## Chapter B11. Eigensystems

```
SUBROUTINE jacobi(a,d,v,nrot)
USE nrtype; USE nrutil, ONLY : assert_eq,get_diag,nrerror,unit_matrix,&
    upper_triangle
IMPLICIT NONE
INTEGER(I4B), INTENT(OUT) :: nrot
REAL(SP), DIMENSION(:), INTENT(OUT) :: d
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
REAL(SP), DIMENSION(:,:), INTENT(OUT) :: v
    Computes all eigenvalues and eigenvectors of a real symmetric N}\timesN\mathrm{ matrix a. On output,
    elements of a above the diagonal are destroyed. d is a vector of length N that returns the
    eigenvalues of a. v is an N}N\timesN\mathrm{ matrix whose columns contain, on output, the normalized
    eigenvectors of a. nrot returns the number of Jacobi rotations that were required.
INTEGER(I4B) :: i,ip,iq,n
REAL(SP) :: c,g,h,s,sm,t,tau,theta,tresh
REAL(SP), DIMENSION(size(d)) :: b,z
n=assert_eq((/size(a,1),size(a,2),size(d),size(v,1),size(v,2)/),'jacobi')
call unit_matrix(v(:,:)) Initialize v to the identity matrix.
b}(:)=get_diag(a(:,:)) Initialize b and d to the diagonal o
d(:)=b(:)
z(:)=0.0 This vector will accumulate terms of
nrot=0
do i=1,50
    sm=sum(abs(a),mask=upper_triangle(n,n)) Sum off-diagonal elements.
    if (sm == 0.0) RETURN
    The normal return, which relies on quadratic convergence to machine underflow.
    tresh=merge(0.2_sp*sm/n**2,0.0_sp, i < 4 )
        On the first three sweeps, we will rotate only if tresh exceeded.
        do ip=1,n-1
            do iq=ip+1,n
                g=100.0_sp*abs(a(ip,iq))
                    After four sweeps, skip the rotation if the off-diagonal element is small.
            if ((i > 4) .and. (abs(d(ip))+g == abs(d(ip))) &
                    .and. (abs(d(iq))+g == abs(d(iq)))) then
                    a(ip,iq)=0.0
            else if (abs(a(ip,iq)) > tresh) then
                h=d(iq)-d(ip)
                if (abs(h)+g== abs(h)) then
                        t=a(ip,iq)/h}\quadt=1/(20
                else
                            theta=0.5_sp*h/a(ip,iq) Equation (11.1.10).
                            t=1.0_sp/(abs(theta)+sqrt(1.0_sp+theta**2))
                    if (theta < 0.0) t=-t
                end if
                    c=1.0_sp/sqrt (1+t**2)
                    s=t*c
                    tau=s/(1.0_sp+c)
                    h=t*a(ip,iq)
                    z(ip)=z(ip)-h
                    z(iq)=z(iq)+h
                    d(ip)=d(ip)-h
                    d(iq)=d(iq)+h
                    a(ip,iq)=0.0
```

```
                    call jrotate(a(1:ip-1,ip),a(1:ip-1,iq))
                            Case of rotations 1 \leq < < p
                            call jrotate(a(ip,ip+1:iq-1),a(ip+1:iq-1,iq))
                            Case of rotations p<j<q.
                            call jrotate(a(ip,iq+1:n),a(iq,iq+1:n))
                            Case of rotations q<j\leqn.
                    call jrotate(v(:,ip),v(:,iq))
                    nrot=nrot+1
                end if
            end do
    end do
    b(:)=b(:)+z(:)
        d(:)=b(:) Update d with the sum of ta mq,
        z(:)=0.0 and reinitialize z
end do
call nrerror('too many iterations in jacobi')
CONTAINS
SUBROUTINE jrotate(a1,a2)
REAL(SP), DIMENSION(:), INTENT(INOUT) :: a1,a2
REAL(SP), DIMENSION(size(a1)) :: wk1
wk1(:)=a1(:)
a1(:)=a1(:)-s*(a2(:)+a1(:)*tau)
a2(:)=a2(:)+s*(wk1(:)-a2(:)*tau)
END SUBROUTINE jrotate
END SUBROUTINE jacobi
```

inAs discussed in Volume 1, jacobi is generally not competitive with tqli in terms of efficiency. However, jacobi can be parallelized whereas tqli uses an intrinsically serial algorithm. The version of jacobi implemented here is likely to be adequate for a small-scale parallel (SSP) machine, but is probably still not competitive with tqli. For a massively multiprocessor (MMP) machine, the order of the rotations needs to be chosen in a more complicated pattern than here so that the rotations can be executed in parallel. In this case the Jacobi algorithm may well turn out to be the method of choice. Parallel replacements for tqli based on a divide and conquer algorithm have also been proposed. See the discussion after tqli on p. 1229.
call unit_matrix...b(:)=get_diag... These routines in nrutil both require access to the diagonal of a matrix, an operation that is not conveniently provided for in Fortran 90. We have split them off into nrutil in case your compiler provides parallel library routines so you can replace our standard versions.
sm=sum (abs (a), mask=upper_triangle (n, n)) The upper_trianglefunction in nrutil returns an upper triangular logical mask. As used here, the mask is true everywhere in the upper triangle of an $n \times n$ matrix, excluding the diagonal. An optional integer argument extra allows additional diagonals to be set to true. With extra=1 the upper triangle including the diagonal would be true. By using the mask, we can conveniently sum over the desired matrix elements in parallel.

SUBROUTINE jrotate(a1,a2) This internal subroutine also uses the values of s and tau from the calling subroutine jacobi. Variables in the calling routine are visible to an internal subprogram, but you should be circumspect in making use of this fact. It is easy to overwrite a value in the calling program inadvertently, and it is
often difficult to figure out the logic of an internal routine if not all its variables are declared explicitly. However, jrotate is so simple that there is no danger here.

```
SUBROUTINE eigsrt(d,v)
USE nrtype; USE nrutil, ONLY : assert_eq,imaxloc,swap
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: d
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: v
    correspondingly. The method is straight insertion.
INTEGER(I4B) :: i,j,n
n=assert_eq(size(d),size(v,1),size(v,2),'eigsrt')
do i=1,n-1
    j=imaxloc(d(i:n))+i-1
    if (j /= i) then
        call swap(d(i),d(j))
        call swap(v(:,i),v(:,j))
    end if
end do
END SUBROUTINE eigsrt
```

    Given the eigenvalues d and eigenvectors v as output from jacobi (§11.1) or tqli (§11.3),
    this routine sorts the eigenvalues into descending order, and rearranges the columns of v
    90 j=imaxloc... See discussion of imaxloc on p. 1017.
call swap... See discussion of overloaded versions of swap after amoeba on p. 1210.

SUBROUTINE tred2(a,d,e, novectors)
USE nrtype; USE nrutil, ONLY : assert_eq, outerprod
IMPLICIT NONE
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
REAL(SP), DIMENSION(:), INTENT(OUT) :: d,e
LOGICAL(LGT), OPTIONAL, INTENT(IN) : : novectors
Householder reduction of a real, symmetric, $N \times N$ matrix a. On output, a is replaced by the orthogonal matrix $\mathbf{Q}$ effecting the transformation. $d$ returns the diagonal elements of the tridiagonal matrix, and e the off-diagonal elements, with $e(1)=0$. If the optional argument novectors is present, only eigenvalues are to be found subsequently, in which case a contains no useful information on output.
INTEGER(I4B) : : i,j,l,n
REAL (SP) : : f,g,h,hh,scale
REAL(SP), DIMENSION(size(a,1)) :: gg
LOGICAL(LGT), SAVE : : yesvec=.true.
$\mathrm{n}=$ assert_eq(size $(\mathrm{a}, 1)$, size $(\mathrm{a}, 2)$, size (d), size (e), 'tred2')
if (present(novectors)) yesvec=.not. novectors
do $i=n, 2,-1$
$1=\mathrm{i}-1$
$\mathrm{h}=0.0$
if (l > 1) then
scale $=\operatorname{sum}(\operatorname{abs}(a(i, 1: 1)))$
if (scale $==0.0$ ) then Skip transformation.
$e(i)=a(i, l)$
else
a(i,1:1)=a(i,1:1)/scale Use scaled $a$ 's for transformation. $\mathrm{h}=\operatorname{sum}(\mathrm{a}(\mathrm{i}, 1: 1) * * 2) \quad$ Form $\sigma$ in h .

```
            f=a(i,l)
            g=-sign(sqrt(h),f)
            e(i)=scale*g
            h=h-f*g Now h is equation (11.2.4).
            a(i,l)=f-g
                    Store \mathbf{u}}\mathrm{ in the ith row of a.
            a(1.1,1)=a(1,1.1)/h
                    u/H in ith column of a
            do j=1,l Store elements of p in temporarily
                e(j)=(dot_product(a(j,1:j),a(i,1:j)) & unused elements of e.
                +dot_product(a(j+1:l,j),a(i,j+1:l)))/h
            end do
            f=dot_product(e(1:l),a(i,1:1))
            hh=f/(h+h)
                    Form K, equation (11.2.11).
            e(1:1)=e(1:1)-hh*a(i,1:l)
                    Form q}\mathrm{ and store in e overwriting p.
                do j=1,1 Reduce a, equation (11.2.13).
                a(j,1:j)=a(j,1:j)-a(i,j)*e(1:j)-e(j)*a(i,1:j)
            end do
        end if
    else
        e(i)=a(i,l)
    end if
    d(i)=h
end do
if (yesvec) d(1)=0.0
e(1)=0.0
do i=1,n Begin accumulation of transforma-
    if (yesvec) then
        l=i-1
        if (d(i) /= 0.0) then
            This block skipped when i=1. Use u and \mathbf{u}/H\mathrm{ stored in a to form P}\mathbf{P}\mathrm{ .}
            gg(1:1)=matmul(a(i,1:l),a(1:l,1:1))
                a(1:1,1:1)=a(1:1,1:1)-outerprod(a(1:l,i),gg(1:1))
        end if
        d(i)=a(i,i)
        a(i,i)=1.0 Reset row and column of a to iden-
        a(i,1:1)=0.0 tity matrix for next iteration.
        a(1:1,i)=0.0
    else
        d(i)=a(i,i)
    end if
end do
END SUBROUTINE tred2 eset row and column of a to ide
tity matrix for next iteration.
egin accumulation of transformaif (yesvec) then tion matrices.
\[
\text { if }(d(i) /=0.0) \text { then }
\]
This block skipped when \(i=1\). Use \(\mathbf{u}\) and \(\mathbf{u} / H\) stored in a to form \(\mathbf{P} \cdot \mathbf{Q}\). \(a(1: 1,1: 1)=a(1: 1,1: 1)\)-outerprod(a(1:1,i), gg(1:1))
end if
(i)=a(i,i)
\(a(i, i)=1.0\)
\(a(i, 1: l)=0.0\)
else
if
END SUBROUTINE tred2
```

This routine gives a nice example of the usefulness of optional arguments. The routine is written under the assumption that usually you will want to find both eigenvalues and eigenvectors. In this case you just supply the arguments $a, d$, and e. If, however, you want only eigenvalues, you supply the additional logical argument novectors with the value .true.. The routine then skips the unnecessary computations. Supplying novectors with the value .false. has the same effect as omitting it.

- $\overline{90}$-
$\S 11.2$. d is a vector of length $N$. On input, its elements are the diagonal elements of the tridiagonal matrix. On output, it returns the eigenvalues. The vector e inputs the subdiagonal elements of the tridiagonal matrix, with e(1) arbitrary. On output e is destroyed. When finding only the eigenvalues, the optional argument $\mathbf{z}$ is omitted. If the eigenvectors of a tridiagonal matrix are desired, the $N \times N$ matrix $\mathbf{z}$ is input as the identity matrix. If the eigenvectors of a matrix that has been reduced by tred2 are required, then $z$ is input as the matrix output by tred2. In either case, the $k$ th column of $z$ returns the normalized eigenvector corresponding to $\mathrm{d}(k)$.
INTEGER(I4B) : : i,iter, $1, m, n$, ndum
REAL(SP) : : b, c, dd,f,g,p,r,s
REAL(SP), DIMENSION(size(e)) :: ff
n=assert_eq(size(d), size(e),'tqli: n')
if (present(z)) ndum=assert_eq(n,size( $z, 1$ ),size( $z, 2$ ),'tqli: ndum')
$e(:)=\operatorname{eoshift}(e(:), 1) \quad$ Convenient to renumber the elements of
do $l=1, n$ e.
iter=0
iterate: do
do $\mathrm{m}=\mathrm{l}, \mathrm{n}-1 \quad$ Look for a single small subdiagonal ele$d d=\operatorname{abs}(d(m))+\operatorname{abs}(d(m+1))$ ment to split the matrix. if (abs(e(m))+dd == dd) exit
end do
if (m == l) exit iterate
if (iter == 30) call nrerror('too many iterations in tqli')
iter=iter+1
$\mathrm{g}=(\mathrm{d}(1+1)-\mathrm{d}(1)) /\left(2.0 \_\right.$sp*e(l)) Form shift.
r=pythag (g,1.0_sp)
$\mathrm{g}=\mathrm{d}(\mathrm{m})-\mathrm{d}(\mathrm{l})+\mathrm{e}(\mathrm{l}) /(\mathrm{g}+\operatorname{sign}(\mathrm{r}, \mathrm{g})) \quad$ This is $d_{m}-k_{s}$.
$\mathrm{s}=1.0$
$\mathrm{c}=1.0$
$\mathrm{p}=0.0$
do $\mathrm{i}=\mathrm{m}-1,1,-1 \quad$ A plane rotation as in the original $Q L$,
$\mathrm{f}=\mathrm{s} * \mathrm{e}$ (i) followed by Givens rotations to re-
$\mathrm{b}=\mathrm{c} * \mathrm{e}$ (i) store tridiagonal form.
r=pythag (f,g)
$e(i+1)=r$
if ( $\mathrm{r}==0.0$ ) then Recover from underflow.
$d(i+1)=d(i+1)-p$
e(m)=0.0
cycle iterate
end if
$\mathrm{s}=\mathrm{f} / \mathrm{r}$
$\mathrm{c}=\mathrm{g} / \mathrm{r}$
$\mathrm{g}=\mathrm{d}(\mathrm{i}+1)-\mathrm{p}$
$r=(\mathrm{d}(\mathrm{i})-\mathrm{g}) * \mathrm{~s}+2.0 \_\mathrm{sp} * \mathrm{c} * \mathrm{~b}$
$\mathrm{p}=\mathrm{s} * \mathrm{r}$
$\mathrm{d}(\mathrm{i}+1)=\mathrm{g}+\mathrm{p}$
$\mathrm{g}=\mathrm{c} * \mathrm{r}-\mathrm{b}$
if (present ( $z$ ) ) then Form eigenvectors.
$\mathrm{ff}(1: n)=\mathrm{z}(1: \mathrm{n}, \mathrm{i}+1)$
$z(1: n, i+1)=s * z(1: n, i)+c * f f(1: n)$
$z(1: n, i)=c * z(1: n, i)-s * f f(1: n)$
end if
end do
$d(1)=d(1)-p$
$e(1)=g$
$e(m)=0.0$
end do iterate
end do
END SUBROUTINE tqli
the routine tqli is intrinsically serial. A parallel replacement based on a divide and conquer algorithm has been proposed $[1,2]$. The idea is to split the tridiagonal matrix recursively into two tridiagonal matrices of
half the size plus a correction. Given the eigensystems of the two smaller tridiagonal matrices, it is possible to join them together and add in the effect of the correction. When some small size of tridiagonal matrix is reached during the recursive splitting, its eigensystem is found directly with a routine like tqli. Each of these small problems is independent and can be assigned to an independent processor. The procedures for sewing together can also be done independently. For very large matrices, this algorithm can be an order of magnitude faster than tqli even on a serial machine, and no worse than a factor of 2 or 3 slower, depending on the matrix. Unfortunately the parallelism is not well expressed in Fortran 90. Also, the sewing together requires quite involved coding. For an implementation see the LAPACK routine SSTEDC. Another parallel strategy for eigensystems uses inverse iteration, where each eigenvalue and eigenvector can be found independently [3].


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routine uses $z$ as an optional argument that is required only if eigenvectors are being found as well as eigenvalues.
iterate: do See discussion of named do loops after simplx on p. 1219.

```
SUBROUTINE balanc(a)
USE nrtype; USE nrutil, ONLY : assert_eq
IMPLICIT NONE
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
REAL(SP), PARAMETER :: RADX=radix(a),SQRADX=RADX**2
    Given an N}\timesN\mathrm{ matrix a, this routine replaces it by a balanced matrix with identical
    eigenvalues. A symmetric matrix is already balanced and is unaffected by this procedure
    The parameter RADX is the machine's floating-point radix.
INTEGER(I4B) :: i,last,ndum
REAL(SP) :: c,f,g,r,s
ndum=assert_eq(size(a,1),size(a,2),'balanc')
do
    last=1
    do i=1,size(a,1)
        Calculate row and column norms.
        c=sum(abs(a(:,i)))-a(i,i)
        r=sum(abs(a(i,:)))-a(i,i)
        if (c /= 0.0 .and. r /= 0.0) then If both are nonzero,
                g=r/RADX
            f=1.0
            s=c+r
            do
                if (c >= g) exit
                f=f*RADX
                    c=c*SQRADX
            end do
            g=r*RADX
            do
                if (c <= g) exit
                    f=f/RADX
                    c=c/SQRADX
            end do
            if ((c+r)/f < 0.95_sp*s) then
                    last=0
                    g=1.0_sp/f
                    a(i,:)=a(i,:)*g Apply similarity transformation.
                    a(:,i)=a(:,i)*f
            end if
        end if
```

```
    end do
    if (last /= 0) exit
end do
```

END SUBROUTINE balanc

$\overline{90}$REAL (SP), PARAMETER : : RADX=radix (a)... Fortran 90 provides a nice collection of numeric inquiry intrinsic functions. Here we find the machine's floating-point radix. Note that only the type of the argument a affects the returned function value.

```
SUBROUTINE elmhes(a)
USE nrtype; USE nrutil, ONLY : assert_eq,imaxloc,outerprod,swap
IMPLICIT NONE
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    Reduction to Hessenberg form by the elimination method. The real, nonsymmetric, N\timesN
    matrix a is replaced by an upper Hessenberg matrix with identical eigenvalues. Recom-
    mended, but not required, is that this routine be preceded by balanc. On output, the
    Hessenberg matrix is in elements a(i,j) with i\leqj+1. Elements with i>j+1 are to be
    thought of as zero, but are returned with random values.
INTEGER(I4B) :: i,m,n
REAL(SP) :: x
REAL(SP), DIMENSION(size(a,1)) :: y
n=assert_eq(size(a,1),size(a,2),'elmhes')
do m=2,n-1 m is called r+1 in the text.
    i=imaxloc(abs(a(m:n,m-1)))+m-1 Find the pivot.
    x=a(i,m-1)
    if (i /= m) then Interchange rows and columns.
        call swap(a(i,m-1:n),a(m,m-1:n))
        call swap(a(:,i),a(:,m))
    end if
    if (x /= 0.0) then Carry out the elimination.
        y(m+1:n)=a(m+1:n,m-1)/x
        a(m+1:n,m-1)=y(m+1:n)
        a(m+1:n,m:n)=a(m+1:n,m:n)-outerprod}(\textrm{y}(\textrm{m}+1:\textrm{n}),\textrm{a}(\textrm{m},\textrm{m}:\textrm{n})
        a(:,m)=a(:,m)+matmul (a(:,m+1:n),y(m+1:n))
    end if
end do
END SUBROUTINE elmhes
```


$y(m+1: n)=\ldots \quad$ If the four lines of code starting here were all coded for a serial machine in a single do-loop starting with do $i=m+1, n$ (see Volume 1), it would pay to test whether y was zero because the next three lines could then be skipped for that value of $i$. There is no convenient way to do this here, even with a where, since the shape of the arrays on each of the three lines is different. For a parallel machine it is probably best just to do a few unnecessary multiplies and skip the test for zero values of $y$.

```
SUBROUTINE hqr(a,wr,wi)
USE nrtype; USE nrutil, ONLY : assert_eq,diagadd,nrerror,upper_triangle
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(OUT) :: wr,wi
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    Finds all eigenvalues of an N}\timesN\mathrm{ upper Hessenberg matrix a. On input a can be exactly
    as output from elmhes §11.5; on output it is destroyed. The real and imaginary parts of
    the N eigenvalues are returned in wr and wi, respectively.
INTEGER(I4B) :: i,its,k,l,m,n,nn,mnnk
REAL(SP) :: anorm,p,q,r,s,t,u,v,w,x,y,z
REAL(SP), DIMENSION(size(a,1)) :: pp
n=assert_eq(size(a,1),size(a,2),size(wr),size(wi),'hqr')
anorm=sum(abs(a),mask=upper_triangle(n,n,extra=2))
    Compute matrix norm for possible use in locating single small subdiagonal element.
nn=n
t=0.0
do
    if (nn < 1) exit
    its=0
    iterate: do
        do l=nn,2,-1
            s=abs(a(l-1,l-1))+abs(a(l, l))
                if (s == 0.0) s=anorm
                if (abs(a(l,l-1))+s == s) exit
        end do
        x=a(nn,nn)
        if (l == nn) then One root found.
            wr}(nn)=x+
            wi(nn)=0.0
            nn=nn-1
            exit iterate Go back for next eigenvalue.
        end if
        y=a(nn-1,nn-1)
        w=a(nn,nn-1)*a(nn-1,nn)
        if (l == nn-1) then Two roots found ...
            p=0.5_sp*(y-x)
            q=p**2+w
            z=sqrt(abs(q))
            x=x+t
            if (q >= 0.0) then ...a real pair ...
                    z=p+sign(z,p)
                    wr}(nn)=x+
                    wr}(nn-1)=wr(nn
                    if (z/= 0.0) wr (nn)=x-w/z
                    wi (nn)=0.0
                wi}(nn-1)=0.
            else ...a complex pair.
                wr(nn)=x+p
                    wr}(nn-1)=wr (nn
                    wi (nn)=z
                wi}(nn-1)=-
            end if
            nn=nn-2
            exit iterate Go back for next eigenvalue.
        end if
            No roots found. Continue iteration.
        if (its == 30) call nrerror('too many iterations in hqr')
        if (its == 10.or. its == 20) then Form exceptional shift.
            t=t+x
            call diagadd(a(1:nn,1:nn),-x)
            s=abs(a(nn,nn-1))+abs(a(nn-1,nn-2))
            x=0.75_sp*s
            y=x
            w=-0.4375_sp*s**2
```

```
end if
its=its+1
do m=nn-2,1,-1 Form shift and then look for 2 consecu-
    z=a(m,m) tive small subdiagonal elements.
    r=x-z
    s=y-z
    p=(r*s-w)/a(m+1,m)+a(m,m+1) Equation (11.6.23).
    q=a(m+1,m+1)-z-r-s
    r=a(m+2,m+1) , _
    s=abs(p)+abs(q)+abs(r) Scale to prevent overflow or underflow.
    p=p/s
    q=q/s
    r=r/s
    if (m == l) exit
    u}=\textrm{abs}(\textrm{a}(\textrm{m},\textrm{m}-1))*(\textrm{abs}(\textrm{q})+\textrm{abs}(\textrm{r})
    v=abs(p)*(abs(a(m-1,m-1))+abs(z)+abs}(\textrm{a}(\textrm{m}+1,\textrm{m}+1))
    if (u+v == v) exit Equation (11.6.26).
end do
do i=m+2,nn
    a(i,i-2)=0.0
    if (i /= m+2) a(i,i-3)=0.0
end do
do k=m,nn-1 Double QR step on rows l to nn and
    if (k/= m) then
    columns m to nn.
        p=a(k,k-1)
        Begin setup of Householder vector.
        q=a(k+1,k-1)
        r=0.0
        if (k /= nn-1) r=a(k+2,k-1)
        x=abs(p)+abs(q)+abs(r)
        if (x /= 0.0) then
            p=p/x Scale to prevent overflow or underflow.
            q=q/x
            r=r/x
        end if
    end if
    s=sign(sqrt(p**2+q**2+r**2),p)
    if (s /= 0.0) then
            if (k == m) then
                if (l /= m) a(k,k-1)=-a(k,k-1)
            else
                a(k,k-1)=-s*x
            end if
            p=p+s Equations (11.6.24).
            x=p/s
            y=q/s
            z=r/s
            q=q/p
            r=r/p Ready for row modification.
            pp(k:nn)=a(k,k:nn)+q*a(k+1,k:nn)
            if (k /= nn-1) then
                    pp(k:nn)=pp(k:nn)+r*a(k+2,k:nn)
                    a(k+2,k:nn)=a(k+2,k:nn)-pp(k:nn)*z
            end if
            a(k+1,k:nn)=a(k+1,k:nn)-pp(k:nn)*y
            a(k,k:nn)=a(k,k:nn)-pp(k:nn)*x
            mnnk=min(nn,k+3) Column modification.
            pp(l:mnnk)=x*a(l:mnnk,k)+y*a(l:mnnk,k+1)
            if (k /= nn-1) then
                    pp(l:mnnk)=pp(l:mnnk)+z*a(l:mnnk,k+2)
                    a(l:mnnk,k+2)=a(l:mnnk,k+2)-pp(l:mnnk)*r
            end if
            a(l:mnnk,k+1)=a(l:mnnk,k+1)-pp(l:mnnk)*q
            a(l:mnnk,k)=a(l:mnnk,k)-pp(l:mnnk)
    end if
```

end do
end do iterate Go back for next iteration on current eigenend do
END SUBROUTINE hqr

Go back for next iteration on current eigenvalue.

Foanorm=sum(abs(a), mask=upper_triangle(n,n,extra=2) See the discussion of upper_triangle after jacobi on p. 1226. Setting extra=2 here picks out the upper Hessenberg part of the matrix.
iterate: do We use a named loop to improve the readability and structuring of the routine. The if-blocks that test for one or two roots end with exit iterate, transferring control back to the outermost loop and thus starting a search for the next root.
call diagadd... The routines that operate on the diagonal of a matrix are collected in nrutil partly so you can write clear code and partly in the hope that compiler writers will provide parallel library routines. Fortran 90 does not provide convenient parallel access to the diagonal of a matrix.

CITED REFERENCES AND FURTHER READING:
Golub, G.H., and Van Loan, C.F. 1989, Matrix Computations, 2nd ed. (Baltimore: Johns Hopkins University Press), $\S 8.6$ and references therein. [1]
Sorensen, D.C., and Tang, P.T.P. 1991, SIAM Journal on Numerical Analysis, vol. 28, pp. 17521775. [2]

Lo, S.-S., Philippe, B., and Sameh, A. 1987, SIAM Journal on Scientific and Statistical Computing, vol. 8, pp. s155-s165. [3]

