999999994460+02	15	5.00999999999999999999999999993110+02
16	1.2850612730374960298078907970+02	17	1.2849999999999999999999999999991960+02	18	1.2848774391990981037535311210+02
19	1.259999999999999999999999999999500+02	20	1.26000000000000000000000000003270+02	21	1.1960972814430339943549566570+00
22	1.1103047208117066218246862570+00	23	1.0490243203607584985841852720+00	24	1.0122560800901896246482376080+00
25	1.00000000000000000000000000661240+00	26	1.00000000000000000000000021930510+00	27	1.0000000000000000000000001835120+00
28	1.00000000000000000000000014391130+00	29	-1.2650612730374960298078910670+02	30	-5.0902450921499841192315644820+02
31	-1.1465551457337464268271022490+03	32	-2.0390980368599936476926273600+03		

EIGENVECTOR NO. 8
-.03116033079_ .01558016540_ -.01558016540_ .03116033081_ -.15734439439_ .15734439439_ .31468878878_ -.31468878878_

EIGENVECTOR NO. 16
-.31622396690_ -.15811198349_ -.15811198349_ -.31622396690_ .00077504015_ .00077504009_ -.00155008022_ -.00155008026_

EIGENVECTOR NO. 24
-.31468878869_ .15734439432_ -.15734439432_ .31468878869_ .01558016525_ -.01558016524_ -.03116033086_ .03115033071_

EIGENVECTOR NO. 32
-.00155008024_ -.00077504012_ -.00077504012_ -.00155008024_ -.15811198346_ -.15811198346_ .31622396691_ .31622396691_

EIGEN SYSTEM CALCULATION TOOK 2.434 SECONDS

PREVIOUS KRONECKER PRODUCT + IDENTITY

	EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH		EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH
1	1.996141619561E+00	9.91E-21	1.440-08	6.890-13	2	1.996093750000E+00	6.31E-21	1.150-08	5.490-13
3	1.995997999374E+00	2.91E-21	5.510-09	5.280-13	4	1.976562500000E+00	-1.00E+00	6.000-13	6.000-13
5	1.976562500000E+00	-1.00E+00	6.270-13	6.270-13	6	1.560329661003E+00	7.82E-21	1.700-08	4.590-13
7	1.560302734375E+00	5.34E-21	1.410-08	3.790-13	8	1.560248874648E+00	2.26E-21	6.480-09	3.490-13
9	1.549316406250E+00	-1.00E+00	3.380-13	3.380-13	10	1.549316406250E+00	-1.00E+00	4.420-13	4.420-13
11	1.249035404890E+00	7.51E-21	2.500-08	3.000-13	12	1.249023437500E+00	5.69E-21	2.180-08	2.610-13
13	1.248999499844E+00	2.30E-21	9.800-09	2.350-13	14	1.244140625000E+00	-1.00E+00	2.150-13	2.150-13
15	1.244140625000E+00	-1.00E+00	3.010-13	3.010-13	16	1.062258851223E+00	1.64E-20	7.840-08	2.350-13
17	1.062255859375E+00	1.02E-20	5.840-08	1.750-13	18	1.062249874961E+00	4.24E-21	2.660-08	1.590-13
19	1.061035156250E+00	-1.00E+00	1.190-13	1.190-13	20	1.061035156250E+00	-1.00E+00	2.610-13	2.010-13
21	1.000095750626E+00	4.36E-22	3.230-09	1.350-13	22	1.000053859727E+00	8.34E-22	5.280-09	1.580-13
23	1.000023937656E+00	1.37E-21	8.750-09	1.570-13	24	1.000005984414E+00	4.94E-21	2.870-08	1.720-13
25	1.000000000000E+00	-1.00E+00	1.010-13	1.010-13	26	1.000000000000E+00	-1.00E+00	1.740-13	1.740-13
27	1.000000000000E+00	-1.00E+00	2.020-13	2.020-13	28	1.000000000000E+00	-1.00E+00	2.140-13	2.140-13
29	9.377411487775E-01	1.15E-25	1.360-12	8.450-14	30	7.509645951099E-01	1.06E-25	7.550-13	1.410-13
31	4.396703389972E-01	2.64E-25	9.550-13	2.970-13	32	3.858380439456E-03	8.37E-26	4.380-13	1.910-13

1	1.9961416195605437732874132560+00	2	1.99609374999999999999999999995710+00	3	1.9959979993742953935574453760+00
4	1.976562499999999999999999999996080+00	5	1.97656249999999999999999999999590+00	6	1.5603296610028058724741698970+00
7	1.560302734374999999999999999993460+00	8	1.5602488746480411588760734460+00	9	1.54931640624999999999999999999400+00
10	1.549316406249999999999999999997570+00	11	1.2490354048901359433218510650+00	12	1.249023437499999999999999999991580+00
13	1.2489994998435738483893731830+00	14	1.24414062499999999999999999999290+00	15	1.244140624999999999999999999998630+00
16	1.0622588512225339858304632230+00	17	1.0622558593749999999999999999954300+00	18	1.06224987496089346209738505320+00
19	1.0610351562500000000000001060+00	20	1.0610351562500000000000001070+00	21	1.0000957506257046064425429820+00
22	1.0000538597269588411239423880+00	23	1.0000239376564261516106244440+00	24	1.0000059844141065379026127900+00
25	1.00000000000000000000000214010+00	26	1.00000000000000000000000076740+00	27	1.000000000000000000000000303680+00
28	1.000000000000000000000000105940+00	29	9.3774114877746601416953647700-01	30	7.5096459510986405667814617530-01
31	4.3967033899719412752582884350-01	32	3.8583804394562267125842685530-03		

EIGENVECTOR NO. 8
 .03116033081 -.01558016552 .01558016528 -.03116033079 .15734439442 -.15734439442 -.31468878873 .31468878873

EIGENVECTOR NO. 16
 .31622396690 .15811198347 .15811198347 .31622396691 -.00077504014 -.00077504010 .00155008025 .00155008023

EIGENVECTOR NO. 24
 .31468878889 -.15734439472 .15734439472 -.31468878889 -.01558016693 .01558016388 .03116033006 -.03116033158

EIGENVECTOR NO. 32
 -.00155008024 -.00077504012 -.00077504012 -.00155008024 -.15811198346 -.15811198346 .31622396691 .31622396691

EIGEN SYSTEM CALCULATION TOOK 2.424 SECONDS

8 BY 8 HADAMARD PRODUCT WITH EIGENVALUES 1.0, 1.0+2.**(-K), K=38 TO 44

I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)			
1	1	1.000E+00	1	2	3.055E-13	1	3	5.471E-13	1	4	1.776E-13	1	5	8.029E-13	1	6	2.629E-13	1	7	4.761E-13
1	8	1.634E-13	2	2	1.000E+00	2	3	1.776E-13	2	4	5.471E-13	2	5	2.629E-13	2	6	8.029E-13	2	7	1.634E-13
2	8	4.761E-13	3	3	1.000E+00	3	4	3.055E-13	3	5	4.761E-13	3	6	1.634E-13	3	7	8.029E-13	3	8	2.629E-13
4	4	1.000E+00	4	5	1.634E-13	4	6	4.761E-13	4	7	2.629E-13	4	8	8.029E-13	5	5	1.000E+00	5	6	3.055E-13
5	7	5.471E-13	5	8	1.776E-13	6	6	1.000E+00	6	7	1.776E-13	6	8	5.471E-13	7	7	1.000E+00	7	8	3.055E-13
8	8	1.000E+00																		

	EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH		EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH
1	1.00000000000004E+00	2.62E-15	3.96D-02	6.62D-14	2	1.0000000000002E+00	8.95E-15	1.08D-01	8.25D-14
3	1.0000000000001E+00	1.51E-14	2.27D-01	6.54D-14	4	1.0000000000000E+00	1.75E-13	1.81D+00	9.67D-14
5	1.0000000000000E+00	-1.00E+00	8.67D-14	8.67D-14	6	1.0000000000000E+00	-1.00E+00	7.59D-14	7.59D-14
7	1.0000000000000E+00	-1.00E+00	1.13D-13	1.13D-13	8	1.0000000000000E+00	-1.00E+00	7.22D-14	7.22D-14

1	1.0000000000003637865571844389D+00	2	1.0000000000001818640641051371D+00	3	1.0000000000000909159883310092D+00
4	1.0000000000000453816983811930D+00	5	1.00000000000000217036163953934D+00	6	1.0000000000000112451213730881D+00
7	1.0000000000000065057432047925D+00	8	1.0000000000000005106305572026D+00		

EIGENVECTOR NO. 1	.35137470152	-.35348363843	-.35156967021	-.35559229298	-.35124933787	-.35676462594	-.35035161593	-.35825327496
EIGENVECTOR NO. 2	.35476267545	-.34463231480	.35588036826	-.35821163833	.35261386114	-.34027085947	.36064810770	-.36085696182
EIGENVECTOR NO. 3	.34334931916	.36285830964	-.33896973303	-.34896813823	.34556956410	.36346253367	-.36124357821	-.36306387119
EIGENVECTOR NO. 4	.37647519702	-.37164756723	-.33777308215	.30509934017	.35116118347	-.33312187382	-.37043559577	.37611358253
EIGENVECTOR NO. 5	.27354733003	.23701606394	.38387002433	.47750286817	-.26461202441	-.26353078902	-.38828835941	-.45099247078
EIGENVECTOR NO. 6	.34641879028	-.19990765410	.40220348720	-.43191148369	-.39191306059	.23816548205	-.35931811724	.39024046873
EIGENVECTOR NO. 7	-.27517281591	-.55498759644	.23196389938	.26651432411	.26410038114	.55009570342	-.22490901635	.26171204355
EIGENVECTOR NO. 8	.46980159455	-.20694755779	-.39727283350	.21179602047	-.46496288597	.29168988866	.38601270594	-.20972605153

GRAM MATRIX

1	1.0E+00	2.0E-14	0.	0.	8.9E-16	-3.6E-15	4.4E-16	1.3E-15
2	1.0E+00	5.3E-15	-8.9E-16	5.3E-15	4.4E-15	3.1E-15	2.2E-15	
3	1.0E+00	8.9E-16	4.4E-15	-2.7E-15	2.7E-15	-4.4E-16		
4	1.0E+00	3.6E-15	1.1E-14	-1.3E-15	0.			
5	1.0E+00	-3.6E-15	2.2E-14	8.9E-16				
6	1.0E+00	7.1E-15	-4.0E-15					
7	1.0E+00	-8.2E-15						
8	1.0E+00							

EIGEN SYSTEM CALCULATION TOOK .056 SECONDS

16 BY 16 HADAMARD PRODUCT WITH EIGENVALUES 1.0, 1.0 + 2.0(-K), K = 24 TO 38

	EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH		EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH
1	1.000000059605E+00	5.22E-19	4.18D-06	1.25D-13	2	1.000000029802E+00	5.94E-19	6.83D-06	1.02D-13
3	1.000000014901E+00	1.80E-18	1.55D-05	1.16D-13	4	1.000000007451E+00	3.51E-18	3.11D-05	1.16D-13
5	1.000000003725E+00	7.18E-18	6.21D-05	1.16D-13	6	1.000000001853E+00	1.45E-17	1.25D-04	1.16D-13
7	1.000000000931E+00	3.34E-17	2.68D-04	1.25D-13	8	1.000000000466E+00	5.66E-17	5.35D-04	1.24D-13
9	1.000000000233E+00	1.19E-16	1.01D-03	1.17D-13	10	1.000000000116E+00	3.81E-16	2.56D-03	1.48D-13
11	1.000000000058E+00	6.20E-16	4.64D-03	1.34D-13	12	1.000000000029E+00	2.13E-15	1.22D-02	1.74D-13
13	1.000000000015E+00	3.57E-15	2.26D-02	1.58D-13	14	1.000000000007E+00	6.15E-15	4.28D-02	1.44D-13
15	1.000000000004E+00	5.43E-15	4.02D-02	1.35D-13	16	1.000000000000E+00	3.75E-15	3.33D-02	1.13D-13
1	1.0000000596046447753292255D+00				2	1.000000029802322387680290331D+00			
4	1.000000007450580596822306418D+00				5	1.000000003725290298355786174D+00			
7	1.000000000931322873210923629D+00				8	1.000000000465661286520516187D+00			
10	1.000000000115415312457815231D+00				11	1.000000000058207643928589381D+00			
13	1.000000000014551219488325371D+00				14	1.000000000007276017905483600D+00			
16	1.000000000000000321071519284D+00				15	1.0000000000003637845208766657D+00			

EIGENVECTOR NO. 1	-.24999994027	-.25000008320	-.24999998902	-.24999990545	-.24999999445	-.24999997286	-.24999996414	-.25000005315
EIGENVECTOR NO. 2	-.24999994011	.249999956374	-.24999999602	.24999996798	-.25000008757	.24999967387	-.25000003997	.25000013798
EIGENVECTOR NO. 3	.24999953042	.25000011258	-.24999979238	-.24999948328	.24999949967	.25000021392	-.25000032565	-.25000005527
EIGENVECTOR NO. 4	.25000003955	-.24999952463	-.24999987525	.24999861373	.25000075423	-.25000004890	-.25000032012	.24999985048
EIGENVECTOR NO. 5	.24999895945	.25000065059	.24999818884	.25000143246	-.24999955142	-.24999981964	-.25000007171	-.24999745204
EIGENVECTOR NO. 6	-.25000133029	.24999782513	-.24999903281	.25000119234	.25000364038	-.24999519868	.25000229876	-.24999928243
EIGENVECTOR NO. 7	.24998855396	.25001091363	-.24999291262	-.25001543002	-.24998956859	-.25001461863	.25000326876	.24999036375
EIGENVECTOR NO. 8	.25001490960	-.25000542746	-.24999339273	.24998120107	-.24999467854	.24999314766	.25001949545	-.24996820661

EIGEN SYSTEM CALCULATION TOOK .346 SECONDS

W21+ SEC 6.4

I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)			
1	1	1.000E+01	1	2	1.000E+00	2	2	9.000E+00	2	3	1.000E+00	3	3	8.000E+00	3	4	1.000E+00	4	4	7.000E+00
4	5	1.000E+00	5	5	6.000E+00	5	6	1.000E+00	6	6	5.000E+00	6	7	1.000E+00	7	7	4.000E+00	7	8	1.000E+00
8	8	3.000E+00	8	9	1.000E+00	9	9	2.000E+00	9	10	1.000E+00	10	10	1.000E+00	10	11	1.000E+00	11	12	1.000E+00
12	12	1.000E+00	12	13	1.000E+00	13	13	2.000E+00	13	14	1.000E+00	14	14	3.000E+00	14	15	1.000E+00	15	15	4.000E+00
15	16	1.000E+00	16	16	5.000E+00	16	17	1.000E+00	17	17	6.000E+00	17	18	1.000E+00	18	18	7.000E+00	18	19	1.000E+00
19	19	8.000E+00	19	20	1.000E+00	20	20	9.000E+00	20	21	1.000E+00	21	21	1.000E+01						

	EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH		EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH
1	1.074619418290E+01	-1.00E+00	1.110-13	1.110-13	2	1.074619418290E+01	-1.00E+00	1.280-13	1.280-13
3	9.210678647361E+00	1.23E-16	1.480-03	8.310-14	4	9.210678647305E+00	1.71E-16	1.740-03	9.810-14
5	8.038941122829E+00	2.78E-18	1.990-05	1.400-13	6	8.038941115814E+00	1.87E-18	1.630-05	1.140-13
7	7.003952209529E+00	8.44E-20	4.530-07	1.860-13	8	7.003951798616E+00	9.14E-20	4.720-07	1.940-13
9	6.000234031584E+00	5.38E-21	1.800-08	2.980-13	10	6.000217522257E+00	5.95E-21	1.900-08	3.130-13
11	5.000244425002E+00	4.25E-22	9.590-10	4.430-13	12	4.999782477743E+00	3.51E-22	8.720-10	4.030-13
13	4.004354023441E+00	6.58E-23	8.900-11	7.390-13	14	3.996048201384E+00	6.30E-23	8.710-11	7.230-13
15	3.043099292579E+00	1.37E-23	1.290-11	1.060-12	16	2.961058884186E+00	1.39E-23	1.300-11	1.070-12
17	2.130209219362E+00	4.65E-24	3.690-12	1.260-12	18	1.789321352695E+00	5.70E-24	4.090-12	1.390-12
19	9.475343675293E-01	5.21E-24	2.740-12	1.900-12	20	2.538058170967E-01	6.70E-24	3.110-12	2.160-12
21	-1.125441522120E+00	3.39E-24	1.570-12	2.160-12					

1	1.0746194182903357513429992190+01	2	1.0746194182903357750717378270+01	3	9.2106786473613320536760919970+00
4	9.2106786473049186481968758470+00	5	8.0389411228290232359051641020+00	6	8.0389411158142733087434060580+00
7	7.0039522095286756738128988650+00	8	7.0039517986163749692715866630+00	9	6.0002340315841670166171874030+00
10	6.0002175222570581400137905160+00	11	5.0002444250019130080653914520+00	12	4.9997824777429018599865223710+00
13	4.0043540234408567350974690880+00	14	3.9960482013836250307295016860+00	15	3.0430992925788237393316432530+00
16	2.9610588841857266916133742310+00	17	2.1302092193625059944850954420+00	18	1.7893213526950814060446742850+00
19	9.4753436752929327885064110970-01	20	2.5380581709667816771009218500-01	21	-1.1254415221199642222987733470+00

EIGEN SYSTEM CALCULATION TOOK .714 SECONDS

W21- SEC 6.4

I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)
1	1	1.000E+01	1	2	1.000E+00	2	2	9.000E+00	2	3	1.000E+00	3	3	8.000E+00	3	4	1.000E+00
4	5	1.000E+00	5	5	6.000E+00	5	6	1.000E+00	6	6	5.000E+00	6	7	1.000E+00	7	7	4.000E+00
8	8	3.000E+00	8	9	1.000E+00	9	9	2.000E+00	9	10	1.000E+00	10	10	1.000E+00	10	11	1.000E+00
12	12	-1.000E+00	12	13	1.000E+00	13	13	-2.000E+00	13	14	1.000E+00	14	14	-3.000E+00	14	15	1.000E+00
15	16	1.000E+00	16	16	-5.000E+00	16	17	1.000E+00	17	17	-6.000E+00	17	18	1.000E+00	18	18	-7.000E+00
19	19	-8.000E+00	19	20	1.000E+00	20	20	-9.000E+00	20	21	1.000E+00	21	21	-1.000E+01	18	19	1.000E+00

EIGENVALUE				VALUE	VECTOR	RESIDUAL	EIGENVALUE				VALUE	VECTOR	RESIDUAL
				ERROR	ERROR	LENGTH				ERROR	ERROR	LENGTH	
1	1.074619418290E+01	7.23E-27	6.86D-14	1.05D-13	2	9.210678647333E+00	2.14E-27	4.27D-14	5.00D-14				
3	8.038941119306E+00	2.27E-27	4.68D-14	4.85D-14	4	7.003952002665E+00	2.10E-26	1.45D-13	1.45D-13				
5	6.000225680185E+00	5.22E-26	2.26D-13	2.26D-13	6	5.000008158673E+00	9.06E-26	3.01D-13	3.01D-13				
7	4.000000205070E+00	1.51E-25	3.88D-13	3.88D-13	8	3.00000003808E+00	4.05E-25	6.30D-13	6.30D-13				
9	2.000000000054E+00	8.70E-25	9.33D-13	9.33D-13	10	1.000000000001E+00	1.50E-24	1.22D-12	1.22D-12				
11	6.890201209496E-25	2.53E-24	1.59D-12	1.59D-12	12	-1.000000000001E+00	2.64E-24	1.62D-12	1.62D-12				
13	-2.000000000054E+00	3.21E-24	1.79D-12	1.79D-12	14	-3.00000000380E+00	4.57E-24	2.14D-12	2.14D-12				
15	-4.000000205070E+00	7.71E-24	2.78D-12	2.78D-12	16	-5.000008158673E+00	1.07E-23	3.26D-12	3.26D-12				
17	-6.000225680185E+00	1.29E-23	3.59D-12	3.59D-12	18	-7.003952002665E+00	1.78E-23	4.21D-12	4.22D-12				
19	-8.038941119306E+00	2.10E-23	4.51D-12	4.67D-12	20	-9.210678647333E+00	1.86E-23	3.99D-12	4.67D-12				
21	-1.074619418290E+01	5.46E-24	1.89D-12	2.89D-12									

1	1.074619418290335757058688396D+01	2	9.210678647333046488327699630D+00	3	8.038941119306440889767405898D+00
4	7.003952002665361328366114594D+00	5	6.000225680185170344125272784D+00	6	5.000008158672945010464050387D+00
7	4.000000205070437800318642310D+00	8	3.000000003808126883535345643D+00	9	2.000000000054488107703379498D+00
10	1.00000000000619745380019122D+00	11	6.890201209495886620299839136D-25	12	-1.00000000000619745380017775D+00
13	-2.000000000054488107703378268D+00	14	-3.000000003808126883535344360D+00	15	-4.000000205070437800318640558D+00
16	-5.000008158672945010464047851D+00	17	-6.000225680185170344125269998D+00	18	-7.003952002665361328366111171D+00
19	-8.038941119306440889767402375D+00	20	-9.210678647333046488327696531D+00	21	-1.074619418290335757058688244D+01

EIGEN SYSTEM CALCULATION TOOK .726 SECONDS

THE MATRIX R8 WITH RANDOM PURTERBATIONS ON THE LAST TWO BITS OF EACH ELEMENT

I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)	I	J	A(I,J)			
1	1	6.110E+02	1	2	1.960E+02	1	3	-1.920E+02	1	4	4.070E+02	1	5	-8.000E+00	1	6	-5.200E+01	1	7	-4.900E+01
1	8	2.900E+01	2	2	8.990E+02	2	3	1.130E+02	2	4	-1.920E+02	2	5	-7.100E+01	2	6	-4.300E+01	2	7	-8.000E+00
2	8	-4.400E+01	3	3	8.990E+02	3	4	1.960E+02	3	5	6.100E+01	3	6	4.900E+01	3	7	8.000E+00	3	8	5.200E+01
4	4	6.110E+02	4	5	8.000E+00	4	6	4.400E+01	4	7	5.900E+01	4	8	-2.300E+01	5	5	4.110E+02	5	6	-5.990E+02
5	7	2.080E+02	5	8	2.080E+02	6	6	4.110E+02	6	7	2.080E+02	6	8	2.080E+02	7	7	9.900E+01	7	8	-9.110E+02
8	8	9.900E+01																		

	EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH		EIGENVALUE	VALUE ERROR	VECTOR ERROR	RESIDUAL LENGTH
1	1.020049018430E+03	6.02E-20	1.11D-09	5.43D-11	2	1.020000000000E+03	3.63E-20	8.61D-10	4.22D-11
3	1.019901951359E+03	1.28E-20	3.62D-10	3.55D-11	4	1.000000000000E+03	-1.00E+00	3.33D-11	3.33D-11
5	1.000000000000E+03	-1.0CE+00	5.22D-11	5.22D-11	6	9.804864072211E-02	1.49E-20	3.90D-10	3.82D-11
7	-7.339622242113E-13	3.25E-20	5.79D-10	5.68D-11	8	-1.020049018430E+03	6.66E-24	8.21D-14	8.38D-11

1	1.020049018430002007959563330D+03	2	1.020000000000004865796653261D+03	3	1.019901951359282897094886675D+03
4	1.000000000000004666978094841D+03	5	1.000000000000004479810120908D+03	6	9.804864072210512597422682421D-02
7	-7.339622242113050923997203486D-13	8	-1.020049018430001189414331787D+03		

EIGENVECTOR NO. 1	.63244793382	.31622396693	.31622396692	.63244793382	-.00155008025	-.00155008023	.00310016048	.00310016048
EIGENVECTOR NO. 2	.22360679776	-.44721359549	-.44721359550	.22360679777	.44721359547	-.44721359547	.22360679782	-.22360679782
EIGENVECTOR NO. 3	-.06232066162	.03116033085	-.03116033075	.06232066157	-.31468878883	.31468878883	.62937757754	-.62937757754
EIGENVECTOR NO. 4	-.13883586915	.58872126327	.27767173831	-.29435063163	.41097867757	-.45541432400	.20548933879	-.22770716200
EIGENVECTOR NO. 5	.35878210858	.49538598504	-.71756421716	-.24769299252	-.19772841621	.02444981590	-.09886420811	.01222490795
EIGENVECTOR NO. 6	.62937757756	-.31468878878	.31468878878	-.62937757756	-.03116033082	.03116033078	.06232066159	-.06232066161
EIGENVECTOR NO. 7	-.04472135957	-.08944271909	.08944271909	.04472135957	-.62609903370	-.62609903370	-.31304951685	-.31304951685
EIGENVECTOR NO. 8	.00310016048	.00155008024	.00155008024	.00310016048	.31622396691	.31622396691	-.63244793383	-.63244793383

GRAM MATRIX

1	1.0E+00	1.7E-15	-1.4E-15	4.0E-16	8.8E-15	1.8E-14	-1.5E-15	5.6E-17
2	1.0E+00	-1.8E-14	1.8E-15	-2.2E-15	4.0E-15	0.	8.9E-15	
3	1.0E+00	-5.3E-15	1.5E-15	-6.7E-16	1.6E-14	2.3E-14		
4	1.0E+00	1.4E-16	5.3E-15	1.8E-15	8.9E-15			
5	1.0E+00	-1.6E-15	-3.3E-15	-2.8E-15				
6	1.0E+00	-4.1E-15	2.0E-15					
7	1.0E+00	8.0E-15						
8	1.0E+00							

EIGEN SYSTEM CALCULATION TOOK .056 SECONDS

APPENDIX C

Control Cards for Using SEVER on the CDC 6600

APPENDIX C

Control Cards for Using SEVER on the CDC 6600

SEVER is maintained in a library file for the convenience of the Control Data 6600 users at Sandia Laboratories, Albuquerque, New Mexico. The name of the file is MATHLIB. Questions concerning the availability of SEVER on the Control Data 6600 at Sandia Laboratories, Livermore, California, should be directed to the Numerical Applications Division 8321.

One control card, COLLECT, is required for using the mathematical library file. The COLLECT processor operates on one relocatable binary file and from one to six library files. The library files are searched for routines which contain entry points matching external references in the relocatable binary file. Such routines are added to the relocatable binary file.

A complete typical example follows:

```
JOB CARD
ACCOUNT CARD
FUN,S.
COLLECT,LGO,MATHLIB.
REDUCE.
LGO.
7/8/9 punch in column 1
Program
7/8/9 punch in column 1
Data
6/7/8/9 punch in column 1
```

In the above example, external references in LGO are satisfied, if possible, by selectively adding routines to LGO from MATHLIB. Additional information on the COLLECT processor with examples is contained in UR0004/6600.

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