

ALGORITHM 342

GENERATOR OF RANDOM NUMBERS SATISFYING THE POISSON DISTRIBUTION [G5]

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CR CATEGORIES: 5.12, 5.5

integer procedure *poisson carlo* (*np_x*, *np_{x1}*, *random*); **value** *np_x*, *random*; **real** *np_x*, *np_{x1}*, *random*;
comment The Poisson distribution gives the probability that *px* events will occur in a certain interval or volume, where the expected or mean value of events is *np_x*. Applications are described by B. W. Lindgren and G. W. McElrath [1]. For a Monte Carlo calculation we wish to generate numbers *px* that satisfy the Poisson distribution, that is to find the inverse of the Poisson function. To do this we generate a pseudo-random number in the interval 0, 1 and find the number *px* such that *random* ≤ (probability that the number is *px* or less) and *random* > (the probability that the number is *px* - 1 or less).

poisson carlo returns the value -1 to signal that the procedure was called with a value of *np_x* < 0 or too large for the precision of the computer. It is the responsibility of the user to test the calculated value if there is any possibility of the occurrence of the error condition.

In order to save computing time, values of the Poisson distribution computed at a previous entry for the same value of *np_x* are stored in the **own** array *pson*. The previous value of *np_x* is *np_{x1}*. The actual parameter corresponding to *np_{x1}* must be a real identifier, not a constant or an expression. Before the first call of *poisson carlo* the calling program must set *np_{x1}* to a value ≠ *np_x*. The number of *pson* elements that were previously computed and stored is computed. If it is desired to save storage space at the expense of computing time, the upper bound 84 of *pson* may be reduced, but then the limit of *computed* near the end of the procedure must also be decreased accordingly.

The procedure which generates *random* is preferably algorithm 266 [3] or 294 [2]. It can be called as the actual parameter in the procedure call of *poisson carlo*.

The author thanks Mr. I. D. Hill for numerous suggestions and corrections which greatly improved the algorithm.

REFERENCES:

1. LINDGREN, B. W., AND McELRATH, G. W. *Introduction to Probability and Statistics*, 2 ed. Macmillan, New York, 1966, pp. 64-68.
2. PIKE, M. C., AND HILL, I. D. Algorithm 266, pseudo-random numbers. *Comm. ACM* 8 (Oct. 1965), 605.
3. STROME, W. M. Algorithm 294, uniform random. *Comm. ACM* 10 (Jan. 1967), 40;

begin

own integer *computed*; **own** real *pnc*;
own real array *pson* [0:84];

integer *n*; **real** *ps*;
if *np_x* < 0 **then go to error**;
if *np_x* ≠ *np_{x1}* **then**
begin
 computed := 0;
 pnc := *pson* [0] := *exp* (-*np_x*);
 if *pnc* = 0 **then go to error**;
 comment *pson* [0] is the probability that *poisson carlo* = 0. It cannot be zero unless -*np_x* underflows the argument range of procedure *exp*. For most computers this sets an upper limit of 85 for *np_x*;
 np_{x1} := *np_x*
end new np_x;
 ps := *pson* [*computed*];
 if *random* ≤ *ps* **then**
 begin
 integer *nmin*, *nmax*;
 comment The probability term can be found by searching the stored values;
 nmin := 0; *nmax* := *computed* + 1;
 for *n* := (*nmax*+*nmin*-1) ÷ 2 **while** *nmax* - *nmin* > 1 **do**
 if *random* > *pson*[*n*] **then** *nmin* := *n* + 1 **else** *nmax* := *n* + 1;
 poisson carlo := *nmin*
 end search
 else
 begin
 real *psc*, *pn*; *pn* := *pnc*;
 comment Additional probability terms must be computed;
 for *n* := *computed* + 1, *n* + 1 **while** *random* > *ps* **do**
 begin
 pn := *pn* × *np_x*/*n*;
 psc := *ps*; *ps* := *ps* + *pn*;
 comment *ps* = cumulative probability of terms up to *n*, and *pn* = probability of *n*th term;
 if *ps* = *psc* **then go to error**;
 if *n* ≤ 84 **then begin** *pson*[*n*] := *ps*;
 pnc := *pn*; *computed* := *n* **end**;
 poisson carlo := *n*
 end
 end more;
 go to fin;
error: *poisson carlo* := -1;
fin:
end poisson carlo;
comment The following is an example of a calling program for the case where *poisson carlo* is compiled within the calling program rather than separately. Instead of **own** variables, non-local variables may then be used. The program is within the IFIP subset if this change is made, and if the expression (*nmax*+*nmin*-1) ÷ 2 is replaced by the less efficient expression .501 × (*nmax*+*nmin*-2);
begin
 integer *x*, *computed*; **real** array *pson* [0:84];
 real *pnc*, *np_x*, *np_{x1}*;
 real procedure *random* (*x*);

```

comment Procedure body random is inserted here;
integer procedure poisson carlo (npx, npz1, random);
comment Procedure body of poisson carlo is inserted here
after deleting declarations of own variables;
ininteger (2, x); npz1 := -1;
in1: inreal (2, npz);
outinteger (1, poisson carlo (npx, npz1, random (x)));
go to in1
end

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ALGORITHM 343 EIGENVALUES AND EIGENVECTORS OF A REAL GENERAL MATRIX [F2]

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KEY WORDS AND PHRASES: eigenvalues, eigenvectors, latent roots, latent vectors, Householder's method, QR algorithm, inverse iteration

CR CATEGORIES: 5.14

ABSTRACT:

Purpose. This subroutine finds all the eigenvalues and eigenvectors of a real general matrix. The eigenvalues are computed by the QR double-step method and the eigenvectors by inverse iteration.

Method. Firstly the following preliminary modifications are carried out to improve the accuracy of the computed results. (i) The matrix is scaled by a sequence of similarity transformations so that the absolute sums of corresponding rows and columns are roughly equal. (ii) The scaled matrix is normalized so that the value of the Euclidean norm is equal to one.

The main part of the process commences with the reduction of the matrix to an upper-Hessenberg form by means of similarity transformations (Householder's method). Then the QR double-step iterative process is performed on the Hessenberg matrix until all elements of the subdiagonal that converge to zero are in modulus less than $2^{-t} \|H\|_E$, where t is the number of significant digits in the mantissa of a binary floating-point number. The eigenvalues are then extracted from this reduced form.

Inverse iteration is performed on the upper-Hessenberg matrix until the absolute value of the largest component of the right-hand side vector is greater than the bound $2^t/(100N)$, where N is the order of the matrix. Normally after this bound is achieved, one step more is performed to obtain the computed eigenvector, but at each step the residuals are computed, and if the residuals of one particular step are greater in absolute value than the residuals of the previous step, then the vector of the previous step is accepted as the computed eigenvector.

Program. The subroutine EIGENP is completely self-contained (composed of five subroutines

EIGENP, SCALE, HESQR, REALVE, and COMPVE) and communication to it is solely through the argument list. The entrance to the subroutine is achieved by CALL EIGENP (N, NM, A, T, EVR, EVI, VECR, VECI, INDIC) The meaning of the parameters is described in the comments at the beginning of the subroutine EIGENP.

REFERENCES:

1. WILKINSON, J. H. *The Algebraic Eigenvalue Problem*. Clarendon Press, Oxford, 1965, pp. 347-353, 485-567, 619-633.

Test results. All tests have been performed on a KDF9 computer ($t = 39$). No breakdown of the method has occurred and in general very accurate computed eigenvalues and eigenvectors have been obtained.

Some examples:

(i) The matrix

$$\begin{bmatrix} -.5 & -1 & -1 & -.5 & -1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

has all eigenvalues with modulus equal to one. The computed eigenvalues are

$-1.00000\ 0000$, $-.25000\ 0000 \pm i.96824\ 58366$, $.50000\ 0000 \pm i.86602\ 54038$.

The computed eigenvectors are

x_1	x_2, x_3	x_4, x_5
.447213595	1.000000000	$-.500000000 \pm i.866025404$
$-.447213595$	$-.250000000 \pm i.968245837$	$-1.000000000 \pm i.16E-10$
.447213595	$-.875000000 \pm i.484122918$	$-.500000000 \pm i.866025404$
$-.447213595$	$.687500000 \pm i.726184377$	$.500000000 \pm i.866025404$
.447213595	$.531250000 \pm i.847215107$	1.000000000

and the computed residuals are in modulus less than $.3E - 10$.

(ii) The matrix

$$\begin{bmatrix} -2 & 1 & 1 & 1 \\ -7 & -5 & -2 & -4 \\ 0 & -1 & -3 & -2 \\ -1 & 0 & -1 & 0 \end{bmatrix}$$

has the eigenvalues

$-4 \pm i2$ and $-1 \pm \sqrt{2}$.

The computed eigenvalues are

$-4.000000000 \pm i2.000000000$, -2.414213562 , $.4142135624$.

The computed eigenvectors are

x_1, x_2	x_3	x_4
$-.2000000000 \pm i.4000000000$	.60E-12	$-.12E-11$
1.0000000000	$-.7941044878$	.4759631495
$.2000000000 \pm i.4000000000$	.5615166683	.3365567706
.14E-10 $\pm i.63E-11$	.2325878195	$-.8125199201$

and the computed residuals are in modulus less than $.7E - 10$.

(iii) The matrix A

$$A = \begin{bmatrix} 1 & 0 & 0.01 \\ 0.1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

is transformed by the process of scaling into the form B

$$B = \begin{bmatrix} .574423 & 0 & .066333 \\ .053454 & .574423 & 0 \\ 0 & .053454 & .574423 \end{bmatrix}$$

with the elements given to six decimal places. The obtained matrix B is essentially invariant under the QR double-step process. This kind of trouble was overcome by introducing the statements

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R = DABS(X) + DABS(Y)
IF(R.EQ.0.0)SHIFT = A(M,M-1)
IF(R.EQ.0.0)GO TO 21

```

in the subroutine HESQR.

The exact eigenvalues of A are

1.1, $0.95 \pm i0.5\sqrt{0.03}$.

The computed eigenvalues are

1.100000000, $0.9500000000 \pm i0.0866025404$.

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SUBROUTINE EIGENP(N,NM,A,T,EVR,EVI,VECR,VECI,INDIC)
DOUBLE PRECISION D1,D2,D3,PRFACT
INTEGER I,IVEC,J,K,K1,KON,L,L1,M,N,NM
REAL ENORM,EPS,EX,R,R1,T
DIMENSION A(NM,1),VECR(NM,1),VECI(NM,1),
1EVR(NM),EVI(NM),INDIC(NM)
DIMENSION IWORK(100),LOCAL(100),PRFACT(100)
1,SUBDIA(100),WORK1(100),WORK2(100),WORK(100)

C
C THIS SUBROUTINE FINDS ALL THE EIGENVALUES AND THE
C EIGENVECTORS OF A REAL GENERAL MATRIX OF ORDER N.
C
C FIRST IN THE SUBROUTINE SCALE THE MATRIX IS SCALED SO THAT
C THE CORRESPONDING ROWS AND COLUMNS ARE APPROXIMATELY
C BALANCED AND THEN THE MATRIX IS NORMALISED SO THAT THE
C VALUE OF THE EUCLIDIAN NORM OF THE MATRIX IS EQUAL TO ONE.
C
C THE EIGENVALUES ARE COMPUTED BY THE QR DOUBLE-STEP METHOD
C IN THE SUBROUTINE HESQR.
C THE EIGENVECTORS ARE COMPUTED BY INVERSE ITERATION IN
C THE SUBROUTINE REALVE, FOR THE REAL EIGENVALUES, OR IN THE
C SUBROUTINE COMPVE, FOR THE COMPLEX EIGENVALUES.
C
C THE ELEMENTS OF THE MATRIX ARE TO BE STORED IN THE FIRST N
C ROWS AND COLUMNS OF THE TWO DIMENSIONAL ARRAY A. THE
C ORIGINAL MATRIX IS DESTROYED BY THE SUBROUTINE.
C N IS THE ORDER OF THE MATRIX.
C NM DEFINES THE FIRST DIMENSION OF THE TWO DIMENSIONAL
C ARRAYS A,VECR,VECI AND THE DIMENSION OF THE ONE
C DIMENSIONAL ARRAYS EVR,EVI AND INDIC. THEREFORE THE
C CALLING PROGRAM SHOULD CONTAIN THE FOLLOWING DECLARATION
C DIMENSION A(NM,NN),VECR(NM,NN),VECI(NM,NN),
C 1EVR(NM),EVI(NM),INDIC(NM)
C WHERE NM AND NN ARE ANY NUMBERS EQUAL TO OR GREATER THAN N
C THE UPPER LIMIT FOR NM IS EQUAL TO 100 BUT MAY BE
C INCREASED TO THE VALUE MAX BY REPLACING THE DIMENSION
C STATEMENT
C DIMENSION IWORK(100),LOCAL(100), ... ,WORK(100)
C IN THE SUBROUTINE EIGENP WITH
C DIMENSION IWORK(MAX),LOCAL(MAX), ... ,WORK(MAX)
C NM AND NN ARE OF COURSE BOUNDED BY THE SIZE OF THE STORE.
C
C THE REAL PARAMETER T MUST BE SET EQUAL TO THE NUMBER OF
C BINARY DIGITS IN THE MANTISSA OF A SINGLE PRECISION
C FLOATING-POINT NUMBER.
C
C THE REAL PARTS OF THE N COMPUTED EIGENVALUES WILL BE FOUND
C IN THE FIRST N PLACES OF THE ARRAY EVR AND THE IMAGINARY
C PARTS IN THE FIRST N PLACES OF THE ARRAY EVI.
C THE REAL COMPONENTS OF THE NORMALISED EIGENVECTOR I
C (I=1,2,...,N) CORRESPONDING TO THE EIGENVALUE STORED IN
C EVR(I) AND EVI(I) WILL BE FOUND IN THE FIRST N PLACES OF
C THE COLUMN I OF THE TWO DIMENSIONAL ARRAY VECR AND THE
C IMAGINARY COMPONENTS IN THE FIRST N PLACES OF THE COLUMN I
C OF THE TWO DIMENSIONAL ARRAY VECI.
C
C THE REAL EIGENVECTOR IS NORMALISED SO THAT THE SUM OF THE
C SQUARES OF THE COMPONENTS IS EQUAL TO ONE.
C THE COMPLEX EIGENVECTOR IS NORMALISED SO THAT THE
C COMPONENT WITH THE LARGEST VALUE IN MODULUS HAS ITS REAL
C PART EQUAL TO ONE AND THE IMAGINARY PART EQUAL TO ZERO.
C
C THE ARRAY INDIC INDICATES THE SUCCESS OF THE SUBROUTINE
C EIGENP AS FOLLOWS
C VALUE OF INDIC(I) EIGENVALUE I EIGENVECTOR I
C 0 NOT FOUND NOT FOUND
C 1 FOUND NOT FOUND
C 2 FOUND FOUND
C
C IF(N.NE.1)GO TO 1
EVR(1) = A(1,1)
EVI(1) = 0.0
VECR(1,1) = 1.0
VECI(1,1) = 0.0
INDIC(1) = 2
GO TO 25

C
1 CALL SCALE(N,NM,A,VECI,PRFACT,ENORM)
C THE COMPUTATION OF THE EIGENVALUES OF THE NORMALISED
C MATRIX.
EX = EXP(-T*ALOG(2.0))
CALL HESQR(N,NM,A,VECI,EVR,EVI,SUBDIA,INDIC,EPS,EX)

C
C THE POSSIBLE DECOMPOSITION OF THE UPPER-HESSENBERG MATRIX
C INTO THE SUBMATRICES OF LOWER ORDER IS INDICATED IN THE
C ARRAY LOCAL. THE DECOMPOSITION OCCURS WHEN SOME
C SUBDIAGONAL ELEMENTS ARE IN MODULUS LESS THAN A SMALL
C POSITIVE NUMBER EPS DEFINED IN THE SUBROUTINE HESQR. THE
C AMOUNT OF WORK IN THE EIGENVECTOR PROBLEM MAY BE
C DIMINISHED IN THIS WAY.
J = N
I = 1
LOCAL(1) = 1
IF(J.EQ.1)GO TO 4
2 IF(ABS(SUBDIA(J-1)).GT.EPS)GO TO 3
I = I+1
LOCAL(I)=0
3 J = J-1
LOCAL(I)=LOCAL(I)+1
IF(J.NE.1)GO TO 2

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C
C THE EIGENVECTOR PROBLEM.
4 K = 1
KON = 0
L = LOCAL(1)
M = N
DO 10 I=1,N
IVEC = N-I+1
IF(I.LE.L)GO TO 5
K = K+1
M = N-L
L = L+LOCAL(K)
5 IF(INDIC(IVEC).EQ.0)GO TO 10
IF(EVI(IVEC).NE.0.0)GO TO 8

C
C TRANSFER OF AN UPPER-HESSENBERG MATRIX OF THE ORDER M FROM
C THE ARRAYS VECI AND SUBDIA INTO THE ARRAY A.
DO 7 K1=1,M
DO 6 L1=K1,M
6 A(K1,L1) = VECI(K1,L1)
IF(K1.EQ.1)GO TO 7
A(K1,K1-1) = SUBDIA(K1-1)
7 CONTINUE

C
C THE COMPUTATION OF THE REAL EIGENVECTOR IVEC OF THE UPPER-
C HESSENBERG MATRIX CORRESPONDING TO THE REAL EIGENVALUE
C EVR(IVEC).
CALL REALVE(N,NM,M,IVEC,A,VECR,EVR,EVI,IWORK,
1 WORK,INDIC,EPS,EX)
GO TO 10

C
C THE COMPUTATION OF THE COMPLEX EIGENVECTOR IVEC OF THE
C UPPER-HESSENBERG MATRIX CORRESPONDING TO THE COMPLEX
C EIGENVALUE EVR(IVEC) + I*EVI(IVEC). IF THE VALUE OF KON IS
C NOT EQUAL TO ZERO THEN THIS COMPLEX EIGENVECTOR HAS
C ALREADY BEEN FOUND FROM ITS CONJUGATE.
8 IF(KON.NE.0)GO TO 9
KON = 1
CALL COMPVE(N,NM,M,IVEC,A,VECR,VECI,EVR,EVI,INDIC,
1 IWORK,SUBDIA,WORK1,WORK2,WORK,EPS,EX)
GO TO 10
9 KON = 0
10 CONTINUE

C
C THE RECONSTRUCTION OF THE MATRIX USED IN THE REDUCTION OF
C MATRIX A TO AN UPPER-HESSENBERG FORM BY HOUSEHOLDER METHOD
DO 12 I=1,N
DO 11 J=I,N
A(I,J) = 0.0
11 A(J,I) = 0.0
12 A(I,I) = 1.0
IF(N.LE.2)GO TO 15
M = N-2
DO 14 K=1,M
L = K+1
DO 14 J=2,N
D1 = 0.0
DO 13 I=L,N
D2 = VECI(I,K)
D1 = D1+ D2*A(J,I)
13 DO 14 I=L,N
A(J,I) = A(J,I)-VECI(I,K)*D1

C
C THE COMPUTATION OF THE EIGENVECTORS OF THE ORIGINAL NON-
C SCALED MATRIX.
15 KON = 1
DO 24 I=1,N
L = 0
IF(EVI(I).EQ.0.0)GO TO 16
L = 1
IF(KON.EQ.0)GO TO 16
KON = 0
GO TO 24
16 DO 18 J=1,N
D1 = 0.0
D2 = 0.0
DO 17 K=1,N
D3 = A(J,K)
D1 = D1+D3*VECR(K,I)
IF(L.EQ.0)GO TO 17
D2 = D2+D3*VECR(K,I-1)
17 CONTINUE
WORK(J) = D1/PRFACT(J)
IF(L.EQ.0)GO TO 18
SUBDIA(J)=D2/PRFACT(J)
18 CONTINUE

C
C THE NORMALISATION OF THE EIGENVECTORS AND THE COMPUTATION
C OF THE EIGENVALUES OF THE ORIGINAL NON-NORMALISED MATRIX.
IF(L.EQ.1)GO TO 21
D1 = 0.0
DO 19 M=1,N
D1 = D1+WORK(M)**2
19 D1 = DSQRT(D1)
DO 20 M=1,N
VECI(M,1) = 0.0
20 VECR(M,1) = WORK(M)/D1
EVR(I) = EVR(I)*ENORM
GO TO 24

C
21 KON = 1
EVR(I) = EVR(I)*ENORM

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EVR(I-1) = EVR(I)
EVI(I) = EVI(I)*ENORM
EVI(I-1) = -EVI(I)
R = 0.0
DO 22 J=1,N
  R1 = WORK(J)**2 + SUBDIA(J)**2
  IF(R.GE.R1)GO TO 22
  R = R1
  L = J
22 CONTINUE
D3 = WORK(L)
R1 = SUBDIA(L)
DO 23 J=1,N
  D1 = WORK(J)
  D2 = SUBDIA(J)
  VECR(J,I) = (D1*D3+D2*R1)/R
  VECI(J,I) = (D2*D3-D1*R1)/R
  VECR(J,I-1) = VECR(J,I)
23 VECI(J,I-1) = -VECI(J,I)
24 CONTINUE
C
25 RETURN
END

SUBROUTINE SCALE(N,NM,A,H,PRFACT,ENORM)
DOUBLE PRECISION COLUMN,FACTOR,FNORM,PRFACT,Q,ROW
INTEGER I,J,ITER,N,NCOUNT,NM
REAL BOUND1,BOUND2,ENORM
DIMENSION A(NM,1),H(NM,1),PRFACT(NM)
C
C THIS SUBROUTINE STORES THE MATRIX OF THE ORDER N FROM THE
C ARRAY A INTO THE ARRAY H. AFTERWARD THE MATRIX IN THE
C ARRAY A IS SCALED SO THAT THE QUOTIENT OF THE ABSOLUTE SUM
C OF THE OFF-DIAGONAL ELEMENTS OF COLUMN I AND THE ABSOLUTE
C SUM OF THE OFF-DIAGONAL ELEMENTS OF ROW I LIES WITHIN THE
C VALUES OF BOUND1 AND BOUND2.
C THE COMPONENT I OF THE EIGENVECTOR OBTAINED BY USING THE
C SCALED MATRIX MUST BE DIVIDED BY THE VALUE FOUND IN THE
C PRFACT(I) OF THE ARRAY PRFACT. IN THIS WAY THE EIGENVECTOR
C OF THE NON-SCALED MATRIX IS OBTAINED.
C
C AFTER THE MATRIX IS SCALED IT IS NORMALISED SO THAT THE
C VALUE OF THE EUCLIDIAN NORM IS EQUAL TO ONE.
C IF THE PROCESS OF SCALING WAS NOT SUCCESSFUL THE ORIGINAL
C MATRIX FROM THE ARRAY H WOULD BE STORED BACK INTO A AND
C THE EIGENPROBLEM WOULD BE SOLVED BY USING THIS MATRIX.
C NM DEFINES THE FIRST DIMENSION OF THE ARRAYS A AND H. NM
C MUST BE GREATER OR EQUAL TO N.
C THE EIGENVALUES OF THE NORMALISED MATRIX MUST BE
C MULTIPLIED BY THE SCALAR ENORM IN ORDER THAT THEY BECOME
C THE EIGENVALUES OF THE NON-NORMALISED MATRIX.
C
DO 2 I=1,N
  DO 1 J=1,N
1    H(I,J) = A(I,J)
2    PRFACT(I) = 1.0
  BOUND1 = 0.75
  BOUND2 = 1.33
  ITER = 0
3  NCOUNT = 0
  DO 8 I=1,N
    COLUMN = 0.0
    ROW = 0.0
    DO 4 J=1,N
      IF(I.EQ.J)GO TO 4
      COLUMN = COLUMN+ ABS(A(J,I))
      ROW = ROW + ABS(A(I,J))
4    CONTINUE
    IF(COLUMN.EQ.0.0)GO TO 5
    IF(ROW.EQ.0.0)GO TO 5
    Q = COLUMN/ROW
    IF(Q.LT.BOUND1)GO TO 6
    IF(Q.GT.BOUND2)GO TO 6
5    NCOUNT = NCOUNT + 1
    GO TO 8
6    FACTOR = DSQRT(Q)
    DO 7 J=1,N
      IF(I.EQ.J)GO TO 7
      A(I,J) = A(I,J)*FACTOR
      A(J,I) = A(J,I)/FACTOR
7    CONTINUE
    PRFACT(I) = PRFACT(I)*FACTOR
8  CONTINUE
  ITER = ITER+1
  IF(ITER.GT.30)GO TO 11
  IF(NCOUNT.LT.N)GO TO 3
C
FNORM = 0.0
DO 9 I=1,N
  DO 9 J=1,N
    Q = A(I,J)
9  FNORM = FNORM+Q*Q
FNORM = DSQRT(FNORM)
DO 10 I=1,N
  DO 10 J=1,N
    A(I,J)=A(I,J)/FNORM
10 ENORM = FNORM
GO TO 13

```

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C
11 DO 12 I=1,N
  DO 12 J=1,N
12   A(I,J) = H(I,J)
  ENORM = 1.0
C
13 RETURN
END

SUBROUTINE HESQR(N,NM,A,H,EVR,EVI,SUBDIA,INDIC,EPS,EX)
DOUBLE PRECISION S,SR,SR2,X,Y,Z
INTEGER I,J,K,L,M,MAXST,M1,N,NM,NS
REAL EPS,EX,R,SHIFT,T
DIMENSION A(NM,1),H(NM,1),EVR(NM),EVI(NM),SUBDIA(NM)
DIMENSION INDIC(NM)
C
C THIS SUBROUTINE FINDS ALL THE EIGENVALUES OF A REAL
C GENERAL MATRIX. THE ORIGINAL MATRIX A OF ORDER N IS
C REDUCED TO THE UPPER-HESSBERG FORM H BY MEANS OF
C SIMILARITY TRANSFORMATIONS(HOUSEHOLDER METHOD). THE MATRIX
C H IS PRESERVED IN THE UPPER HALF OF THE ARRAY H AND IN THE
C ARRAY SUBDIA. THE SPECIAL VECTORS USED IN THE DEFINITION
C OF THE HOUSEHOLDER TRANSFORMATION MATRICES ARE STORED IN
C THE LOWER PART OF THE ARRAY H.
C NM IS THE FIRST DIMENSION OF THE ARRAYS A AND H. NM MUST
C BE EQUAL TO OR GREATER THAN N.
C THE REAL PARTS OF THE N EIGENVALUES WILL BE FOUND IN THE
C FIRST N PLACES OF THE ARRAY EVR,AND
C THE IMAGINARY PARTS IN THE FIRST N PLACES OF THE ARRAY EVI
C THE ARRAY INDIC INDICATES THE SUCCESS OF THE ROUTINE AS
C FOLLOWS
C   VALUE OF INDIC(I)   EIGENVALUE I
C   0                     NOT FOUND
C   1                     FOUND
C EPS IS A SMALL POSITIVE NUMBER THAT NUMERICALLY REPRESENTS
C ZERO IN THE PROGRAM. EPS = (EUCLIDIAN NORM OF H)*EX ,WHERE
C EX = 2**(-T). T IS THE NUMBER OF BINARY DIGITS IN THE
C MANTISSA OF A FLOATING POINT NUMBER.
C
C
C REDUCTION OF THE MATRIX A TO AN UPPER-HESSBERG FORM H.
C THERE ARE N-2 STEPS.
  IF(N-2)14,1,2
1  SUBDIA(1) = A(2,1)
  GO TO 14
2  M = N-2
  DO 12 K=1,M
    L = K+1
    S = 0.0
    DO 3 I=L,N
      H(I,K) = A(I,K)
3    S = S+ABS(A(I,K))
    IF(S.NE.ABS(A(K+1,K)))GO TO 4
    SUBDIA(K) = A(K+1,K)
    H(K+1,K) = 0.0
    GO TO 12
4  SR2 = 0.0
    DO 5 I=L,N
      SR = A(I,K)
      SR = SR/S
5    A(I,K) = SR
      SR2 = SR2+SR*SR
    SR = DSQRT(SR2)
    IF(A(L,K).LT.0.0)GO TO 6
    SR = -SR
6  SR2 = SR2-SR*A(L,K)
    A(L,K) = A(L,K)-SR
    H(L,K) = H(L,K)-SR*S
    SUBDIA(K) = SR*S
    X = S*DSQRT(SR2)
    DO 7 I=L,N
      H(I,K) = H(I,K)/X
7  SUBDIA(I) = A(I,K)/SR2
C PREMULTIPLICATION BY THE MATRIX PR.
  DO 9 J=L,N
    SR = 0.0
    DO 8 I=L,N
      SR = SR+A(I,K)*A(I,J)
8  DO 9 I=L,N
    A(I,J) = A(I,J)-SUBDIA(I)*SR
C POSTMULTIPLICATION BY THE MATRIX PR.
  DO 11 J=1,N
    SR=0.0
    DO 10 I=L,N
      SR = SR+A(J,I)*A(I,K)
10  DO 11 I=L,N
    A(J,I) = A(J,I)-SUBDIA(I)*SR
12 CONTINUE
  DO 13 K=1,M
13  A(K+1,K) = SUBDIA(K)
C TRANSFER OF THE UPPER HALF OF THE MATRIX A INTO THE
C ARRAY H AND THE CALCULATION OF THE SMALL POSITIVE NUMBER
C EPS.
  SUBDIA(N-1) = A(N,N-1)
14 EPS = 0.0
  DO 15 K=1,N
    INDIC(K) = 0

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        IF(K.NE.N)EPS = EPS+SUBDIA(K)**2
        DO 15 I=K,N
            H(K,I) = A(K,I)
15      EPS = EPS + A(K,I)**2
        EPS = EX*SQRT(EPS)
C
C THE QR ITERATIVE PROCESS. THE UPPER-HESSSENBERG MATRIX H IS
C REDUCED TO THE UPPER-MODIFIED TRIANGULAR FORM.
C
C DETERMINATION OF THE SHIFT OF ORIGIN FOR THE FIRST STEP OF
C THE QR ITERATIVE PROCESS.
        SHIFT = A(N,N-1)
        IF(N.LE.2)SHIFT = 0.0
        IF(A(N,N).NE.0.0)SHIFT = 0.0
        IF(A(N-1,N).NE.0.0)SHIFT = 0.0
        IF(A(N-1,N-1).NE.0.0)SHIFT = 0.0
        M = N
        NS = 0
        MAXST = N*10
C
C TESTING IF THE UPPER HALF OF THE MATRIX IS EQUAL TO ZERO.
C IF IT IS EQUAL TO ZERO THE QR PROCESS IS NOT NECESSARY.
        DO 16 I=2,N
            DO 16 K=I,N
                IF(A(I-1,K).NE.0.0)GO TO 18
16      CONTINUE
        DO 17 I=1,N
            INDIC(I)=1
            EVR(I) = A(I,I)
17      EVI(I) = 0.0
        GO TO 37
C
C START THE MAIN LOOP OF THE QR PROCESS.
18 K=M-1
        M1=K
        I = K
C FIND ANY DECOMPOSITIONS OF THE MATRIX.
C JUMP TO 34 IF THE LAST SUBMATRIX OF THE DECOMPOSITION IS
C OF THE ORDER ONE.
C JUMP TO 35 IF THE LAST SUBMATRIX OF THE DECOMPOSITION IS
C OF THE ORDER TWO.
        IF(K)37,34,19
19 IF(ABS(A(M,K)).LE.EPS)GO TO 34
        IF(M-2.EQ.0)GO TO 35
20 I = I-1
        IF(ABS(A(K,I)).LE.EPS)GO TO 21
        K = I
        IF(K.GT.1)GO TO 20
21 IF(K.EQ.M1)GO TO 35
C TRANSFORMATION OF THE MATRIX OF THE ORDER GREATER THAN TWO
        S = A(M,M)+A(M1,M1)+SHIFT
        SR= A(M,M)*A(M1,M1)-A(M,M1)*A(M1,M)+0.25*SHIFT**2
        A(K+2,K) = 0.0
C CALCULATE X1,Y1,Z1, FOR THE SUBMATRIX OBTAINED BY THE
C DECOMPOSITION.
        X = A(K,K)*(A(K,K)-S)+A(K,K+1)*A(K+1,K)+SR
        Y = A(K+1,K)*(A(K,K)+A(K+1,K+1)-S)
        R = DABS(X)+DABS(Y)
        IF(R.EQ.0.0)SHIFT = A(M,M-1)
        IF(R.EQ.0.0)GO TO 21
        Z = A(K+2,K+1)*A(K+1,K)
        SHIFT = 0.0
        NS = NS+1
C
C THE LOOP FOR ONE STEP OF THE QR PROCESS.
        DO 33 I=K,M1
            IF(I.EQ.K)GO TO 22
C CALCULATE XR,YR,ZR.
            X = A(I,I-1)
            Y = A(I+1,I-1)
            Z = 0.0
            IF(I+2.GT.M)GO TO 22
            Z = A(I+2,I-1)
22      SR2 = DABS(X)+DABS(Y)+DABS(Z)
            IF(SR2.EQ.0.0)GO TO 23
            X = X/SR2
            Y = Y/SR2
            Z = Z/SR2
23      S = DSQRT(X*X + Y*Y + Z*Z)
            IF(X.LT.0.0)GO TO 24
            S = -S
24      IF(I.EQ.K)GO TO 25
            A(I,I-1) = S*SR2
25      IF(SR2.NE.0.0)GO TO 26
            IF(I+3.GT.M)GO TO 33
            GO TO 32
26      SR = 1.0-X/S
            S = X-S
            X = Y/S
            Y = Z/S
C PREMULIPLICATION BY THE MATRIX PR.
        DO 28 J=I,M
            S = A(I,J)+A(I+1,J)*X
            IF(I+2.GT.M)GO TO 27
            S = S+A(I+2,J)*Y
27      S = S*SR
            A(I,J) = A(I,J)-S
            A(I+1,J) = A(I+1,J)-S*X
            IF(I+2.GT.M)GO TO 28

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            A(I+2,J) = A(I+2,J)-S*Y
28      CONTINUE
C POSTMULTIPLICATION BY THE MATRIX PR.
        L = I+2
        IF(I.LT.M1)GO TO 29
        L = M
29      DO 31 J=K,L
            S = A(J,I)+A(J,I+1)*X
            IF(I+2.GT.M)GO TO 30
            S = S + A(J,I+2)*Y
30      S = S*SR
            A(J,I) = A(J,I)-S
            A(J,I+1)=A(J,I+1)-S*X
            IF(I+2.GT.M)GO TO 31
            A(J,I+2)=A(J,I+2)-S*Y
31      CONTINUE
            IF(I+3.GT.M)GO TO 33
            S = -A(I+3,I+2)*Y*SR
32      A(I+3,I) = S
            A(I+3,I+1) = S*X
            A(I+3,I+2) = S*Y + A(I+3,I+2)
33      CONTINUE
C
        IF(NS.GT.MAXST)GO TO 37
        GO TO 18
C
C COMPUTE THE LAST EIGENVALUE.
34 EVR(M) = A(M,M)
        EVI(M) = 0.0
        INDIC(M) = 1
        M = K
        GO TO 18
C
C COMPUTE THE EIGENVALUES OF THE LAST 2X2 MATRIX OBTAINED BY
C THE DECOMPOSITION.
35 R = 0.5*(A(K,K)+A(M,M))
        S = 0.5*(A(M,M)-A(K,K))
        S = S*S + A(K,M)*A(M,K)
        INDIC(K) = 1
        INDIC(M) = 1
        IF(S.LT.0.0)GO TO 36
        T = DSQRT(S)
        EVR(K) = R-T
        EVR(M) = R+T
        EVI(K) = 0.0
        EVI(M) = 0.0
        M = M-2
        GO TO 18
36 T = DSQRT(-S)
        EVR(K) = R
        EVI(K) = T
        EVR(M) = R
        EVI(M) = -T
        M = M-2
        GO TO 18
C
37 RETURN
        END
        SUBROUTINE REALVE(N,NM,M,IVEC,A,VECR,EVR,EVI,
        I1WORK,WORK,INDIC,EPS,EX)
        DOUBLE PRECISION S,SR
        INTEGER I,IVEC,ITER,J,K,L,M,N,NM,NS
        REAL BOUND,EPS,EVALUE,EX,PREVIS,R,R1,T
        DIMENSION A(NM,1),VECR(NM,1),EVR(NM)
        DIMENSION EVI(NM),I1WORK(NM),WORK(NM),INDIC(NM)
C
C THIS SUBROUTINE FINDS THE REAL EIGENVECTOR OF THE REAL
C UPPER-HESSSENBERG MATRIX IN THE ARRAY A, CORRESPONDING TO
C THE REAL EIGENVALUE STORED IN EVR(IVEC). THE INVERSE
C ITERATION METHOD IS USED.
C NOTE THE MATRIX IN A IS DESTROYED BY THE SUBROUTINE.
C N IS THE ORDER OF THE UPPER-HESSSENBERG MATRIX.
C NM DEFINES THE FIRST DIMENSION OF THE TWO DIMENSIONAL
C ARRAYS A AND VECR. NM MUST BE EQUAL TO OR GREATER THAN N.
C M IS THE ORDER OF THE SUBMATRIX OBTAINED BY A SUITABLE
C DECOMPOSITION OF THE UPPER-HESSSENBERG MATRIX IF SOME
C SUBDIAGONAL ELEMENTS ARE EQUAL TO ZERO. THE VALUE OF M IS
C CHOSEN SO THAT THE LAST N-M COMPONENTS OF THE EIGENVECTOR
C ARE ZERO.
C IVEC GIVES THE POSITION OF THE EIGENVALUE IN THE ARRAY EVR
C FOR WHICH THE CORRESPONDING EIGENVECTOR IS COMPUTED.
C THE ARRAY EVI WOULD CONTAIN THE IMAGINARY PARTS OF THE N
C EIGENVALUES IF THEY EXISTED.
C
C THE M COMPONENTS OF THE COMPUTED REAL EIGENVECTOR WILL BE
C FOUND IN THE FIRST M PLACES OF THE COLUMN IVEC OF THE TWO
C DIMENSIONAL ARRAY VECR.
C
C IWORK AND WORK ARE THE WORKING STORES USED DURING THE
C GAUSSIAN ELIMINATION AND BACKSUBSTITUTION PROCESS.
C THE ARRAY INDIC INDICATES THE SUCCESS OF THE ROUTINE AS
C FOLLOWS
        VALUE OF INDIC(I)      EIGENVECTOR I
C          1                      NOT FOUND
C          2                      FOUND
C EPS IS A SMALL POSITIVE NUMBER THAT NUMERICALLY REPRESENTS
C ZERO IN THE PROGRAM. EPS = (EUCLIDIAN NORM OF A)*EX, WHERE
C EX = 2**(1-T). T IS THE NUMBER OF BINARY DIGITS IN THE

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C MANTISSA OF A FLOATING POINT NUMBER.
  VECR(1,IVEC) = 1.0
  IF(M.EQ.1)GO TO 24
C SMALL PERTURBATION OF EQUAL EIGENVALUES TO OBTAIN A FULL
C SET OF EIGENVECTORS.
  EVALUE = EVR(IVEC)
  IF(IVEC.EQ.M)GO TO 2
  K = IVEC+1
  R = 0.0
  DO 1 I=K,M
    IF(EVALUE.NE.EVR(I))GO TO 1
    IF(EV(I).NE.0.0)GO TO 1
    R = R+3.0
  1 CONTINUE
  EVALUE = EVALUE+R*EX
  DO 3 K=1,M
  2 A(K,K) = A(K,K)-EVALUE
C
C GAUSSIAN ELIMINATION OF THE UPPER-HESSSENBERG MATRIX A. ALL
C ROW INTERCHANGES ARE INDICATED IN THE ARRAY IWORK.ALL THE
C MULTIPLIERS ARE STORED AS THE SUBDIAGONAL ELEMENTS OF A.
  K = M-1
  DO 8 I=1,K
    L = I+1
    IWORK(I) = 0
    IF(A(I+1,I).NE.0.0)GO TO 4
    IF(A(I,I).NE.0.0)GO TO 8
    A(I,I) = EPS
    GO TO 8
  4 IF(ABS(A(I,I)).GE.ABS(A(I+1,I)))GO TO 6
    IWORK(I) = 1
    DO 5 J=I,M
      R = A(I,J)
      A(I,J) = A(I+1,J)
      A(I+1,J) = R
    5 R = -A(I+1,I)/A(I,I)
      A(I+1,I) = R
      DO 7 J=L,M
      7 A(I+1,J) = A(I+1,J)+R*A(I,J)
    8 CONTINUE
    IF(A(M,M).NE.0.0)GO TO 9
    A(M,M) = EPS
C
C THE VECTOR {1,1,...,1} IS STORED IN THE PLACE OF THE RIGHT
C HAND SIDE COLUMN VECTOR.
  DO 11 I=1,N
    IF(I.GT.M)GO TO 10
    WORK(I) = 1.0
    GO TO 11
  10 WORK(I) = 0.0
  11 CONTINUE
C
C THE INVERSE ITERATION IS PERFORMED ON THE MATRIX UNTIL THE
C INFINITE NORM OF THE RIGHT-HAND SIDE VECTOR IS GREATER
C THAN THE BOUND DEFINED AS 0.01/(N*EX).
  BOUND = 0.01/(EX * FLOAT(N))
  NS = 0
  ITER = 1
C
C THE BACKSUBSTITUTION.
  DO 12 I=N,1
  12 R = 0.0
  DO 15 J=I,M
    J = M-I+1
    S = WORK(J)
    IF(J.EQ.M)GO TO 14
    L = J+1
    DO 13 K=L,M
      SR = WORK(K)
      S = S - SR*A(J,K)
    13 WORK(J) = S/A(J,J)
    T = ABS(WORK(J))
    IF(R.GE.T)GO TO 15
    R = T
  15 CONTINUE
C
C THE COMPUTATION OF THE RIGHT-HAND SIDE VECTOR FOR THE NEW
C ITERATION STEP.
  DO 16 I=1,M
  16 WORK(I) = WORK(I)/R
C
C THE COMPUTATION OF THE RESIDUALS AND COMPARISON OF THE
C RESIDUALS OF THE TWO SUCCESSIVE STEPS OF THE INVERSE
C ITERATION.IF THE INFINITE NORM OF THE RESIDUAL VECTOR IS
C GREATER THAN THE INFINITE NORM OF THE PREVIOUS RESIDUAL
C VECTOR THE COMPUTED EIGENVECTOR OF THE PREVIOUS STEP IS
C TAKEN AS THE FINAL EIGENVECTOR.
  R1 = 0.0
  DO 18 I=1,M
    T = 0.0
    DO 17 J=I,M
      T = T+A(I,J)*WORK(J)
    17 T = ABS(T)
    IF(R1.GE.T)GO TO 18
    R1 = T
  18 CONTINUE
  IF(ITER.EQ.1)GO TO 19
  IF(PREVIS.LE.R1)GO TO 24
  DO 20 I=1,M
  20 VECR(I,IVEC) = WORK(I)

  PREVIS = R1
  IF(NS.EQ.1)GO TO 24
  IF(ITER.GT.6)GO TO 25
  ITER = ITER+1
  IF(R.LT.BOUND)GO TO 21
  NS = 1
C
C GAUSSIAN ELIMINATION OF THE RIGHT-HAND SIDE VECTOR.
  DO 21 K = M-1
  21 K = M-1
  DO 23 I=1,K
    R = WORK(I+1)
    IF(IWORK(I).EQ.0)GO TO 22
    WORK(I+1)=WORK(I)+WORK(I+1)*A(I+1,I)
    WORK(I) = R
    GO TO 23
  22 WORK(I+1)=WORK(I+1)+WORK(I)*A(I+1,I)
  23 CONTINUE
  GO TO 12
C
  24 INDIC(IVEC) = 2
  25 IF(M.EQ.N)GO TO 27
  J = M+1
  DO 26 I=J,N
  26 VECR(I,IVEC) = 0.0
  27 RETURN
  END

  SUBROUTINE COMPVE(N,NM,M,IVEC,A,VECR,H,EVR,EVI,INDIC,
  IWORK,SUBDIA,WORK1,WORK2,WORK,EPS,EX)
  DOUBLE PRECISION D,D1
  INTEGER I,I1,I2,ITER,IVEC,J,K,L,M,N,NM,NS
  REAL B,BOUND,EPS,ETA,EX,FKSI,PREVIS,R,S,U,V
  DIMENSION A(NM,1),VECR(NM,1),H(NM,1),EVR(NM),EVI(NM),
  IINDIC(NM),IWORK(NM),SUBDIA(NM),WORK1(NM),WORK2(NM),
  2WORK(NM)
C
C THIS SUBROUTINE FINDS THE COMPLEX EIGENVECTOR OF THE REAL
C UPPER-HESSSENBERG MATRIX OF ORDER N CORRESPONDING TO THE
C COMPLEX EIGENVALUE WITH THE REAL PART IN EVR(IVEC) AND THE
C CORRESPONDING IMAGINARY PART IN EVI(IVEC). THE INVERSE
C ITERATION METHOD IS USED MODIFIED TO AVOID THE USE OF
C COMPLEX ARITHMETIC.
C THE MATRIX ON WHICH THE INVERSE ITERATION IS PERFORMED IS
C BUILT UP IN THE ARRAY A BY USING THE UPPER-HESSSENBERG
C MATRIX PRESERVED IN THE UPPER HALF OF THE ARRAY H AND IN
C THE ARRAY SUBDIA.
C NM DEFINES THE FIRST DIMENSION OF THE TWO DIMENSIONAL
C ARRAYS A,VECR AND H. NM MUST BE EQUAL TO OR GREATER
C THAN N.
C M IS THE ORDER OF THE SUBMATRIX OBTAINED BY A SUITABLE
C DECOMPOSITION OF THE UPPER-HESSSENBERG MATRIX IF SOME
C SUBDIAGONAL ELEMENTS ARE EQUAL TO ZERO. THE VALUE OF M IS
C CHOSEN SO THAT THE LAST N-M COMPONENTS OF THE COMPLEX
C EIGENVECTOR ARE ZERO.
C
C THE REAL PARTS OF THE FIRST M COMPONENTS OF THE COMPUTED
C COMPLEX EIGENVECTOR WILL BE FOUND IN THE FIRST M PLACES OF
C THE COLUMN WHOSE TOP ELEMENT IS VECR(1,IVEC) AND THE
C CORRESPONDING IMAGINARY PARTS OF THE FIRST M COMPONENTS OF
C THE COMPLEX EIGENVECTOR WILL BE FOUND IN THE FIRST M
C PLACES OF THE COLUMN WHOSE TOP ELEMENT IS VECR(1,IVEC-1).
C
C THE ARRAY INDIC INDICATES THE SUCCESS OF THE ROUTINE AS
C FOLLOWS
C   VALUE OF INDIC(I)   EIGENVECTOR I
C   1                     NOT FOUND
C   2                     FOUND
C THE ARRAYS IWORK,WORK1,WORK2 AND WORK ARE THE WORKING
C STORES USED DURING THE INVERSE ITERATION PROCESS.
C EPS IS A SMALL POSITIVE NUMBER THAT NUMERICALLY REPRESENTS
C ZERO IN THE PROGRAM. EPS = (EUCLIDIAN NORM OF H)*EX, WHERE
C EX = 2**(-T). T IS THE NUMBER OF BINARY DIGITS IN THE
C MANTISSA OF A FLOATING POINT NUMBER.
C
  FKSI = EVR(IVEC)
  ETA = EVI(IVEC)
C THE MODIFICATION OF THE EIGENVALUE (FKSI + I*ETA) IF MORE
C EIGENVALUES ARE EQUAL.
  IF(IVEC.EQ.M)GO TO 2
  K = IVEC+1
  R = 0.0
  DO 1 I=K,M
    IF(FKSI.NE.EVR(I))GO TO 1
    IF(ABS(ETA).NE.ABS(EVI(I)))GO TO 1
    R = R + 3.0
  1 CONTINUE
  R = R*EX
  FKSI = FKSI+R
  ETA = ETA +R
C
C THE MATRIX ((H-FKSI*I)*(H-FKSI*I) + (ETA*ETA)*I) IS
C STORED INTO THE ARRAY A.
  DO 2 R = FKSI*FKSI + ETA*ETA
  2 R = 2.0*FKSI
  S = M-1
  DO 5 I=1,M
    DO 4 J=I,M
      D = 0.0

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      A(J,I) = 0.0
      DO 3 K = 1,J
3       D = D+H(I,K)*H(K,J)
4       A(I,J) = D-S*H(I,J)
5       A(I,I) = A(I,I)+R
      DO 9 I=1,L
        R = SUBDIA(I)
        A(I+1,I) = -S*R
        I1 = I+1
        DO 6 J=1,I1
9         A(J,I) = A(J,I)+R*H(J,I+1)
        IF(I.EQ.1)GO TO 7
        A(I+1,I-1) = R*SUBDIA(I-1)
        DO 8 J=I,M
8         A(I+1,J) = A(I+1,J)+R*H(I,J)
9       CONTINUE
C
C THE GAUSSIAN ELIMINATION OF THE MATRIX
C ((H-FKSI*I)*(H-FKSI*I) + (ETA*ETA)*I) IN THE ARRAY A. THE
C ROW INTERCHANGES THAT OCCUR ARE INDICATED IN THE ARRAY
C IWORK. ALL THE MULTIPLIERS ARE STORED IN THE FIRST AND IN
C THE SECOND SUBDIAGONAL OF THE ARRAY A.
      K = M-1
      DO 18 I=1,K
        I1 = I+1
        I2 = I+2
        IWORK(I) = 0
        IF(I.EQ.K)GO TO 10
        IF(A(I+2,I).NE.0.0)GO TO 11
10       IF(A(I+1,I).NE.0.0)GO TO 11
        IF(A(I,I).NE.0.0)GO TO 18
        A(I,I) = EPS
        GO TO 18
C
11      IF(I.EQ.K)GO TO 12
        IF(ABS(A(I+1,I)).GE.ABS(A(I+2,I)))GO TO 12
        IF(ABS(A(I,I)).GE.ABS(A(I+2,I)))GO TO 16
        L = I+2
        IWORK(I) = 2
        GO TO 13
12      IF(ABS(A(I,I)).GE.ABS(A(I+1,I)))GO TO 15
        L = I+1
        IWORK(I) = 1
C
13      DO 14 J=I,M
        R = A(I,J)
        A(I,J) = A(L,J)
14      A(L,J) = R
15      IF(I.NE.K)GO TO 16
        I2 = I1
16      DO 17 L=I1,I2
        R = -A(L,I)/A(I,I)
        A(L,I) = R
        DO 17 J=I1,M
17       A(L,J) = A(L,J)+R*A(I,J)
18      CONTINUE
        IF(A(M,M).NE.0.0)GO TO 19
        A(M,M) = EPS
C
C THE VECTOR (1,1,...,1) IS STORED INTO THE RIGHT-HAND SIDE
C VECTORS VECR(,IVEC) AND VECR(,IVEC-1) REPRESENTING THE
C COMPLEX RIGHT-HAND SIDE VECTOR.
19      DO 21 I=1,N
        IF(I.GT.M)GO TO 20
        VECR(I,IVEC) = 1.0
        VECR(I,IVEC-1) = 1.0
        GO TO 21
20      VECR(I,IVEC) = 0.0
        VECR(I,IVEC-1) = 0.0
21      CONTINUE
C
C THE INVERSE ITERATION IS PERFORMED ON THE MATRIX UNTIL THE
C INFINITE NORM OF THE RIGHT-HAND SIDE VECTOR IS GREATER
C THAN THE BOUND DEFINED AS 0.01/(N*EX).
      BOUND = 0.01/(EX*FLOAT(N))
      NS = 0
      ITER = 1
      DO 22 I=1,M
22      WORK(I) = H(I,I)-FKSI
C
C THE SEQUENCE OF THE COMPLEX VECTORS Z(S) = P(S)+I*Q(S) AND
C W(S+1) = U(S+1)+I*V(S+1) IS GIVEN BY THE RELATIONS
C (A - (FKSI-I*ETA)*I)*W(S+1) = Z(S) AND
C Z(S+1) = W(S+1)/MAX(W(S+1)).
C THE FINAL W(S) IS TAKEN AS THE COMPUTED EIGENVECTOR.
C
C THE COMPUTATION OF THE RIGHT-HAND SIDE VECTOR
C (A-FKSI*I)*P(S)-ETA*Q(S). A IS AN UPPER-HESSSENBERG MATRIX.
23      DO 27 I=1,M
        D = WORK(I)*VECR(I,IVEC)
        IF(I.EQ.1)GO TO 24
        D = D+SUBDIA(I-1)*VECR(I-1,IVEC)
24      L = I+1
        IF(L.GT.M)GO TO 26
        DO 25 K=L,M
25       D = D+H(I,K)*VECR(K,IVEC)
26      VECR(I,IVEC-1) = D-ETA*VECR(I,IVEC-1)
27      CONTINUE
C
C GAUSSIAN ELIMINATION OF THE RIGHT-HAND SIDE VECTOR.
      K = M-1
      DO 28 I=1,K
        L = I+IWORK(I)
        R = VECR(L,IVEC-1)
        VECR(L,IVEC-1) = VECR(I,IVEC-1)
        VECR(I,IVEC-1) = R
        VECR(I+1,IVEC-1) = VECR(I+1,IVEC-1)+A(I+1,I)*R
        IF(I.EQ.K)GO TO 28
        VECR(I+2,IVEC-1) = VECR(I+2,IVEC-1)+A(I+2,I)*R
28      CONTINUE
C
C THE COMPUTATION OF THE REAL PART U(S+1) OF THE COMPLEX
C VECTOR W(S+1). THE VECTOR U(S+1) IS OBTAINED AFTER THE
C BACKSUBSTITUTION.
      DO 31 I=1,M
        J = M-I+1
        D = VECR(J,IVEC-1)
        IF(J.EQ.M)GO TO 30
        L = J+1
        DO 29 K=L,M
29         D1 = A(J,K)
        D = D-D1*VECR(K,IVEC-1)
30      VECR(J,IVEC-1) = D/A(J,J)
31      CONTINUE
C
C THE COMPUTATION OF THE IMAGINARY PART V(S+1) OF THE VECTOR
C W(S+1), WHERE V(S+1) = (P(S)-(A-FKSI*I)*U(S+1))/ETA.
      DO 35 I=1,M
        D = WORK(I)*VECR(I,IVEC-1)
        IF(I.EQ.1)GO TO 32
        D = D+SUBDIA(I-1)*VECR(I-1,IVEC-1)
32      L = I+1
        IF(L.GT.M)GO TO 34
        DO 33 K=L,M
33         D = D+H(I,K)*VECR(K,IVEC-1)
34      VECR(I,IVEC) = (VECR(I,IVEC)-D)/ETA
35      CONTINUE
C
C THE COMPUTATION OF (INFIN. NORM OF W(S+1))**2 .
      L = 1
      S = 0.0
      DO 36 I=1,M
        R = VECR(I,IVEC)**2 + VECR(I,IVEC-1)**2
        IF(R.LE.S)GO TO 36
        S = R
        L = I
36      CONTINUE
C
C THE COMPUTATION OF THE VECTOR Z(S+1),WHERE Z(S+1)= W(S+1)/
C (COMPONENT OF W(S+1) WITH THE LARGEST ABSOLUTE VALUE) .
      U = VECR(L,IVEC-1)
      V = VECR(L,IVEC)
      DO 37 I=1,M
        B = VECR(I,IVEC)
        R = VECR(I,IVEC-1)
        VECR(I,IVEC) = (R*U + B*V)/S
        VECR(I,IVEC-1) = (B*U-R*V)/S
37      CONTINUE
C
C THE COMPUTATION OF THE RESIDUALS AND COMPARISON OF THE
C RESIDUALS OF THE TWO SUCCESSIVE STEPS OF THE INVERSE
C ITERATION. IF THE INFINITE NORM OF THE RESIDUAL VECTOR IS
C GREATER THAN THE INFINITE NORM OF THE PREVIOUS RESIDUAL
C VECTOR THE COMPUTED VECTOR OF THE PREVIOUS STEP IS TAKEN
C AS THE COMPUTED APPROXIMATION TO THE EIGENVECTOR.
      B = 0.0
      DO 41 I=1,M
        R = WORK(I)*VECR(I,IVEC-1) - ETA*VECR(I,IVEC)
        U = WORK(I)*VECR(I,IVEC) + ETA*VECR(I,IVEC-1)
        IF(I.EQ.1)GO TO 38
        R = R+SUBDIA(I-1)*VECR(I-1,IVEC-1)
        U = U+SUBDIA(I-1)*VECR(I-1,IVEC)
38      L = I+1
        IF(L.GT.M)GO TO 40
        DO 39 J=L,M
39         R = R+H(I,J)*VECR(J,IVEC-1)
        U = U+H(I,J)*VECR(J,IVEC)
40      U = R*R + U*U
        IF(B.GE.U)GO TO 41
        B = U
41      CONTINUE
        IF(ITER.EQ.1)GO TO 42
        IF(PREVIS.LE.B)GO TO 44
42      DO 43 I=1,N
        WORK1(I) = VECR(I,IVEC)
43      WORK2(I) = VECR(I,IVEC-1)
        PREVIS = B
        IF(NS.EQ.1)GO TO 46
        IF(ITER.GT.6)GO TO 47
        ITER = ITER+1
        IF(BOUND.GT.SQRT(S))GO TO 23
        NS = 1
        GO TO 23
C
44      DO 45 I=1,N
        VECR(I,IVEC) = WORK1(I)
45      VECR(I,IVEC-1) = WORK2(I)
46      INDIC(IVEC-1) = 2
47      INDIC(IVEC) = 2
47      RETURN
      END

```

ADDED IN PROOF. A small alteration to the program is desirable. The four statements in the subroutine SCALE, page 822, lines 3-6, should be replaced by the four statements below. The alteration is necessary so that the program will also give correct eigenvectors for the case when no convergence of the process of scaling occurs.

```

      PRFACT (I) = 1.0
      DO 12 J = 1, N
12      A (I, J) = H (I, J)
      ENORM = 1.0

```

REMARKS ON ALGORITHM 32 [D1]

MULTINT [R. Don Freeman, Jr., *Comm. ACM* 4 (Feb. 1961), 106]

AND

CERTIFICATION OF ALGORITHM 32 [Henry C. Thacher, Jr., *Comm. ACM* 6 (Feb. 1963), 69]

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KEY WORDS AND PHRASES: numerical integration, multi-dimensional integration, Gaussian integration

CR CATEGORIES: 5.16

The real procedure *MULTINT* was corrected according to the certification. It was then compiled on a CDC 3800 computer and tested on the second integral given in the certification. It became apparent that

(i) Equation (2) of the certification should read

$$\int_{-1}^1 \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \int_{-\sqrt{1-x^2-y^2}}^{\sqrt{1-x^2-y^2}} \frac{dz \, dy \, dx}{x^2 + y^2 + (z - k)^2} = \pi \left(2 + \left(\frac{1}{k} - k \right) \log \left| \frac{1+k}{1-k} \right| \right) \quad (2)$$

It should be noted that the right-hand side of equation (2) as printed in the certification does not correspond either to the original limits or to those given above.

(ii) the statement

$Low := 0;$

in the real procedure *Low* should be replaced by

$Low := -Upp(j, x);$

(iii) the second line of the **for** statement in the real procedure *Upp* should read

$temp := temp - x[i] \times x[i];$

After making these corrections, it is possible to obtain results corresponding to a permuted version of the table given in the certification, which should be replaced by the following:

k	$\frac{1}{2}$	2		
true	11.46027375	1.10609686		
s	1	2	1	2
$P = 2$	5.454466	9.361670	1.0368787	1.1184317
$P = 3$	11.838664	12.408983	1.1343568	1.1094294

In addition, since several compilers require specifications, it would be desirable

(i) to change the last specification in the heading of *MULTINT* to read

integer $n, P;$

(ii) to insert the specifications

integer $j;$ array $x;$

in the heading of the real procedures *Low*, *Upp*, and *Funev*.

Some of these additions were necessary in order to ensure correct results with the compiler used for the tests.



Howard and Tashjian—cont'd from page 818

and the invariance of tensor quantities with respect to coordinate transformations, it is possible to reduce the derivations to routine computer operations. As was shown in [3 and 4], this technique can be applied with equal facility to the problem of deriving the equations of motion of a particle in any curvilinear coordinate system. In fact, any equation or system of equations which can be expressed in tensor form is amenable to automatic formulation by the methods described.

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D2	9	RUNGE-KUTTA	5-60(312),4-66(273)	F1	42	INVERSION	4-61(176),11-61(498),
D2	194	ZEROS OF O.D.E. SYSTEM	8-63(441)	F1	42	1-63(38),8-63(445)	
D2	218	KUTTA-MERSON	12-63(737),10-64(585),	F1	50	INVERSE OF HILBERT MATRIX	4-61(179),1-62(50),
D2	218	4-66(273)		F1	50	1-63(38)	
D2		EXTRAPOLATION METHOD	NUM.MATH.V8(10)	F1	51	INVERSE OF PERTURBED MATRIX	4-61(180),7-62(391)
D3		<u>PARTIAL DIFFERENTIAL EQUATIONS</u>		F1	52	INVERSE OF TEST MATRIX	4-61(180),8-61(339),
D3		CONFORMAL MAP-ELLIPSE TO CIRCLE	BIT 1962(243)	F1	52	11-61(498),8-62(438),1-63(39),8-63(446)	
D3		PDE SOLNS.BY INTEGRAL OPERATORS	STANFORD UNIV.-	F1	58	INVERSION-GAUSSIAN ELIMINATION	5-61(236),6-62(347),
D3		APPL.MATH.STAT.REP.NONR 225(37)NO.24		F1	58	8-62(438),12-62(606)	
D3		KERNEL FCN.IN BNDY.VALUE PROBS.	NUM.MATH.V3(209)	F1	66	INVERSION-SORT METHOD	7-61(322),1-62(50),
D3		LINEAR ELLIPTIC BNDY.VAL.PROB.	AUTOMATISIERTE	F1	66	6-62(348)	
D3		BNDY.VALUE PROBS.-INTEGRAL OPRS	NUM.MATH.V7(56)	F1	67	GRAM MATRIX	7-61(322),6-62(348)
D3		BEHANDLUNG ELLIPTISCHER RANDWERTPROBLEME(PUB.1962)		F1	120	INVERSION-GAUSSIAN ELIMINATION	8-62(437),1-63(40),
D4		<u>DIFFERENTIATION</u>		F1	120	8-63(445)	
D4	79	DIFFERENCE EXPRESSION COEFF.	2-62(97),3-63(104)	F1	140	INVERSION	11-62(556),8-63(448)
D4		DIFFN.BY NEVILLES FORMULAS	NUM.MATH.V8(462)	F1	150	INVERSE OF SYMMETRIC MATRIX	2-63(67),7-63(390),
D5		<u>INTEGRAL EQUATIONS</u>		F1	150	3-64(148)	
D5		SYSTEM OF VOLTERRA EQNS.	ZH.VYCH.MAT.MAT.FIZ.-	F1	166	MONTE CARLO INVERSE	4-63(164),9-63(523)
D5		1965(933)		F1	197	MATRIX DIVISION	8-63(443),3-64(148)
E1		<u>INTERPOLATION</u>		F1	230	MATRIX PERMUTATION	6-64(347)
E1	18	RATIONAL INTERP.-CONT.FRACT.	9-60(508),8-62(437)	F1	231	INVERSION-GAUSS.ELIM.-COMP.PIV.	6-64(347),4-65(220)
E1	70	AITKEN INTERPOLATION	11-61(497),7-62(392)	F1	274	HILBERT DERIVED TEST MATRIX	1-66(11)
E1	77	INTERPOLATION,DIFFN.,INTEGRN.	2-62(96),6-62(348),	F1	287	INTEGER MATRIX TRIANGULATION	7-66(513)
E1	77	8-63(446),11-63(663)		F1	298	SQ. RT.OF A POS.DEFINITE MATRIX	3-67(182)
E1	167	CONFLUENT DIVIDED DIFFERENCES	4-63(164),9-63(523)	F1	319	TRIANG FCNRS OF MODIFIED MATRIX	1-68(12)
				F1	325	ADJUST INVERSE OF SYM MATRIX	2-68(118)
				F1		INVERSE-CONFL. VANDERMONDE MTX	NUM.MATH.V5(429)
				F1		EQUIVALENCE OF MATRICES	ICC BULL.-1964(62)
				F1		SYMM.DECCOMP.OF POS.DEF.BAND MTX	NUM.MATH.V7(368)
				F1		SYMM.DECCOMP.OF POS.DEF.MTX.	NUM.MATH.V7(368)
				F1		SYMM.DECCOMP.OF POS.DEF.BAND MTX	COMPUTING V1(77)
				F1		INVERSION-SYMM.POS.DEF.MTX.	COMP.J.V9(321)
				F1		SMITH NORMAL FORM	BIT 1967(163)
				F1		PERMUTATIONS OF ROWS AND COLS.	COMP.J.V10(206)
				F1		ADJUST INVERSE OF SYM MATRIX	COMPUTING V3(76)
				F1		HOUSEHOLDER TRIDIAG OF SYM MTRX	NUM.MATH.V11(184)

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