The determination of eigenvalues of symmetric quindiagonal matrices

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Evans (1975) has described a method for finding the eigenvalues of quindiagonal matrices A based on the bisection and the Sturm sequence property of the leading principal minors $P_i(\lambda)$ of $A - \lambda I$. The algorithms there presented contained certain typographical errors, but even with these removed the procedures give incorrect results for certain matrices which have some zero $P_i(\lambda)$ at the point of bisection. This paper describes a modification, based on earlier work on general band matrices, in which the sign of $P_i(\lambda)$ is determined without calculating its value. Thus there are no problems with underflow or overflow.

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1. Introduction

One of the best methods for determining the eigenvalues of a symmetric tridiagonal matrix A is based on the Sturm sequence property of the leading principal minors of $(A - \lambda I)$. This has proved itself to be reliable and robust and is available on a number of machines both through the auspices of the NAG library and manufacturers' provided software. On account of its well established behaviour an attempt was made, in a paper by Evans (1975), to extend this method to quindiagonal matrices. This included two ALGOL procedures: quindiageigen based on a Newton iteration method to find the eigenvalues of a general pentadiagonal matrix and quindibisect which used the method of bisection to determine the eigenvalues of a symmetric quindiagonal matrix. A summary of Evans's paper is given in Section 2. It was decided to include the procedure quindibisect in a comparative study of methods currently available for the location of eigenvalues of band symmetric matrices (Cliff, 1977). During its implementation, a number of typographical errors were found. These, together with their corrections, are given by Cliff. However, even with these corrections, the algorithm gave wrong results in certain cases and in Section 3 we explain why this is so. In Section 4 the modifications of the method to avoid such errors are described. Some numerical examples of the modified method are given in Section 5 and the new ALGOL procedures in Section 6.

2. Summary of Evans's method

The eigenvalues of the symmetric quindiagonal matrix A are given by

$$\det \begin{vmatrix} c_1-\lambda & b_2 & d_3 & & & & & & \\ b_2 & c_2-\lambda & b_3 & d_4 & & & & & 0 \\ d_3 & b_3 & c_3-\lambda & b_4 & d_5 & & & & \\ & d_4 & b_4 & c_4-\lambda & b_5 & d_6 & & & \\ & & \cdot & \cdot & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \cdot & d_n & \\ & 0 & & & \cdot & b_{n-1} & c_{n-1}-\lambda & b_n & \\ & & & & & d_n & b_n & c_n-\lambda & \end{vmatrix} = 0$$

Evans developed a recursive sequence for $P_i(\lambda)$, $i = 0, 1, 2, \ldots n$, the leading principal minors of order i of the matrix $A - \lambda I$. This sequence of polynomials, with $P_i(\lambda)$ being of degree i in λ, can be shown to form a Sturm sequence of polynomials in the interval $(-\infty, +\infty)$. Thus the number of disagreements in sign $s(\lambda)$, in the sequence $P_i(\lambda)$, $i = 0, 1, 2, \ldots n$, is equal to the number of roots of $P_n(\lambda) = 0$ smaller than λ. This property enables one to use the process of bisection to calculate the eigenvalues of A. In the computation of the sequence $P_i(\lambda)$, $i = 0, \ldots n$, for a particular value of λ both underflow and overflow may occur making it difficult to design a robust algorithm. To overcome this difficulty the sequence of polynomials $P_i(\lambda)$ is replaced by the sequence $p_i(\lambda)$ defined by

$$p_i(\lambda) = \frac{P_i(\lambda)}{P_{i-1}(\lambda)} \qquad i = 1, \ldots n$$

The $p_i(\lambda)$ may be shown to satisfy a modified recurrence relation and with its use we are able to calculate the number of negative $p_i(\lambda)$ which gives $s(\lambda)$ the number of eigenvalues smaller than λ.

3. Errors in the symmetric case

Applying the corrected algorithm to various test matrices, it was first found to give wrong results for matrices in which the elements of the diagonal, the upper and lower sub-subdiagonals all had the value one and the rest of the elements were zero. Inspection of the algorithm showed that there was incorrect treatment of $P_i(\lambda)$ when λ was equal to the element in the first diagonal position. As the situation was further complicated by the zeros in the upper and lower subdiagonals, the matrix

$$\begin{pmatrix} 2 & 1 & 4 & 0 \\ 1 & 7 & 3 & 1 \\ 4 & 3 & 2 & 3 \\ 0 & 1 & 3 & 5 \end{pmatrix} \qquad (1)$$

was specifically designed to give $\lambda = 2$ on the first iteration while, at the same time, having all the elements in the band non-zero. The output from Evans's corrected algorithm was

$$-2{\cdot}813, \quad 2{\cdot}000, \quad 2{\cdot}000, \quad 10{\cdot}516,$$

whereas the accurate eigenvalues to three decimal places are

$$-2{\cdot}813, \quad 3{\cdot}413, \quad 4{\cdot}883, \quad 10{\cdot}516$$

This discrepancy may be explained by examining the method used to obtain the recurrence relation for $p_i(\lambda)$. The calculation of the $P_i(\lambda)/P_{i-1}(\lambda)$ involves expressions of the form $P_r(\lambda)/P_{i-1}(\lambda)$ for $r < i - 1$ which may be evaluated in terms of the previously computed $p_k(\lambda)$, $k \leqslant i - 1$ using the algebraic identity

$$\frac{P_r}{P_{i-1}} = \frac{P_r P_{r+1} \ldots P_{i-2}}{P_{r+1} P_{r+2} \ldots P_{i-1}} = \frac{1}{p_{r+1} p_{r+2} \cdots p_{i-1}} \qquad (r < i - 1) \qquad (2)$$

Such a substitution is satisfactory provided that the P_k, where

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$k = r + 1, r + 2, \ldots i - 1$, are all non-zero. In addition, if one or more of the P_k, where $k = r + 1, r + 2, \ldots i - 2$, are zero, then the above expression contains the indeterminate 0/0. A similar problem arises when dealing with symmetric tridiagonal matrices. In this case, Wilkinson (1960, 1965) has shown that we may replace zero valued $p_k(\lambda)$ by a suitably small quantity, related to the machine precision constant *relfeh*, with little or no loss of accuracy. This technique was followed by Evans who, during the computation of $p_i(\lambda)$ in the **procedure** quindibisect, substituted the quantity *relfeh* for any divisor containing a zero $p_k(\lambda)$ as a factor. However, it is this step which leads to wrong results in the quindiagonal case as may be illustrated by considering the leading submatrix of order 3 of Matrix (1):

$$\begin{pmatrix} 2 & 1 & 4 \\ 1 & 7 & 3 \\ 4 & 3 & 2 \end{pmatrix}$$

If we take $\lambda = 2$, the sequence $P_i(\lambda)$ has the values:

$$P_0 = 1, \quad P_1 = 0, \quad P_2 = -1, \quad P_3 = -56$$

Hence, the correct values of the sequence $p_i(\lambda)$ are:

$$p_0 = 1 \text{ (by definition)}, \quad p_1 = 0, \quad p_2 = -\infty, \quad p_3 = 56 \tag{3}$$

Using formulae derived through the application of (2), Evans's corrected algorithm yields:

$$p_0 = 1, \quad p_1 = 0, \quad p_2 = 5 - (relfeh)^{-1},$$
$$p_3 = \frac{-9}{[5 - (relfeh)^{-1}]} - 56(relfeh)^{-1} \tag{4}$$

The computed value of p_3 will be $-56(relfeh)^{-1}$ and its sign is different from that of the correct p_3 in Eqns (3). This is due to the replacement of P_0/P_2 by $P_0P_1/P_1P_2 = (p_1p_2)^{-1}$ and leads to a true value of -1 being replaced by $(relfeh)^{-1}$; a fact borne out when one compares the two values of $p_3(2)$. If one assigns a positive sign to the zero $p_i(\lambda)$, then Eqns (3) give the correct value: $s(2) = 1$, whereas Eqns (4) give $s(2) = 2$.

4. Reduction to upper triangular form

The errors described in Section 3 may be circumvented by basing the calculation of $s(\lambda)$ on a method described by Wilkinson (1965). This involves using a variation of Gauss elimination with pivoting to decompose $A - \lambda I$ into upper triangular form. The same approach was adopted by Peters and Wilkinson (1969) in the determination of the eigenvalues of $Ax = \lambda Bx$ with band symmetric A and B and made use of a previously published algorithm bandet2 described by Martin and Wilkinson (1967). However, this procedure was more general than our application required. In particular, it dealt with general band matrices, took no account of symmetry and also produced the LU decomposition with interchanges of $A - \lambda I$. The present authors have extracted the relevant parts from bandet2 and have made it more efficient by using both the symmetrical and quindiagonal properties of the input matrix. The new algorithm is named quindet2 and appears in Section 6. For quindiagonal A there are only three rows and five columns to be considered in each major step of the Gauss elimination, the values of these elements being held in the array r. For further details of this method readers may consult the above references together with Wilkinson and Reinsch (1971). The **procedure** quindibisect was altered so that $s(\lambda)$ was calculated using a call to **procedure** quindet2. In addition, since it now no longer used the values of the squared subdiagonal and sub-subdiagonal elements of the matrix, these were removed from its parameter list. The improved procedure has been named quindibisect2 and will also be found in Section 6.

5. Numerical results

The procedures have been tested using several matrices with *eps*1 $= 10^{-8}$ and *relfeh* $= 2^{-37}$, the machine precision constant relevant to the ICL 1900 series. We quote here a selection of results.

(*a*) The 10 × 10 matrix used in Evans (1975). Results expressed in floating decimal form correct to eight significant figures are:

2·058 889 1, 1; 1·733 686 8, 1; 1·461 648 1, 1;
1·194 331 1, 1; 9·472 946 0, 0; 7·541 211 6, 0;
5·976 448 2, 0; 4·353 020 4, 0; 2·571 821 8, 0;
5·990 008 9, −1;

(*b*) The 10 × 10 matrix in which

the diagonal $c_i = 1{\cdot}0 \quad i = 1, \ldots 10$
the subdiagonal $b_i = 0{\cdot}0 \quad i = 2, \ldots 10$
the sub-subdiagonal $d_i = 1{\cdot}0 \quad i = 3, \ldots 10$

Results correct to seven decimal places are:

2·000 000 0, 2·000 000 0, 1·000 000 0, 1·000 000 0,
0·000 000 0, 2·732 050 8, 2·732 050 8, −0·732 050 8,
−0·732 050 8, 0·000 000 0

(*c*) The 14 × 14 matrix in which

$c_i = 1{\cdot}0 \quad i = 1, \ldots 4, \quad c_i = 0{\cdot}0 \quad i = 5, \ldots 14$
$b_i = 0{\cdot}0 \quad i = 2, \ldots 14$
$d_i = 1{\cdot}0 \quad i = 3, 4, \quad d_i = 0{\cdot}0 \quad i = 5, \ldots 14$

This matrix would give underflow problems if the values of $P_i(\lambda)$ themselves were computed. During this test (and others too), on the occasions in which various $P_i(\lambda)$ were found to be zero, we printed out the values of λ and $s(\lambda)$. In every case $s(\lambda)$ was the correct number of eigenvalues $< \lambda$. Results correct to seven decimal places are:

2·000 000 0, 2·000 000 0, with all the rest 0·000 000 0

6. ALGOL programs

```
procedure quindet2(c,b,d,n,mu,no);
value n,mu;
integer n,no;
real mu;
array c,b,d;
comment The arrays c, b and d contain the diagonal, sub-
diagonal and sub-subdiagonal elements of a symmetric quin-
diagonal matrix of order n. The value of the output parameter
no is the number of eigenvalues greater than mu;
begin
integer i,j,k,rr,w;
real x;
array r[1:3, 1:5];
comment Initialise the array r;
 r[2,1] := c[1] - mu;
 r[2,2] := r[3,1] := b[2];
 r[2,3] := d[3];
 r[3,2] := c[2] - mu;
 r[3,3] := b[3];
 r[3,4] := d[4];
 r[2,4] := r[2,5] := r[3,5] := 0;
 no := if r[2,1] ≧ 0 then 1 else 0;
 comment k counts the major stages;
 for k := 2 step 1 until n do
 begin rr := 1;
  for i := 2, 1 do
  if k > i then
  begin w := 3 - i;
   comment Interchange row w and row 3 if necessary;
   if abs(r[3,1]) > abs(r[w,1]) then
   begin for j := 1 step 1 until i + 3 do
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```
    begin x := r[3,j];
     r[3,j] := r[w,j];
     r[w,j] := x
    end;
   if r[3,1] ≧ 0 ≡ r[w,1] ≧ 0 then rr := −rr
   end;
   comment Elimination of subdiagonal elements;
   x := if r[w,1] = 0 then 0 else r[3,1]/r[w,1];
   for j := 2 step 1 until i + 3 do
   r[3, j − 1] := r[3,j] − x * r[w,j];
   r[3, i + 3] := 0
  end i;
  if r[3,1] < 0 then rr := −rr;
  if rr > 0 then no := no + 1;
  comment Update elements of array r;
  for i := 1, 2 do
  for j := 1 step 1 until 5 do r[i,j] := r[i + 1,j];
  if k + 1 ≦ n then
  begin r[3,1] := d[k + 1];
   r[3,2] := b[k + 1];
   r[3,3] := c[k + 1] − mu
  end;
  r[3,4] := if k + 2 ≦ n then b[k + 2] else 0;
  r[3,5] := if k + 3 ≦ n then d[k + 3] else 0;
 end k;
end quindet2;

procedure quindibisect2(c,b,d,n,m1,m2,eps1,relfeh) res:(eps2,z,
 x);
value n,m1,m2,eps1,relfeh;
real eps1,eps2,relfeh;
integer n,m1,m2,z;
array c,b,d,x;
comment c is the diagonal, b the subdiagonal and d the sub-
subdiagonal of a symmetric quindiagonal matrix of order n.
Input to vectors b[i] and d[i] should begin with i = 2 and 3
respectively. The value of relfeh is machine dependent and
is the precision of the arithmetic used, i.e. for a t digit
binary mantissa relfeh is of the order of 2^-t.

The eigenvalues lambda[m1], . . . lambda[m2], where m2 is not
less than m1 and lambda[i + 1] is not less than lambda[i], are
calculated by the method of bisection and stored in the vector
x. Bisection is continued until the upper and lower bounds for
an eigenvalue differ by less than eps1, unless at some earlier
stage, the upper and lower bounds differ only in the least
significant digits. eps2 gives an extreme upper bound for the
error in any eigenvalue, but for certain types of matrices the
small eigenvalues are determined to a very much higher
accuracy. In this case, eps1 should be set equal to the error to be
tolerated in the smallest eigenvalue. It must not be set to zero;

begin real h,xmin,xmax; integer i;
 comment calculation of xmin and xmax;
 d[1] := d[2] := 0;
 b[1] := 0;
 xmin := c[n] − abs(b[n]) − abs(d[n]);
 xmax := c[n] + abs(b[n]) + abs(d[n]);
 h := abs(b[n − 1]) + abs(d[n − 1]) + abs(b[n]);
 if c[n − 1] + h > xmax then xmax := c[n − 1] + h;
 if c[n − 1] − h < xmin then xmin := c[n − 1] − h;
 for i := n − 2 step −1 until 1 do
 begin
  h := abs(b[i]) + abs(d[i]) + abs(b[i + 1])
    + abs(d [i + 2]);
  if c[i] + h > xmax then xmax := c[i] + h;
  if c[i] − h < xmin then xmin := c[i] − h
 end i;
 eps2 := relfeh * (if xmin + xmax > 0 then xmax else
  −xmin);
 if eps1 < 0 then eps1 := eps2;
 eps2 := 0·5 * eps1 + 7 * eps2;
 comment inner block;
 begin integer a,k; real x1,xu,xo; array wu[m1:m2];
  xo := xmax;
  for i := m1 step 1 until m2 do
  begin x[i] := xmax; wu[i] := xmin
  end i;
  z := 0;
  comment Loop for the kth eigenvalue;
  for k := m2 step −1 until m1 do
  begin xu := xmin;
   for i := k step −1 until m1 do
   begin if xu < wu[i] then
    begin xu := wu[i]; goto contin
    end
   end i;
   contin: if xo > x[k] then xo := x[k];
   for x1 := (xu + xo)/2 while xo − xu >
   2 * relfeh * (abs(xu) + abs(xo)) + eps1 do
   begin z := z + 1;
    quindet2(c,b,d,n,x1,a);
    a := n − a;
    if a < k then
    begin if a < m1 then xu := wu[m1] := x1
     else
     begin xu := wu[a + 1] := x1;
      if x[a] > x1 then x[a] := x1
     end
    end
    else xo := x1
   end x1;
   x[k] := (xo + xu)/2
  end k;
 end inner block;
end of quindibisect2;
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