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ALGORITMY

40. NEGEIG

DISTRIBUTION OF THE EIGENVALUES OF EIGENPROBLEM $\mathbf{Ax} = \lambda \mathbf{Bx}$

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An individual eigenvalue is of little significance for very large matrices. Frequently only the distribution of eigenvalues is needed. A procedure (based on the negative eigenvalue theorem) which determines the distribution of eigenvalues of the generalized eigenproblem $\mathbf{Ax} = \lambda \mathbf{Bx}$ is described here. It makes it possible to find the number of eigenvalues less than any given real number. This procedure is efficient especially for band matrices of high order.

Given the generalized eigenproblem

$$\mathbf{Ax} = \lambda \mathbf{Bx}, \text{ where}$$

\mathbf{A} , \mathbf{B} are hermitian matrices of order n , \mathbf{B} positive definite, then the number of eigenvalues $I(\mu)$ less than a given real number μ equals to

$$I(\mu) = \sum_{i=1}^n \Theta(-X_i), \text{ where}$$

$\Theta(x) = 1$ for $x > 0$, otherwise $\Theta(x) = 0$. Numbers X_i are the (1, 1) elements of the partitioned matrices \mathbf{U}_i , where

$$(1) \quad \mathbf{U}_1 = \mathbf{A} - \mu \mathbf{B},$$

$$(2) \quad \mathbf{U}_i = \mathbf{Z}_{i-1} - \mathbf{Y}_{i-1} X_{i-1}^{-1} \mathbf{Y}_{i-1}^*, \quad i = 2, \dots, n,$$

$$(3) \quad \mathbf{U}_i = \left[\begin{array}{c|c} X_i & \mathbf{Y}_i^* \\ \hline \mathbf{Y}_i & \mathbf{Z}_i \end{array} \right].$$

(The asterisk designates hermitian conjugation). For the proof see [1]–[3].

The procedure *NEGEIG* may be used to calculate the number of eigenvalues of any real symmetric eigenproblem $\mathbf{Ax} = \lambda \mathbf{Bx}$ (\mathbf{B} pos. def.) which are less than a given real number. However, it is most efficient if \mathbf{A} , \mathbf{B} are band matrices of very high order.

The matrices \mathbf{A} , \mathbf{B} are assumed to be band matrices ($a_{ij} = b_{ij} = 0$ for $|i - j| \geq m$). For the sake of efficiency, just the (i, j) elements ($0 \leq i - j < m$) of the matrix $\mathbf{A} - \mu \mathbf{B}$ are stored, column by column, in one-dimensional array a . E.g. for $m = 2$, $n = 3$ the matrix

$$\begin{bmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{bmatrix}$$

is re-stored as $a = (a_{11}, a_{21}, a_{22}, a_{32}, a_{33})$.

The theorem fails if some $X_i = 0$. In such a case X_i is replaced by $-rel \times \max_{j=1, \dots, k} |(\mathbf{Y}_i)_j|$, $i = 1, \dots, n - 1$ where $k = \min(m - 1, n - i)$, like in [4]. It means that the zero X_i is treated as negative. If \mathbf{Y}_i is the zero vector then Eq. (2) is replaced by $\mathbf{U}_i = \mathbf{Z}_{i-1}$. If $\mathbf{A} = \mathbf{0}$, \mathbf{A} is treated as a negative definite matrix.

The number of non-zero elements of the matrix $\mathbf{Y}_{i-1} X_{i-1}^{-1} \mathbf{Y}_{i-1}^*$ is less or equal to $(m - 1)^2$. Hence only $(m - 1)^2$ elements in the left upper corner of \mathbf{Z}_{i-1} are changed in the course of calculation of \mathbf{U}_i . This property may be extremely useful since it is possible to work part by part with matrices of such a large order that $\mathbf{A} - \mu \mathbf{B}$ cannot be localized in the array a .

The procedure *NEGEIG* involves approximately (for large m , n) nm^2 additions and $1/2 nm^2$ multiplications.

integer procedure *NEGEIG* (a , m , n , $const$, eps);

value m , n , $const$, eps ; **real** $const$, eps ; **integer** m , n ; **array** a ;

comment Input to procedure *NEGEIG*

a array a gives the (i, j) elements ($0 \leq i - j < m$) of a band real symmetric matrix $\mathbf{A} - \mu \mathbf{B}$ stored column by column. This elements are lost during the calculation.

m bandwidth of \mathbf{A} , \mathbf{B} is $2m - 1$.

n order of \mathbf{A} , \mathbf{B} .

$const$ $1/rel$, where rel is the smallest number for which $1 + rel > 1$ on the computer.

eps the smallest positive real number representable on the computer.

Output of procedure *NEGEIG*

NEGEIG the number of eigenvalues of the eigenproblem $\mathbf{Ax} = \lambda \mathbf{Bx}$, \mathbf{A} , \mathbf{B} real. sym., \mathbf{B} pos. def., which are less than μ ;

begin real c , x , y_{max} ; **integer** i , $i1$, $i2$, j , k , $l1$, $l2$, $n2$, neg ; **array** $y[2 : m]$;

$neg := 0$;

comment $X_1 = x$;

$x := a[1]$;

```

if  $x < eps$  then  $neg := neg + 1$ ;
 $i1 := 1$ ;
for  $i := 2$  step 1 until  $n$  do
  begin comment  $U_i$  (array  $a$ ) and  $X_i = x$  will be computed;
     $n2 := n - i + 2$ ;
     $l1 := n2 - m$ ;
    if  $l1 < 0$  then  $l1 := 0$ ;
    comment  $l1$  is the number of the last rows of the matrix  $Y_{i-1} X_{i-1}^{-1} Y_{i-1}^*$ 
      having zero elements;
    if  $m < n2$  then  $n2 := m$ ;
    comment The first  $n2 - 1$  non-zero elements of  $Y_{i-1}$  are stored as  $y$ ;
     $y_{max} := 0$ ;
    for  $j := 2$  step 1 until  $n2$  do
      begin  $i1 := i1 + 1$ ;
         $c := a[i1]$ ;
        if  $abs(c) > y_{max}$  then  $y_{max} := abs(c)$ ;
         $y[j] := c$ 
      end  $j$ ;
    comment if  $y_{max} < eps$  then  $U_i = Z_{i-1}$ ;
    if  $y_{max} \geq eps$  then
      begin  $i2 := i1$ ;
        for  $j := 2$  step 1 until  $n2$  do
          begin if  $abs(x) < eps$  then  $c := y[j]/y_{max} \times const$ 
            else  $c := -y[j]/x$ ;
            comment Calculate the  $(j - 1)$ -st column of  $U_i$ ;
            for  $k := j$  step 1 until  $n2$  do
              begin  $i2 := i2 + 1$ ;
                 $a[i2] := a[i2] + c \times y[k]$ 
              end  $k$ ;
            comment From the stored elements in the  $(j - 1)$ -st column
              of  $U_i$  the last  $\min(l1, l2)$  unchanged elements will
              be jumped over;
             $l2 := j - 1$ ;
            if  $l2 < l1$  then  $i2 := i2 + l2$  else  $i2 := i2 + l1$ 
          end  $j$ 
        end;
         $i1 := i1 + 1$ ;
         $x := a[i1]$ ;
        if  $x < eps$  then  $neg := neg + 1$ 
      end  $i$ ;
     $NEGEIG := neg$ 
  end  $NEGEIG$ ;

```

The procedure *NEGEIG* has been tested on MINSK 22 (ALGOL 60) and IBM 360/40 (FORTRAN) computers.

The accuracy of the result is not influenced by close or coincident eigenvalues. The procedure has been tested extensively. To give a formal test of the procedure the matrices [5]

$$\mathbf{A} = \begin{bmatrix} 10 & 2 & 3 & 1 & 1 \\ 2 & 12 & 1 & 2 & 1 \\ 3 & 1 & 11 & 1 & -1 \\ 1 & 2 & 1 & 9 & 1 \\ 1 & 1 & -1 & 1 & 15 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 12 & 1 & -1 & 2 & 1 \\ 1 & 14 & 1 & -1 & 1 \\ -1 & 1 & 16 & -1 & 1 \\ 2 & -1 & -1 & 12 & -1 \\ 1 & 1 & 1 & -1 & 11 \end{bmatrix}$$

were used. The eigenvalues of the corresponding eigenproblem are [5]

$$\begin{aligned} &+4.3278\ 7211\ 020_{10} - 1 \\ &+6.6366\ 2748\ 402_{10} - 1 \\ &+9.4385\ 9004\ 670_{10} - 1 \\ &+1.1092\ 8454\ 002_{10} + 0 \\ &+1.4923\ 5323\ 254_{10} + 0. \end{aligned}$$

The quantities $I(\mu)$ in dependence on μ are given in the following table (we have put $rel = 2^{-28}$ and $eps = 10^{-18}$ on MINSK 22).

Table

μ	$I(\mu)$
+4.3278 7210 ₁₀ -1	0
+4.3278 7220 ₁₀ -1	1
+6.6366 2752 ₁₀ -1	2
+6.6366 2764 ₁₀ -1	2
+9.4385 8992 ₁₀ -1	2
+9.4385 9004 ₁₀ -1	3
+1.1092 8452 ₁₀ +0	3
+1.1092 8455 ₁₀ +0	4
+1.4923 5321 ₁₀ +0	4
+1.4923 5325 ₁₀ +0	5

The procedure has been used already to calculate the distribution of eigenvalues (calculating $I(\mu)$ at about one hundred equidistant points in the eigenvalue spectrum) for a lot of different matrices $n = 100 - 10\ 000$, $m = 2 - 80$.

References

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