ALGORITMY

40. NEGEIG

DISTRIBUTION OF THE EIGENVALUES OF EIGENPROBLEM $\mathbf{A}\mathbf{x} = \lambda\, \mathbf{B}\mathbf{x}$

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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 $\mathbf{A}\mathbf{x} = \lambda\, \mathbf{B}\mathbf{x}$ 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

$$\mathbf{A}\mathbf{x} = \lambda\, \mathbf{B}\mathbf{x}\,, \quad \text{where}$$

$\mathbf{A}$, $\mathbf{B}$ 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

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

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

$$\mathbf{U}_1 = \mathbf{A} - \mu\mathbf{B}\,, \tag{1}$$

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

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

(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 $\mathbf{A}\mathbf{x} = \lambda\, \mathbf{B}\mathbf{x}$ ($\mathbf{B}$ 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 $|i - j| \geqq$ $\geqq m$. For the sake of efficiency, just the (i, j) elements ($0 \leqq i - j < m$) 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 $-rel \times$ $\times \max_{j=1,\dots,k} |(\mathbf{Y}_i)_j|$, $i = 1, \dots, n - 1$ 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 ($0 \leqq i - j < m$) 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 $\mathbf{A}\mathbf{x} = \lambda\, \mathbf{B}\mathbf{x}$, $\mathbf{A}$, $\mathbf{B}$ real. sym., $\mathbf{B}$ pos. def., which are less then μ;

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

    neg := 0;

    comment $X_1 = x$;

    x := *a*[1];

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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;
      ymax := 0;
      for j := 2 step 1 until n2 do
      begin i1 := i1 + 1;
            c := a[i1];
            if abs(c) > ymax then ymax := abs(c);
            y[j] := c
      end j;
comment if ymax < eps then U_i = Z_{i-1};
if ymax ≧ eps then
begin i2 := i1;
      for j := 2 step 1 until n2 do
            begin if abs(x) < eps then c := y[j]/ymax × 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 × 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;
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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]

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

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

$$\begin{aligned} &+4{\cdot}3278\ 7211\ 020_{10} - 1 \\ &+6{\cdot}6366\ 2748\ 402_{10} - 1 \\ &+9{\cdot}4385\ 9004\ 670_{10} - 1 \\ &+1{\cdot}1092\ 8454\ 002_{10} + 0 \\ &+1{\cdot}4923\ 5323\ 254_{10} + 0\,. \end{aligned}$$

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	$I(\mu)$
$+4{\cdot}3278\ 7210_{10}-1$	0
$+4{\cdot}3278\ 7220_{10}-1$	1
$+6{\cdot}6366\ 2752_{10}-1$	2
$+6{\cdot}6366\ 2764_{10}-1$	2
$+9{\cdot}4385\ 8992_{10}-1$	2
$+9{\cdot}4385\ 9004_{10}-1$	3
$+1{\cdot}1092\ 8452_{10}+0$	3
$+1{\cdot}1092\ 8455_{10}+0$	4
$+1{\cdot}4923\ 5321_{10}+0$	4
$+1{\cdot}4923\ 5325_{10}+0$	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

[1] *Jeffreys H., B. S. Jeffreys:* Methods of Mathematical Physics, At the University Press, Cambridge, 1946, p. 127.

[2] *Dean P.:* The Vibrational Properties of Disordered Systems: Numerical Studies. Rev. Mod. Phys. 44 (1972), 127—168.

[3] *Dean P., J. L. Martin:* A Method for Determining the Frequency Spectra of Disordered Lattices in Two-Dimensions. Proc. Roy. Soc. A 259 (1961), 409—418.

[4] *Barth W., R. S. Martin, J. H. Wilkinson:* Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection. Numer. Math. 9 (1967), 386—393.

[5] *Martin R. S., J. H. Wilkinson:* Reduction of the Symmetric Eigenproblem $Ax = \lambda Bx$ and Related Problems to Standard Form. Numer. Math. 11 (1968), 99—110.

[6] *Wilkinson J. H.:* The Algebraic Eigenvalue Problem. Oxford University Press, London, 1965.