Subroutine ATEIG

This subroutine computes the eigenvalues of a real upper almost-triangular matrix (Hessenberg form -- see subroutine HSBG) using the double QR iteration of J. G. F. Francis.

1. Mathematical background

a. Definition of the QR iteration

Let A be a real or complex nonsingular matrix of order n. Then a decomposition of A exists of the form

$$A = Q R$$

where Q is unitary and R is upper triangular. If the diagonal elements of R are real and positive, Q is unique. Consider now the sequence of matrices $A^{(p)}$ defined recursively by

$$A^{(o)} = A, \quad A^{(p)} = Q^{(p)} R^{(p)}, \quad A^{(p+1)} = R^{(p)} Q^{(p)} \quad p \geq 0.$$

Note that $A^{(p+1)} = Q^{(p)*} A^{(p)} Q^{(p)}$ for $p \geq 0$; hence it follows that $A^{(p)}$ is similar to A for all p.

Furthermore, if A satisfies certain conditions, it can be proved that $A^{(p)}$ tends to an upper triangular matrix as $p \to \infty$; thus the eigenvalues of A are the diagonal elements of this limit matrix.

b. Convergence

If the moduli of the eigenvalues are distinct, the elements $a_{ij}^{(p)}$ below the main diagonal of $A^{(p)}$ tend to zero, as do $|\lambda_i|^p / |\lambda_j|^p$, the eigenvalues being subscripted so that $|\lambda_i| > |\lambda_{i+1}|$.

Thus, in general, the eigenvalues appear on the main diagonal, starting from the last position, in increasing order of moduli.

So, when the smallest eigenvalue λ_n has been found, we can reduce the order of the matrix by neglecting the last row and column and find λ_{n-1} by the same process, without any special deflation.

Note that the speed of convergence is considerably improved when the origin of the eigenvalues is shifted close to λ_n.

Such a shift, say $s^{(p)}$, can be introduced before an iteration and the opposite one afterwards. Then the iteration can be written as:

$$A^{(p)} - s^{(p)} I = Q^{(p)} R^{(p)}$$

$$A^{(p+1)} = R^{(p)} Q^{(p)} + s^{(p)} I$$

In general, $A_{n,n}^{(p)}$, for p large enough, can provide an efficient value for $s^{(p)}$.

c. Use of the Hessenberg form

The Hessenberg form is preserved under the QR iteration. Thus, a reduction of the initial matrix to the Hessenberg form can give a significant saving of computation in each iteration for the QR decomposition, the lower part of the matrix consisting only of the codiagonal terms.

Before each iteration, the codiagonal terms will be inspected. If some of these are zero, the matrix will be split according to this occurrence, and the iteration will be applied to the lower main submatrix only.

d. The double QR iteration

Let A be a diagonalizable real upper Hessenberg matrix. Such a matrix must be expected to have complex conjugate pairs of eigenvalues. If these pairs are the only eigenvalues of equal modulus, it can be shown that they will appear as the latent roots of main submatrices of order 2. In this case, if a shift is close to one of these roots, it will be complex, and we will have to deal with complex matrices, although the initial one is real. The use of the double QR iteration avoids this inconvenience.

Taking $s^{(p+1)} = \bar{s}^{(p)}$, consider the transformation giving $A^{(p+2)}$ from $A^{(p)}$:

$$A^{(p+2)} = Q^{(p+1)*} Q^{(p)*} A^{(p)} Q^{(p)} Q^{(p+1)}$$

It can be proved that the product $Q^{(p)} Q^{(p+1)}$ derives from the QR decomposition of the matrix $M = (A^{(p)} - s^{(p)} I)(A^{(p)} - s^{(p+1)} I)$, which is real.

In fact, Francis (1961, 1962) showed that only the first column m_1 of M is necessary for determining the transformation which gives $A^{(p+2)}$ from $A^{(p)}$, if they both have the Hessenberg form.

Practically, the first part of the double iteration consists of the application of an initial transformation $N_1^* A^{(p)} N_1$ where N_1 is unitary and such that $N_1^* m_1 = \pm \|m_1\| e_1$. This leads to a matrix which no longer has the Hessenberg form.

Thus, the remaining part of the iteration will involve the application of (n-1) successive transformations, which have the same form as the initial one whose matrices N_i are such that the resulting matrix $A^{(p+2)}$ has the Hessenberg form.

This process can fail when a subdiagonal term of the given matrix is zero. In this case, the matrix can be split, and the iteration is performed on the lower main submatrix only.

In the subroutine, N_i are Householder's matrices.

2. Programming considerations

At each iteration, the latent roots x_1 and x_2 of the lower main submatrix of order 2 are computed. Then, the following situations can occur:

a. The term $a_{n-1,n-2}$ can be taken as zero. Then, x_1 and x_2 are eigenvalues of the original matrix, and the order of the matrix is reduced by 2. IANA(N) and IANA(N-1) are set to 0 and 2 respectively.

b. The term $a_{n,n-1}$ can be taken as zero. In this case, $a_{n,n}$ is an eigenvalue of the original matrix, and the order of the matrix is reduced by 1. IANA(N) is set to 1.

c. One of the last two subdiagonal terms is stable through one iteration. Then the smaller one is considered as zero. The corresponding components of IANA are set to 0, 1, or 2, according to a. or b.

d. The maximum number of iterations is reached. In this case, the smaller of the last two subdiagonal elements is taken as zero. The corresponding components of IANA are set to 0, 1, or 2, according to a. or b.

The user can check the results by inspecting the subdiagonal terms of the matrix on return from the subroutine, according to the vector IANA, in the following way:

If for each IANA(I) containing 1 or 2, $2 \leq I \leq M$,

$$\left|A(I,I-1)\right| \leq 10^{-7} \left(\left|RR(I)\right| + \left|RI(I)\right|\right),$$

then RR(I) and RI(I) were computed with a satisfactory accuracy.

For reference see:

(1) J.G.F. Francis, Computer Journal. October, 1961 4-3, January, 1962 4-4.

(2) J.H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.

```
C
C     ..................................................................
C
C        SUBROUTINE ATEIG
C
C        PURPOSE
C           COMPUTE THE EIGENVALUES OF A REAL ALMOST TRIANGULAR MATRIX
C
C        USAGE
C           CALL ATEIG(M,A,RR,RI,IANA,IA)
C
C        DESCRIPTION OF THE PARAMETERS
C           M      ORDER OF THE MATRIX
C           A      THE INPUT MATRIX, M BY M
C           RR     VECTOR CONTAINING THE REAL PARTS OF THE EIGENVALUES
C                  ON RETURN
C           RI     VECTOR CONTAINING THE IMAGINARY PARTS OF THE EIGEN-
C                  VALUES ON RETURN
C           IANA   VECTOR WHOSE DIMENSION MUST BE GREATER THAN OR EQUAL
C                  TO M, CONTAINING ON RETURN INDICATIONS ABOUT THE WAY
C                  THE EIGENVALUES APPEARED (SEE MATH. DESCRIPTION)
C           IA     SIZE OF THE FIRST DIMENSION ASSIGNED TO THE ARRAY A
C                  IN THE CALLING PROGRAM WHEN THE MATRIX IS IN DOUBLE
C                  SUBSCRIPTED DATA STORAGE MODE.
C                  IA=M WHEN THE MATRIX IS IN SSP VECTOR STORAGE MODE.
C
C        REMARKS
C           THE ORIGINAL MATRIX IS DESTROYED
C           THE DIMENSION OF RR AND RI MUST BE GREATER OR EQUAL TO M
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           QR DOUBLE ITERATION
C
C        REFERENCES
C           J.G.F. FRANCIS - THE QR TRANSFORMATION---THE COMPUTER
C           JOURNAL, VOL. 4, NO. 3, OCTOBER 1961, VOL. 4, NO. 4, JANUARY
C           1962.  J. H. WILKINSON - THE ALGEBRAIC EIGENVALUE PROBLEM -
C           CLARENDON PRESS, OXFORD, 1965.
C
C     ..................................................................
C
      SUBROUTINE ATEIG(M,A,RR,RI,IANA,IA)
      DIMENSION A(1),RR(1),RI(1),PRR(2),PRI(2),IANA(1)
      INTEGER P,P1,Q
C
      E7=1.0E-8
      E6=1.0E-6
      E10=1.0E-10
      DELTA=0.5
      MAXIT=30
C
C        INITIALIZATION
C
      N=M
   20 N1=N-1
      IN=N1*IA
      NN=IN+N
      IF(N1) 30,1300,30
   30 NP=N+1
C
C        ITERATION COUNTER
C
      IT=0
C
C        ROOTS OF THE 2ND ORDER MAIN SUBMATRIX AT THE PREVIOUS
C        ITERATION
C
      DO 40 I=1,2
      PRR(I)=0.0
   40 PRI(I)=0.0
C
C        LAST TWO SUBDIAGONAL ELEMENTS AT THE PREVIOUS ITERATION
C
      PAN=0.0
      PAN1=0.0
C
C        ORIGIN SHIFT
C
      R=0.0
      S=0.0
C
C        ROOTS OF THE LOWER MAIN 2 BY 2 SUBMATRIX
C
      N2=N1-1
      IN1=IN-IA
      NN1=IN1+N
      N1N=IN+N1
      N1N1=IN1+N1
   60 T=A(N1N1)-A(NN)
      U=T*T
      V=4.0*A(N1N)*A(NN1)
      IF(ABS(V)-U*E7) 100,100,65
   65 T=U+V
      IF(ABS(T)-AMAX1(U,ABS(V))*E6) 67,67,68
   67 T=0.0
   68 U=(A(N1N1)+A(NN))/2.0
      V=SQRT(ABS(T))/2.0
      IF(T)140,70,70
   70 IF(U) 80,75,75
   75 RR(N1)=U+V
      RR(N)=U-V
      GO TO 130
   80 RR(N1)=U-V
      RR(N)=U+V
      GO TO 130
  100 IF(T)120,110,110
  110 RR(N1)=A(N1N1)
      RR(N)=A(NN)
      GO TO 130
  120 RR(N1)=A(NN)
      RR(N)=A(N1N1)
  130 RI(N)=0.0
      RI(N1)=0.0
      GO TO 160
  140 RR(N1)=U
      RR(N)=U
      RI(N1)=V
      RI(N)=-V
  160 IF(N2)1280,1280,180
C
C        TESTS OF CONVERGENCE
C
  180 N1N2=N1N1-IA
      RMOD=RR(N1)*RR(N1)+RI(N1)*RI(N1)
      EPS=E10*SQRT(RMOD)
      IF(ABS(A(N1N2))-EPS)1280,1280,240
  240 IF(ABS(A(NN1))-E10*ABS(A(NN))) 1300,1300,250
  250 IF(ABS(PAN1-A(N1N2))-ABS(A(N1N2))*E6) 1240,1240,260
  260 IF(ABS(PAN-A(NN1))-ABS(A(NN1))*E6)1240,1240,300
  300 IF(IT-MAXIT) 320,1240,1240
C
C        COMPUTE THE SHIFT
C
  320 J=1
      DO 360 I=1,2
      K=NP-I
      IF(ABS(RR(K)-PRR(I))+ABS(RI(K)-PRI(I))-DELTA*(ABS(RR(K))
     1   +ABS(RI(K)))) 340,360,360
  340 J=J+I
  360 CONTINUE
      GO TO (440,460,460,480),J
  440 R=0.0
      S=0.0
      GO TO 500
  460 J=N+2-J
      R=RR(J)*RR(J)
      S=RR(J)+RR(J)
      GO TO 500
  480 R=RR(N)*RR(N1)-RI(N)*RI(N1)
      S=RR(N)+RR(N1)
C
C        SAVE THE LAST TWO SUBDIAGONAL TERMS AND THE ROOTS OF THE
C        SUBMATRIX BEFORE ITERATION
C
  500 PAN=A(NN1)
      PAN1=A(N1N2)
      DO 520 I=1,2
      K=NP-I
      PRR(I)=RR(K)
  520 PRI(I)=RI(K)
C
C        SEARCH FOR A PARTITION OF THE MATRIX, DEFINED BY P AND Q
C
      P=N2
      IF (N-3)600,600,525
  525 IPI=N1N2
      DO 580 J=2,N2
      IPI=IPI-IA-1
      IF(ABS(A(IPI))-EPS) 600,600,530
```

```
  530 IPIP=IPI+IA
      IPIP2=IPIP+IA
      D=A(IPIP)*(A(IPIP)-S)+A(IPIP2)*A(IPIP+1)+R
      IF(D)540,560,540
  540 IF(ABS(A(IPI))*(ABS(A(IPIP+1))+ABS(A(IPIP)+A(IPIP2+1)-S)+ABS(A(IPIP2+2)
     1 )) -ABS(D)*EPS) 620,620,560
  560 P=N1-J
  580 CONTINUE
  600 Q=P
      GO TO 680
  620 P1=P-1
      Q=P1
      IF (P1-1) 680,680,650
  650 DO 660 I=2, P1
      IPI=IPI-IA-1
      IF(ABS(A(IPI))-EPS)680,680,660
  660 Q=Q-1
C
C        QR DOUBLE ITERATION
C
  680 II=(P-1)*IA+P
      DO 1220 I=P,N1
      II1=II-IA
      IIP=II+IA
      IF(I-P)720,700,720
  700 IPI=II+1
      IPIP=IIP+1
C
C        INITIALIZATION OF THE TRANSFORMATION
C
      G1=A(II)*(A(II)-S)+A(IIP)*A(IPI)+R
      G2=A(IPI)*(A(IPIP)+A(II)-S)
      G3=A(IPI)*A(IPIP+1)
      A(IPI+1)=0.0
      GO TO 780
  720 G1=A(II1)
      G2=A(II1+1)
      IF(I-N2)740,740,760
  740 G3=A(II1+2)
      GO TO 780
  760 G3=0.0
  780 CAP=SQRT(G1*G1+G2*G2+G3*G3)
      IF(CAP)800,860,800
  800 IF(G1)820,840,840
  820 CAP=-CAP
  840 T=G1+CAP
      PSI1=G2/T
      PSI2=G3/T
      ALPHA=2.0/(1.0+PSI1*PSI1+PSI2*PSI2)
      GO TO 880
  860 ALPHA=2.0
      PSI1=0.0
      PSI2=0.0
  880 IF(I-Q)900,960,900
  900 IF(I-P)920,940,920
  920 A(II1)=-CAP
      GO TO 960
  940 A(II1)=-A(II1)
C
C        ROW OPERATION
C
  960 IJ=II
      DO 1040 J=I,N
      T=PSI1*A(IJ+1)
      IF(I-N1)980,1000,1000
  980 IP2J=IJ+2
      T=T+PSI2*A(IP2J)
 1000 ETA=ALPHA*(T+A(IJ))
      A(IJ)=A(IJ)-ETA
      A(IJ+1)=A(IJ+1)-PSI1*ETA
      IF(I-N1)1020,1040,1040
 1020 A(IP2J)=A(IP2J)-PSI2*ETA
 1040 IJ=IJ+IA
C
C        COLUMN OPERATION
C
      IF(I-N1)1080,1060,1060
 1060 K=N
      GO TO 1100
 1080 K=I+2
 1100 IP=IIP-I
      DO 1180 J=Q,K
      JIP=IP+J
      JI=JIP-IA
      T=PSI1*A(JIP)
      IF(I-N1)1120,1140,1140
 1120 JIP2=JIP+IA
      T=T+PSI2*A(JIP2)
 1140 ETA=ALPHA*(T+A(JI))
      A(JI)=A(JI)-ETA
      A(JIP)=A(JIP)-ETA*PSI1
      IF(I-N1)1160,1180,1180
 1160 A(JIP2)=A(JIP2)-ETA*PSI2
 1180 CONTINUE
      IF(I-N2)1200,1220,1220
 1200 JI=II+3
      JIP=JI+IA
      JIP2=JIP+IA
      ETA=ALPHA*PSI2*A(JIP2)
      A(JI)=-ETA
      A(JIP)=-ETA*PSI1
      A(JIP2)=A(JIP2)-ETA*PSI2
 1220 II=IIP+1
      IT=IT+1
      GO TO 60
C
C        END OF ITERATION
C
 1240 IF(ABS(A(NN1))-ABS(A(N1N2))) 1300,1280,1280
C
C        TWO EIGENVALUES HAVE BEEN FOUND
C
 1280 IANA(N)=0
      IANA(N1)=2
      N=N2
      IF(N2)1400,1400,20
C
C        ONE EIGENVALUE HAS BEEN FOUND
C
 1300 RR(N)=A(NN)
      RI(N)=0.0
      IANA(N)=1
      IF(N1)1400,1400,1320
 1320 N=N1
      GO TO 20
 1400 RETURN
      END
```

Subroutine HSBG

This subroutine reduces an n by n real matrix A by a similarity transformation to upper almost-triangular (Hessenberg) form. Each row is reduced in turn, starting from the last one, by applying a suitable right elimination matrix, and similarity is achieved by also applying the left inverse transformation. Thus the eigenvalues of A are preserved.

1. Mathematical background

Let $A^{(p)}$ denote the matrix obtained from $A^{(o)} = A$ after reducing rows $n, n-1, \ldots, n-p+1$. The similarity which transforms $A^{(p)}$ to $A^{(p+1)}$ is as follows:

a. First we determine a pivot element $a^{(p)}_{n-p,k}$ whose column subscript k is such that

$$\left| a^{(p)}_{n-p,k} \right| = \max_i \left| a^{(p)}_{n-p,i} \right| , i = 1, 2, \ldots, n-p-1$$

b. If the pivot element $a^{(p)}_{n-p,k} = 0$, no transformations are necessary; that is, the (p+1)th similarity is the identity transformation. Otherwise, if it is necessary ($k \neq n-p-1$), we interchange the kth and (n-p-1)th columns so that the pivot element is in the subdiagonal position. The same interchange is applied to the rows of $A^{(p)}$. The resulting matrix is similar to $A^{(p)}$, and, to ease the notation, we denote it by $A^{(p)}$.

c. Define multipliers

$$b_j^{(p)} = a^{(p)}_{n-p,j} / a^{(p)}_{n-p,n-p-1} \qquad j=1, 2, \ldots, n-p-2$$

Then the (p+1)th similarity is given by the following.

Right elimination:

$$\bar{a}_{ij}^{(p)} = a_{ij}^{(p)} - b_j^{(p)} \; a^{(p)}_{i,n-p-1}$$

$i=1, 2, \ldots, n-p$
$j=1, 2, \ldots, n-p-2$

$$\bar{a}_{ij}^{(p)} = a_{ij}^{(p)} \qquad \text{other indices}$$

Left inverse transformation:

$$a^{(p+1)}_{n-p-1,j} = \bar{a}^{(p)}_{n-p-1,j} + \sum_{i=1}^{n-p-2} b_i^{(p)} \, \bar{a}_{ij}^{(p)}$$

$$a_{ij}^{(p+1)} = \bar{a}_{ij}^{(p)} \qquad i \neq n-p-1$$

Finally, $A^{(n-2)}$ will have the upper almost-triangular form.

For reference see J. H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.

```
C
C     ..................................................................
C
C        SUBROUTINE HSBG
C
C        PURPOSE
C           TO REDUCE A REAL MATRIX INTO UPPER ALMOST TRIANGULAR FORM
C
C        USAGE
C           CALL HSBG(N,A,IA)
C
C        DESCRIPTION OF THE PARAMETERS
C           N      ORDER OF THE MATRIX
C           A      THE INPUT MATRIX, N BY N
C           IA     SIZE OF THE FIRST DIMENSION ASSIGNED TO THE ARRAY
C                  A IN THE CALLING PROGRAM WHEN THE MATRIX IS IN
C                  DOUBLE SUBSCRIPTED DATA STORAGE MODE.  IA=N WHEN
C                  THE MATRIX IS IN SSP VECTOR STORAGE MODE.
C
C        REMARKS
C           THE HESSENBERG FORM REPLACES THE ORIGINAL MATRIX IN THE
C           ARRAY A.
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           SIMILARITY TRANSFORMATIONS USING ELEMENTARY ELIMINATION
C           MATRICES, WITH PARTIAL PIVOTING.
C
C        REFERENCES
C           J.H. WILKINSON - THE ALGEBRAIC EIGENVALUE PROBLEM -
C           CLARENDON PRESS, OXFORD, 1965.
C
C     ..................................................................
C
      SUBROUTINE HSBG(N,A,IA)
      DIMENSION A(1)
      DOUBLE PRECISION S
      L=N
      NIA=L*IA
      LIA=NIA-IA
C
C        L IS THE ROW INDEX OF THE ELIMINATION
C
   20 IF(L-3) 360,40,40
   40 LIA=LIA-IA
      L1=L-1
      L2=L1-1
C
C        SEARCH FOR THE PIVOTAL ELEMENT IN THE LTH ROW
C
      ISUB=LIA+L
      IPIV=ISUB-IA
      PIV=ABS(A(IPIV))
      IF(L-3) 90,90,50
   50 M=IPIV-IA
      DO 80 I=L,M,IA
      T=ABS(A(I))
      IF(T-PIV) 80,80,60
   60 IPIV=I
      PIV=T
   80 CONTINUE
   90 IF(PIV) 100,320,100
  100 IF(PIV-ABS(A(ISUB))) 180,180,120
C
C        INTERCHANGE THE COLUMNS
C
  120 M=IPIV-L
      DO 140 I=1,L
      J=M+I
      T=A(J)
      K=LIA+I
      A(J)=A(K)
  140 A(K)=T
C
C        INTERCHANGE THE ROWS
C
      M=L2-M/IA
      DO 160 I=L1,NIA,IA
      T=A(I)
      J=I-M
      A(I)=A(J)
  160 A(J)=T
C
C        TERMS OF THE ELEMENTARY TRANSFORMATION
C
  180 DO 200 I=L,LIA,IA
  200 A(I)=A(I)/A(ISUB)
C
C        RIGHT TRANSFORMATION
C
      J=-IA
      DO 240 I=1,L2
      J=J+IA
      LJ=L+J
      DO 220 K=1,L1
      KJ=K+J
      KL=K+LIA
  220 A(KJ)=A(KJ)-A(LJ)*A(KL)
  240 CONTINUE
C
C        LEFT TRANSFORMATION
C
      K=-IA
      DO 300 I=1,N
      K=K+IA
      LK=K+L1
      S=A(LK)
      LJ=L-IA
      DO 280 J=1,L2
      JK=K+J
      LJ=LJ+IA
  280 S=S+A(LJ)*A(JK)*1.0D0
  300 A(LK)=S
C
C        SET THE LOWER PART OF THE MATRIX TO ZERO
C
      DO 310 I=L,LIA,IA
  310 A(I)=0.0
  320 L=L1
      GO TO 20
  360 RETURN
      END
```