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RCSL NO: 55-D61

TYPE : Algol 5 Procedure

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MATHEMATICAL PROCEDURE LIBRARY

jacobi

ABSTRACT

jacobi calculates all the eigenvalues and, if wanted, the corresponding eigenvectors of a symmetric matrix by the method of Jacobi.



..... INFORMATION DEPARTMENT

1. Function and Parameters.

Jacobi calculates all the eigenvalues and, if desired, the corresponding eigenvectors of a symmetric matrix by the method of Jacobi.

Procedure head:

```
real procedure jacobi(a,lambda,x,vect,maxscan);  
value vect,maxscan;  
array a,lambda,x;  
boolean vect;  
integer maxscan;
```

Call parameters:

a : a real array containing the given matrix.

vect : (boolean) . If vect is true, the eigenvectors will be calculated.

maxscan : (integer or real). If the value of maxscan is > 0, at most this number of scans are performed in the procedure. If the value is 0, no limitation is imposed on the number of scans. (see section 2. Method).

Return parameters:

jacobi : (real). Contains the number of rotations in the last two bytes and the number of scans in the first two bytes. If the procedure exits because the maximum number of scans is reached, the negative number of scans is stored. Hence the sign of the procedure value reveals its success.

lambda : (real array). Contains on exit the calculated eigenvalues.

x : (real array). If the eigenvectors are wanted, they are stored as column-vectors in x. The eigenvector associated with the eigenvalue lambda(1) is stored in x(.,1).

Parameter check:

The orders of the matrix a and the vectors x and lambda are not given as parameters, but are checked by the procedure in this way:

First, the upper subscript bound of the array lambda is assigned to the order. Then it is checked that the arrays are declared

```
a(1:order,1:order)      (1)
lambda(1:order)         (2)
x(1:order,1:order)     (4)
```

(this last check is performed only if the eigenvectors are wanted; in fact, if vect=false, x can be any real array and is never touched).

In case of error, the execution is terminated by the error-message on current output

```
jacobi <error-number>
```

where <error-number> is the sum of the numbers attached to each wrong array as stated above. Thus the declaration

```
a(1:order,0:order)
lambda(1:order)
x(1:order)
```

yields the error-number 5 if vect=true, otherwise 1.

This initial check of the parameters implies that there is no need for index-check in the procedure.

2. Method.

The method consists of a number of scans of all the super-diagonal elements of the matrix. If the element in question is greater in absolute value than a certain threshold (approximately the current root-mean-square of all super-diagonal elements), a rotation is performed, so designed that this element becomes zero.

The exit condition is that the current threshold is less than 5×10^{-13} initial threshold (or that the maximum number of scans is reached). Since the procedure converges at least quadratically, little time is saved by reducing the accuracy.

Just before exit, the super- and main-diagonal elements are reestablished so that the matrix is unchanged on exit.

For further details, see [1].

3. Accuracy, Time and Storage Requirement.

Accuracy: The relative error of the eigenvalues and, if the eigenvectors are calculated, the greatest element of $(x^t x x - I)$ is unlikely to exceed $n \times$ (the relative machine accuracy, appr. 3×10^{-11}). This applies also to the greatest element of $(a x x - x x L) / \max(\lambda)$. However, if the magnitudes of the eigenvalues are highly different it may happen that the eigenvalues of low magnitude are determined less accurate. It can be shown (see [1]) that the absolute error of the eigenvalues is bounded by

$$2 \times \|L\| / \sqrt{1-nI} \times (nI / (1-\sqrt{1-nI}) + nA),$$

where

$$\begin{aligned} L &= \text{diag}(\lambda) \\ nI &= \|x^t x x - I\| ; x^t \text{ is } x \text{ transposed.} \\ nA &= \|a x x - x x L\| / \|L\|. \end{aligned}$$

Time : Generally proportional to n^3 when n is large (see section 4. Test and Discussion).

Storage requirement: 5 segments of program
 18 local real variables.

4. Test and Discussion.

Several matrices have been tried by the test program (or slightly modified versions) at the end of this section.

The table below shows the type and order of the matrix in question, the number of scans, the number of rotations, the time consumed by the procedure (in sec.), and the norms nI and nA as defined in section 3. (the infinity-norm is used.)

| type | n | scan | rotation | time | nI | nA |
|------|----|------|----------|------|-----------------------|-----------------------|
| a | 10 | 14 | 180 | 1.9 | 1.7×10^{-9} | 8.3×10^{-10} |
| a | 20 | 17 | 796 | 14.6 | 7.1×10^{-9} | 2.1×10^{-9} |
| b | 15 | 12 | 327 | 4.8 | 1.2×10^{-9} | 9.4×10^{-10} |
| c | 9 | 4 | 12 | .15 | 2.5×10^{-10} | 9.2×10^{-11} |
| d | 8 | 11 | 69 | .68 | 7.6×10^{-10} | 6.1×10^{-10} |

The types represent the following matrices:

- a) HHH-matrices. The general element of a n-th order matrix is given by $a(i,j)=a(j,i)=n-i+1$. The eigenvalues are

$$l(i)=0.25/\sin((2i-1)\pi/(4n+2))\times 2$$

- b) The matrix

$$a(i,j)=a(j,i)=\text{if } i < j \text{ then } 1 \text{ else } 10 \times (i-1)$$

- c) The matrix

$$a(i,j)=a(j,i)=\text{if } i=j \text{ then } 0 \text{ else } 1$$

All eigenvalues are -1 except for one which is n-1.

- d) The matrix and the complete output of the testprogram for this case are:

matrix:

```

611
196 899
-192 113 899
407 -192 196 611
-8 -71 61 8 411
-52 -43 49 44 -599 411
-49 -8 8 59 208 208 99
29 -44 52 -23 208 208 -911 99

```

```

scans= 11 rotations= 69 time= 0.68 sec.
nI = 7.6e-10 nA = 6.1e-10

```

eigenvalues:

```

1.0200490189e 3
1.0000000002e 3
1.0000000003e 3
9.8048646596e -2
2.5609435927e -9
1.0200000004e 3
1.0199019515e 3
-1.0200490187e 3

```

end

Test program:

```

test1 jacobi
begin integer n;
for underflows=-1 while read(in,n)>0 do
begin real x,eli,ela,maxl,normi,norma,la,layout,t0,t1,si,sa;
array a,t(1:n,1:n),l(1:n);
integer i,j,k,layno;

read(in,layno);
for i:=1 step 1 until n do
for j:=1 step 1 until i do
begin read(in,x);
a(i,j):=a(j,i):=x
end;

```

```

t0:=systime(1,0,1a);
for i:=0,i+1 while t1<t0+2.56 do
begin x:=jacobi(a,l,t,true,0);
      t1:=systime(1,0,1a)
end;
t0:=(t1-t0)/i;

maxl:=normi:=norma:=0;
for i:=1 step 1 until n do
begin si:=sa:=0;
  for j:=1 step 1 until n do
begin eli:=ela:=0;
  la:=l(j);
  for k:=1 step 1 until n do
begin eli:=eli+t(k,i)*t(k,j);
      ela:=ela+a(i,k)*t(k,j)
end k;
  if i=j then eli:=eli-1;
  ela:=ela-t(i,j)*la;
  si:=si+abs eli;
  sa:=sa+abs ela
end j;
  if si>normi then normi:=si;
  if sa>norma then norma:=sa;
  if abs l(i)>maxl then maxl:=abs l(i)
end i;

layout:=real(case layno of(<<d>,<<dd>,<<-dd>,<<-ddd>,<<-dddd>,<<d>,<<d>,<<-d.dddd>,<<-d.ddddd));
write(out,<:<12>matrix:>);
for i:=1 step 1 until n do
begin k:=0;
  write(out,<:<10>:>);
  for j:=1 step 1 until i do
begin write(out,string layout,a(i,j));
      k:=k+layno;
      if k>70 and j<i then
begin write(out,<:<10>:>,false add 32,layno);
          k:=layno
end
end
end write matrix;
write(out,<:<10><10>scans=:>,<<-dddd>,x shift(-24) extract 24,
      <: rotations=:>,x extract 24,
      <: time=:>,<< ddd.00>,t0,<: sec.:>,
      <:<10>nI =:>,<< d.dn-dd>,normi,
      <: nA =:>,norma/maxl,
      <:<10><10>eigenvalues:<10>:>);
for i:=1 step 1 until n do
  write(out,<<-d.ddddddddn-dd>,l(i),<:<10>:>)
end read n
end

```

5. References

- [1] Kahan, W. and Green, D. : Eigenvalues and Eigenvectors of a Real Symmetric Matrix. (Unpublished but copies of the paper are achievable on demand)

6. Algorithm

```
jacobi=set 5
jacobi=algol index.no
```

```
external
```

```
real procedure jacobi(a,lambda,x,vect,maxscan);
message jacobi, version 20.11.69, RCSL NO: 55-D61;
value vect,maxscan;
integer maxscan;
boolean vect;
array a,lambda,x;
begin real eps,t,ave,s,u,thresh,dlow,d,c,aij,ajj;
integer i,j,ii,jj,jl,n,nrscan,nrrot;
boolean again;
```

```
i:=if system(3,n,lambda)<1 then 2 else 0;
j:=system(3,ii,a);
if j<n+1 or ii<n*(n+1) then i:=i+1;
j:=system(3,ii,x);
if (j<n+1 or ii<n*(n+1)) and vect then i:=i+4;
if i>0 then system(9,i,<<10>jacobi :>);
```

```
if vect then
for i:=1 step 1 until n do
begin x(i,i):=1;
for j:=i+1 step 1 until n do x(i,j):=x(j,i):=0
end x:=identity;
```

```
d:=0;
for i:=1 step 1 until n do
begin lambda(i):=a(i,i);
for j:=i+1 step 1 until n do d:=d+a(i,j)**2
end i;
```

```
nrscan:=nrrot:=0;
if d>0 then
begin dlow:= $\sqrt[n]{d}$ -7*d;
ave:=(n-1)*n*0.55;
thresh:=sqrt(d/ave);
eps:= $5^n-13$ *thresh;
```

```
scan:again:=false;
nrscan:=nrscan+1;
for i:=n-1 step -1 until 1 do
for j:=i+1 step 1 until n do
begin comment scan;
aij:=a(i,j);
if abs aij >= thresh then
begin ajj:=a(j,j);
s:=ajj-a(i,i);
t:=abs aij;
if s+t<eps then
begin comment rot<0;
again:=true;
nrrot:=nrrot+1;
if abs s< $\sqrt[n]{d}$ -6*t then s:=c:=0.70710678118 else
begin t:=aij/s;
s:=0.25/sqrt(t**2+0.25);
c:=sqrt(s+0.5);
s:=2*t*s/c
end rot<pi/4;
```

```

for ii:=1 step 1 until 1 do
begin t:=a(ii,1); u:=a(ii,j);
  a(ii,1):=cxt-sxu;
  a(ii,j):=sxt+cxu
end;
jl:=j-1;
for ii:=i+1 step 1 until jl do
begin t:=a(i,ii); u:=a(ii,j);
  a(i,ii):=cxt-sxu;
  a(ii,j):=sxt+cxu
end;
a(j,j):=sxaij+cxajj;
a(i,i):=cxa(i,i)-sxcxaij-sxajj;
for ii:=j step 1 until n do
begin t:=a(i,ii); u:=a(j,ii);
  a(i,ii):=cxt-sxu;
  a(j,ii):=sxt+cxu
end;

if vect then
for ii:= 1 step 1 until n do
begin t:=x(ii,1); u:=x(ii,j);
  x(ii,1):=cxt-sxu;
  x(ii,j):=sxt+cxu
end;

d:=d-aij×2;
if d<dlow then
begin d:=0;
  for ii:=n-1 step -1 until 1 do
  for jj:=ii+1 step 1 until n do
  d:=d+a(ii,jj)×2;
  dlow:=n-7×d
end;

thresh:=sqrt(d/ave);
if thresh<eps then goto quit
end rotation
end aij
end scan;
if again and (maxscan>0=>maxscan>nrscan) then goto scan;

if again then nrscan:=-nrscan;

quit:for i:=1 step 1 until n do
begin t:=a(i,i);
  a(i,i):=lambda(i);
  lambda(i):=t;
  for j:=i+1 step 1 until n do a(i,j):=a(j,i)
end i
end d>0;
jacobi:=0.5 add nrscan shift 24 add nrrot
end jacobi;

comment
Call parameters:
  a      : a real array containing the given matrix.
  vect   : (boolean) . If vect is true, the eigenvectors
           will be calculated.
  maxscan : (integer or real). If the value of maxscan is > 0,
           at most this number of scans are performed in the
           procedure. If the value is 0, no limitation is imposed
           on the number of scans.

```


Return parameters:

- jacobi : (real). Contains the number of rotations in the last two bytes and the number of scans in the first two bytes. If the procedure exits because the maximum number of scans is reached, the negative number of scans is stored. Hence the sign of the procedure value reveals its success.
- lambda : (real array). Contains on exit the calculated eigenvalues.
- x : (real array). If the eigenvectors are wanted, they are stored as column-vectors in x. The eigenvector associated with the eigenvalue lambda(1) is stored in x(.,1);