

$$\begin{aligned}
P_3 &= (c_3 - \lambda)P_2 - b_3d_2P_1 - a_3e_1(c_2 - \lambda) \\
&\quad + a_3d_2R_2 + b_3e_1S_2; \\
R_3 &= d_2P_1 - e_1S_2; \quad S_3 = b_3P_1 - a_3R_2 \\
P_4 &= (c_4 - \lambda)P_3 - b_4d_3P_2 - a_4e_2[(c_3 - \lambda)P_1 - a_3e_1P_0] \\
&\quad + a_4d_3R_3 + b_4e_2S_3; \\
R_4 &= d_3P_2 - e_2S_3; \quad S_4 = b_4P_2 - a_4R_3.
\end{aligned}$$

for $i = 5(1)n - 1$,

$$\begin{aligned}
P_i &= (c_i - \lambda)P_{i-1} - b_id_{i-1}P_{i-2} \\
&\quad - a_ie_{i-2}[(c_{i-1} - \lambda)P_{i-3} - a_{i-1}e_{i-3}P_{i-4}] \\
&\quad + a_id_{i-1}R_{i-1} + b_ie_{i-2}S_{i-1}; \\
R_i &= d_{i-1}P_{i-2} - e_{i-2}S_{i-1}; \quad S_i = b_iP_{i-2} - a_iR_{i-1}
\end{aligned}$$

and finally for $i = n$,

$$\det(C - \lambda I) = P_n = (c_n - \lambda)P_{n-1} - b_nd_{n-1}P_{n-2} - a_ne_{n-2}[(c_{n-1} - \lambda)P_{n-3} - a_{n-1}e_{n-3}P_{n-4}] + a_nd_{n-1}R_{n-1} + b_ne_{n-2}S_{n-1}. \quad (2.6)$$

Similarly, the evaluation of $P'_n(\lambda) = \frac{d}{d\lambda} [\det(C - \lambda I)]$ can be

carried out by the formulae listed below:

$$\begin{aligned}
P'_0 &= 0; \quad R'_0 = 0; \quad S'_0 = 0 \\
P'_1 &= -1; \quad R'_1 = 0; \quad S'_1 = 0 \\
P'_2 &= (c_2 - \lambda)P'_1 - b_2d_1P'_0 - P_1; \quad R'_2 = 0; \quad S'_2 = 0 \\
P'_3 &= (c_3 - \lambda)P'_2 - b_3d_2P'_1 - P_2 + a_3e_1; \\
R'_3 &= d_2P'_1; \quad S'_3 = b_3P'_1 \\
P'_4 &= (c_4 - \lambda)P'_3 - b_4d_3P'_2 + a_4e_2P_1 \\
&\quad - a_4e_2[(c_3 - \lambda)P'_1 - a_3e_1P'_0] + a_4d_3R'_3 \\
&\quad + b_4e_2S'_3 - P_3; \\
R'_4 &= d_3P'_2 - e_2S'_3; \quad S'_4 = b_4P'_2 - a_3R'_3
\end{aligned}$$

for $i = 5(1)n - 1$;

$$\begin{aligned}
P'_i &= (c_i - \lambda)P'_{i-1} - b_id_{i-1}P'_{i-2} - P_{i-1} + a_ie_{i-2}P_{i-3} \\
&\quad - a_ie_{i-2}[(c_{i-1} - \lambda)P'_{i-3} - a_{i-1}e_{i-3}P'_{i-4}] \\
&\quad + a_id_{i-1}R'_{i-1} + b_ie_{i-2}S'_{i-1}; \\
R'_i &= d_{i-1}P'_{i-2} - e_{i-2}S'_{i-1}; \quad S'_i = b_iP'_{i-2} - a_iR'_{i-1} \quad (2.7)
\end{aligned}$$

with $i = n$,

$$\begin{aligned}
\frac{d}{d\lambda} [\det(C - \lambda I)] &= P'_n = (c_n - \lambda)P'_{n-1} - b_nd_{n-1}P'_{n-2} \\
&\quad - P_{n-1} + a_ne_{n-2}P_{n-3} \\
&\quad - a_ne_{n-2}[(c_{n-1} - \lambda)P'_{n-3} - a_{n-1}e_{n-3}P'_{n-4}] \\
&\quad + a_nd_{n-1}R'_{n-1} + b_ne_{n-2}S'_{n-1}.
\end{aligned}$$

Finally, the two recursive formulae (2.6) and (2.7) are used in Newton's iterative method for finding an eigenvalue of the matrix C , in the form

$$\lambda_{k+1} = \lambda_k - [P_n(\lambda_k)/P'_n(\lambda_k)], \quad k \geq 0. \quad (2.8)$$

where λ_0 is an initial estimate.

If the root is simple, then this method has quadratic convergence, that is

$$|\lambda_{k+1} - \lambda| \propto |\lambda_k - \lambda|^2. \quad (2.9)$$

However, if the root to which the process is converging is multiple then (2.9) has linear convergence. It is possible to modify the formula to take account of multiplicity of roots if we know the order of multiplicity of the root. In general, we will not have this information available.

Alternatively, having found λ_1 by Newton's method, we may switch to the more efficient Secant iterative method,

$$\lambda_{k+1} = \lambda_k - (\lambda_k - \lambda_{k-1})P_n(\lambda_k)/[P_n(\lambda_k) - P_n(\lambda_{k-1})], \quad k \geq 1. \quad (2.10)$$

The iteration is continued until satisfactory convergence to the eigenvalue λ is obtained, i.e. until $|(\lambda_{k+1} - \lambda_k)/\lambda_k| < \epsilon$, where ϵ is a small specified tolerance.

Having computed one or more of the eigenvalues by any of the above techniques, it is desirable to ensure that in further searches for eigenvalues, we do not redetermine those already

found. Thus, we require some technique of suppressing the known eigenvalues. The recommended technique is as follows. If approximations $\lambda^{(1)}, \dots, \lambda^{(s)}$ to eigenvalues are known, then instead of iterating with $P_n(\lambda)$ use

$$G_n(\lambda) = P_n(\lambda) / \prod_{i=1}^s (\lambda - \lambda^{(i)}). \quad (2.11)$$

Note that $G_n(\lambda)$ is again implicitly defined through the implicit determination of $P_n(\lambda)$ and the derivative of $G_n(\lambda)$ for use in Newton's method is given by

$$G'_n(\lambda) = G_n(\lambda) \left\{ P'_n(\lambda)/P_n(\lambda) - \sum_{i=1}^s (\lambda - \lambda^{(i)})^{-1} \right\}, \quad (2.12)$$

from which an expression for $G'_n(\lambda)/G_n(\lambda)$ can be obtained.

3. The symmetric case

When the quindagonal matrix C is symmetric, i.e.,

$$d_i = b_{i+1}, \quad i = (1)n - 1 \text{ and } e_j = a_{j+2}, \quad j = 1(1)n - 2,$$

the recursive sequence (2.2) and (2.3) become,

$$\begin{aligned}
P_0 &= 1 \\
P_1 &= (c_1 - \lambda)P_0, \\
P_2 &= (c_2 - \lambda)P_1 - b_2^2P_0, \\
P_3 &= (c_3 - \lambda)P_2 - b_3^2P_1 - a_3^2(c_2 - \lambda) + 2a_3b_2b_3, \quad (3.1)
\end{aligned}$$

and

$$\begin{aligned}
P_4 &= (c_4 - \lambda)P_3 - b_4^2P_2 - a_4^2\{(c_3 - \lambda)P_1 - a_3^2P_0\} \\
&\quad + 2a_4b_4\{b_3P_1 - b_2a_3P_0\}.
\end{aligned}$$

Further applications of the bordering technique developed in Section 2, produces the recursive sequence P_i for $i = 5, 6, \dots$ in the simpler form

$$\begin{aligned}
P_i &= (c_i - \lambda)P_{i-1} - b_i^2P_{i-2} - a_i^2\{(c_{i-1} - \lambda)P_{i-3} - a_{i-1}^2P_{i-4}\} \\
&\quad + 2a_ib_i\{b_{i-1}P_{i-3} - b_{i-2}a_{i-1}P_{i-4} \\
&\quad + b_{i-3}a_{i-1}a_{i-2}P_{i-5} - \dots\}
\end{aligned}$$

and finally in a more compact notation, for $i = n$,

$$\begin{aligned}
P_n &= (c_n - \lambda)P_{n-1} - b_n^2P_{n-2} \\
&\quad - a_n^2\{(c_{n-1} - \lambda)P_{n-3} - a_{n-1}^2P_{n-4}\} \\
&\quad + 2 \sum_{j=1}^{n-2} (-1)^{j+1} b_n b_{n-j} \left[\prod_{r=n-j+1}^n a_r \right] P_{n-j+2}. \quad (3.2)
\end{aligned}$$

Now since the polynomials $P_0, P_1, P_2, \dots, P_{n-1}, P_n$ form a sequence consisting of the leading principal minors of $|C - \lambda I|$, where C is a symmetric quindagonal matrix, then they form a properly signed interleaved sequence of polynomials (i.e. all $P_k(\lambda) > 0$ for a sufficiently large value of λ either positive or negative and the zeros of $P_k(\lambda)$ strictly separate those of $P_{k+1}(\lambda)$) and thus with the aid of the separation theorem (Wilkinson, 1965), it can be shown that the sequence of polynomials P_0, P_1, \dots, P_n form a Sturm sequence of polynomials in the interval $(-\infty, +\infty)$.

The fundamental property of such polynomials facilitate the calculation of the roots by the process of bisection, i.e. the number of disagreements in the sign $s(\lambda)$ in the sequence P_i , $i = 0, 1, 2, \dots, n$ being equal to the number of roots of $P_n(\lambda)$ smaller than λ .

From Gerschgorins' theorem, the eigenvalues are all contained in the union of the n intervals

$$c_i \pm (|b_i| + |b_{i+1}| + |a_i| + |a_{i+2}|), \quad i = 1, 2, \dots, n$$

with

$$b_1 = b_{n+1} = a_1 = a_2 = a_{n+1} = a_{n+2} = 0.$$

Hence the expression

$$\max \left\{ c_i \pm (|b_i| + |a_i| + |b_{i+1}| + |a_{i+2}|) \right\}, \quad (3.3)$$

can be input to the bisection process as initial upper and lower bounds for the eigenvalues.

To carry out the above algorithm in floating point arithmetic without the fear of underflow and overflow occurring, we follow

a similar procedure to Barth, *et al.* (1967) and replace the sequence of polynomials $P_i(\lambda)$ by the sequence $p_i(\lambda)$ defined by

$$p_i(\lambda) = P_i(\lambda)/P_{i-1}(\lambda), \quad (i = 1, 2, \dots, n) \quad (3.4)$$

The polynomials $p_i(\lambda)$ can be shown with a little analysis to satisfy the relationships,

$$\begin{aligned} p_0 &= 1, \\ p_1 &= (c_1 - \lambda), \\ p_2 &= (c_2 - \lambda) - b_2^2/p_1, \\ p_3 &= (c_3 - \lambda) - b_3^2/p_2 - a_3^2(c_2 - \lambda)/p_2p_1 + 2a_3b_2b_3/p_2p_1, \\ \dots \\ p_n &= (c_n - \lambda) - b_n^2/p_{n-1} - a_n^2\{(c_{n-1} - \lambda)/p_{n-1}p_{n-2} \\ &\quad - a_{n-1}^2/p_{n-1}p_{n-2}p_{n-3}\} + \\ &\quad 2 \sum_{j=1}^{n-2} (-1)^{j+1} b_n b_{n-j} \left[\frac{(a_n/p_{n-j-1}p_{n-j})}{\prod_{r=n-j+1}^{n-1} (a_r/p_r)} \right]. \quad (3.5) \end{aligned}$$

With the use of the modified sequence of polynomials p_i , $i = 0, 1, 2, \dots, n$ in (3.5), we find that the number of negative p_i now gives $s(\lambda)$, the number of eigenvalues smaller than λ .

The calculation of the products p_1p_2 , $p_1p_2p_3$, etc in the sequence (3.5) also requires careful consideration when λ is close to an eigenvalue to ensure numerical stability.

4. Numerical results

The recursive algorithmic process given by the relationship (2.6) and (2.7) was checked for validity by obtaining the eigenvalues of the quindagonal matrix

$$S = \begin{bmatrix} a^2 + bc, & 2ab, & b^2, & & & 0 \\ 2ca, & a^2 + 2bc, & 2ab, & & & \\ c^2, & 2ca, & a^2 + 2bc, & & & -b^2 \\ & & 2ca, & & & a^2 + 2bc, & 2ab, \\ & 0 & c^2, & 2ca, & & a^2 + bc \end{bmatrix} = J^2$$

where $J = \text{tridiag}(c, a, b)$. The eigenvalues of J are known to be

$$\lambda_s = a + 2\sqrt{bc} \cos \{s\pi/(N + 1)\}, \quad s = 1, 2, \dots, N \quad (4.1)$$

An ALGOL program using equations (2.8) and (2.10) was completed for the Loughborough University ICL 1904A computer and a starting approximation of

$$\lambda_0 = [a + 2\sqrt{bc} \cos(\pi/N)]^2$$

was used in the iteration process. The results obtained for the matrix $S = J^2$ where $J = \text{tridiag}(1, 2, 2)$ of order 10 correct to 7 significant places in decreasing order were as follows:

0.22220438,2; 0.19179357,2; 0.14839644,2; 0.10080441,2;
0.57721367,1; 0.25519195,1; 0.68067270,0; 0.50959032,0;
0.14396281,0; 0.21837196, -1;

which agree exactly with the theoretical results obtained from using (4.1).

Similarly, an ALGOL procedure based on the program given by Barth, *et al.* (1967) which computes the eigenvalues of the (10×10) test matrix, i.e.

$$\begin{bmatrix} 5 & -4 & 1 & & & & & & & \\ -4 & 6 & -4 & 1 & & & & & & 0 \\ 1 & -4 & 7 & -4 & 1 & & & & & \\ & & 1 & -4 & 12 & -4 & & & & -1 \\ & & & & 1 & -4 & 13 & -4 & & \\ & 0 & & & & 1 & -4 & 14 & & \\ & & & & & & & 1 & -4 & 14 \end{bmatrix},$$

by the method of bisection using the Sturm sequence of polynomials p_i , $i = 1, 2, \dots, n$ given by (3.6) yields the following results correct to 7 significant figures

2.0588891,1; 1.7336869,1; 1.4616481,1; 1.1943311,1;
9.4729464,0; 7.5412116,0; 5.9764481,0; 4.3530204,0;
2.5718218,0; 5.9900089, -1.

Both ALGOL programs are presented in section 5.

5. ALGOL programs

```

procedure quindiageigen (a, b, cc, d, e, lambda1, n, eps);
value n;
integer n;
array a, b, cc, d, e;
real lambda1, eps;
comment Procedure determines by the Newton iteration method
the eigenvalue of a pentadiagonal matrix where the array cc
denotes the diagonal, b and d the lower and upper sub-diagonal,
and a and e the lower and upper sub sub-diagonal elements.
Iteration is continued until the eigenvalue lambda1 is obtained
to an accuracy specified by eps, m being the iteration count.
begin
integer i, m;
real lambda2;
array c, p, pd, r, s[0:n];
13: for i := 1 step 1 until n do
begin
c[i] := cc[i] - lambda1;
end;
m := m + 1;
p[0] := 1; r[1] := s[1] := 1; p[1] := c[1];
r[2] := d[1]; s[2] := b[2];
p[2] := c[2] × p[1] - b[2] × d[1] × p[0];
r[3] := d[2] × p[1] - e[1] × s[2];
s[3] := b[3] × p[1] - a[3] × r[2];
p[3] := c[3] × p[2] - b[3] × d[2] × p[1] - a[3] × e[1]
× c[2] + a[3] × d[2] × r[2] + b[3] × e[1] × s[2];
for i := 4 step 1 until n do
begin
r[i] := d[i - 1] × p[i - 2] - e[i - 2] × s[i - 1];
s[i] := b[i] × p[i - 2] - a[i] × r[i - 1];
p[i] := c[i] × p[i - 1] - b[i] × d[i - 1] × p[i - 2]
- a[i] × e[i - 2] × (c[i - 1] × p[i - 3] - a[i - 1]
× e[i - 3] × p[i - 4]) + a[i] × d[i - 1] × r[i - 1]
+ b[i] × e[i - 2] × s[i - 1];
end;
pd[0] := r[1] := s[1] := 0;
pd[1] := -1; r[2] := s[2] := 0;
pd[2] := c[2] × pd[1] - b[2] × d[1] × pd[0] - p[1];
r[3] := d[2] × pd[1]; s[3] := b[3] × pd[1];
pd[3] := c[3] × pd[2] - b[3] × d[2] × pd[1] - p[2] +
a[3] × e[1];
for i := 4 step 1 until n do
begin
r[i] := d[i - 1] × pd[i - 2] - e[i - 2] × s[i - 1];
s[i] := b[i] × pd[i - 2] - a[i] × r[i - 1];
pd[i] := c[i] × pd[i - 1] - b[i] × d[i - 1] ×
pd[i - 2] - p[i - 1] + a[i] × e[i - 2] ×
p[i - 3] - a[i] × e[i - 2] × (c[i - 1] × pd[i - 3] -
a[i - 1] × e[i - 3] × pd[i - 4]) + a[i] × d[i - 1] ×
r[i - 1] + b[i] × e[i - 2] × s[i - 1];
end;
lambda2 := lambda1 - p[n]/pd[n];
if abs((lambda2 - lambda1)/lambda1) < eps then goto 12;
lambda1 := lambda2;
goto 13;
12: end of quindiageigen;
procedure quindibisect (c, b, d, dd, beta, 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 $c, b, d, dd, x, \text{beta}$;
comment c is the diagonal, b the sub-diagonal, d the sub sub-diagonal, beta the squared sub-diagonal and dd the squared sub sub-diagonal of a symmetric quindagonal matrix of order n . Input to vectors $b[i], \text{beta}[i], d[i]$ should begin with $i = 2, 2, 3$ 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 2^{-t} . The eigenvalues $\text{lambda}[m1], \dots, \text{lambda}[m2]$, where $m2$ is not less than $m1$ and $\text{lambda}[i + 1]$ is not less than $\text{lambda}[i]$, 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 equal to zero;

```
begin real h, xmin, xmax; integer i;
comment Calculation of xmin, xmax;
d[1] := d[2] := 0;
dd[1] := dd[2] := 0;
beta[1] := 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(d[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 xl, xu, xo; array wu[m1:m2],
p[1:n];
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 integer r, j;
array p[0:n];
real prod, prod2, sum, prod p;
z := z + 1
comment sturm sequence;
a := 0; p[0] = 0;
p[1] := c[1] - x1;
if p[1] < 0 then a := a + 1;
p[2] := (c[2] - x1) - beta[2]/(if p[1] # 0
then p[1] else relfeh);
if p[2] < 0 then a := a + 1;
p[3] := (c[3] - x1) - beta[3]/(if p[2] # 0
then p[2] else relfeh)
- dd[3] * (c[2] - x1)/(if (p[2] * p[1]) # 0
then (p[2] * p[1]) else relfeh)
+ 2 * d[3] * b[2] * b[3]/(if (p[2] * p[1]) # 0
then (p[2] * p[1]) else relfeh);
if p[3] < 0 then a := a + 1; prodp = p[1] * p[2];
for i := 4 step 1 until n do
begin
sum := 0;
prod2 := 1;
prodp := prodp * p[i - 1];
for j := i - 2 step -1 until 1 do
begin
prod := 1;
For r := i - j + 1 step 1 until i do prod :=
prod * d[r];
prod2 := prod2 * p[i - j - 2];
sum := sum + 2 * ((-1)^(j + 1)) *
b[i - j] * prod * prod2;
end j;
p[i] := (c[i] - x1) - beta[i]/(if p[i - 1] # 0
then p[i - 1] else relfeh) - dd[i]
* ((c[i - 1] - x1)/(if (p[i - 1]
* p[i - 2]) # 0 then (p[i - 1]
* p[i - 2]) else relfeh) - dd[i - 1]/
if (p[i - 1] * p[i - 2] * p[i - 3]) # 0
then (p[i - 1] * p[i - 2] *
* p[i - 3]) else relfeh)) + sum;
if prodp ne 0 then prodp else relfeh);
if p[i] < 0 then a := a + 1;
end i;
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 quindibisect;
```

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