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A RECURSIVE RELATION FOR THE DETERMINANT OF A PENTADIAGONAL MATRIX

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ABSTRACT. A recursive relation is developed for the determinant of a pentadiagonal matrix S which satisfies $s_{i,j} \neq 0$ for $|i - j| = 1$. When S is symmetric, one has a six-term recursive relation. An example is given to illustrate its use in the computation of eigenvalues.

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1. Introduction.

Pentadiagonal matrices arise frequently in numerical analysis. They are usually encountered in approximation to fourth derivatives, high order approximations to second derivatives, and as intermediate steps in Givens' and Householder's method for determining eigenvalues. It seems relevant, therefore, to investigate the structure of the determinant of such a matrix with the hope of developing a good method for determining the eigenvalues. For this task we let

$$\begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & & & \\ s_{21} & s_{22} & s_{23} & s_{24} & & & \\ s_{31} & s_{32} & s_{33} & s_{34} & & & \\ 0 & s_{42} & s_{43} & s_{44} & & & \\ & & & & \cdots & & \\ & & & & & s_{n-1,n-1} & s_{n-1,n} \\ & & & & & s_{n,n-1} & s_{nn} \end{bmatrix} , \qquad (1)$$

where we assume that

$$s_{ij} = 0 , \quad \text{if } |i - j| < 2 , \quad \text{and}$$

$$s_{ij} \neq 0 , \quad \text{if } |i - j| = 1 .$$

2. Properties of the Matrix.

<u>Definition</u>. The product

$$s_{i_1 i_2} s_{i_2 i_3} \cdots s_{i_{k-1} i_k} s_{i_k i_1} , \qquad (2)$$

$i_1, i_2, \ldots, i_k$ distinct, is called a cycle of length k. The cycle is non-zero if the product (2) is non-zero.

Lemma 1. In (1) a non-zero cycle of length k, $3 \leq k \leq n$, can occur only in a principal submatrix with a least k consecutive indices.

Proof: If suffices to show that a non-zero k-cycle cannot occur in the principal submatrix

$$S[i, i+1, \ldots, i+j, i+j+2, i+j+3, \ldots, i+k] ,$$

i.e. the matrix containing the indicated rows and columns. It is clear that any cycle must contain $s_{i+j,i+j+2}$. But now, to return to the index i we cannot use the indices $i+j$ or $i+j+2$. From the band structure of S it is clear that no other indices are available to return to i.

Lemma 2. In a principal submatrix of S consisting of k consecutive indices, $k \geq 3$, there are exactly two non-zero k-cycles.

Proof: Clearly, it suffices to show this for the principal submatrix $S[1, 2, \ldots, k]$.

At the index i, $1 \leq i \leq k-2$, we can proceed to either $i+1$ or $i+2$. If $i+1$ is chosen, then we must return by the index $i+2$. Then we have no choice except to proceed to $i+3$. If $i+2$ is chosen, we must reserve $i+1$ for the return. Hence, we must proceed to $i+4$.

Starting at $i=1$ by either s_{12} or s_{13}, we have only the two k-cycles

$$s_{12} s_{24} s_{46} \cdots s_{53} s_{31} \tag{3}$$

and

$$s_{13} s_{35} s_{57} \cdots s_{42} s_{21} . \tag{4}$$

We will denote (3) by $Cy(1,k)$ and (4) by the suggestive notation $\overset{t}{Cy}(1,k)$. This notation is prompted by the fact that transposing the indices of the elements of the product $Cy(1,k)$ gives the cycle $\overset{t}{Cy}(1,k)$.

For notational convenience let us define the quantities

$$\left.\begin{aligned} a_i &= s_{ii} && (i=1,2,\ldots,n) \\ b_i &= s_{i,i+1}s_{i+1,i} && (i=1,2,\ldots,n-1) \\ \beta_i &= s_{i,i+2}s_{i+2,i} && \\ c_i &= s_{i,i+1}s_{i+1,i+2}s_{i+2,i} && \end{aligned}\right\} \; (i=1,2,\ldots,n-2) . \qquad (5)$$

We see that these are just the one-, two-, and three-cycles of S. By assumption $b_i \neq 0$ $(i=1,2,\ldots,n-1)$.

The key to the recursive relation lies in the fact that all cycles of length greater than three can be written in terms of the quantities in (5). This fact is proved in the following lemma.

Lemma 3. For the matrix S defined in (1) the following formulas are valid for $m = 2,3,\ldots,[\frac{1}{2}n]$,

$$Cy(1,2m) = \frac{c_1 \overset{t}{c}_2 c_3 \overset{t}{c}_4 \cdots c_{2m-3} \overset{t}{c}_{2m-2}}{b_2 b_3 \cdots b_{2m-2}}$$

$$Cy(1,2m+1) = \frac{c_1 \overset{t}{c}_2 \cdots c_{2m-3} \overset{t}{c}_{2m-2} c_{2m-1}}{b_2 b_3 \cdots b_{2m-2} b_{2m-1}} . \qquad (6)$$

Proof: We prove this lemma by induction on m. For $m=2$, we can write

$$Cy(1,4) = s_{12}s_{24}s_{45}s_{53}s_{31} = \frac{(s_{12}s_{23}s_{31})(s_{24}s_{43}s_{32})}{s_{23}s_{32}} = \frac{c_1 \overset{t}{c}_2}{b_2}$$

and

$$Cy(1,5) = s_{12}s_{24}s_{45}s_{53}s_{31} = \frac{(s_{12}s_{24}s_{43}s_{31})(s_{45}s_{53}s_{34})}{s_{34}s_{43}} = Cy(1,4)\frac{c_3}{b_3}$$

$$= \frac{c_1 c_2^t c_3}{b_2 b_3} \quad .$$

Hence, (6) is true for $m=1$. Assume (6) is true for all $m \le k-1$. Then

$$Cy(1,2k) = s_{12}\cdots s_{2k-4,2k-2}s_{2k-2,2k}s_{2k,2k-1}s_{2k-1,2k-3}\cdots s_{31}$$

$$= (s_{12}\cdots s_{2k-4,2k-2}s_{2k-2,2k-1}s_{2k-1,2k-3}\cdots s_{31})$$

$$\cdot \frac{(s_{2k-2,2k}s_{2k,2k-1}s_{2k-1,2k-2})}{s_{2k-2,2k-1}s_{2k-1,2k-2}}$$

Therefore,

$$Cy(1,2k) = Cy(1,2k-1)\frac{c_{2k-2}^t}{b_{2k-2}}$$

$$= \frac{c_1 c_2^t \cdots c_{2k-3} c_{2k-2}^t}{b_2 \cdots b_{2k-3} b_{2k-2}}$$

and

$$Cy(1,2k+1) = s_{12}\cdots s_{2k-2,2k}s_{2k,2k+1}s_{2k+1,2k-1}\cdots s_{31}$$

$$= (s_{12}\cdots s_{2k-2,2k}s_{2k,2k-1}s_{2k-1,2k-3}\cdots s_{31}$$

$$\cdot \frac{(s_{2k,2k+1}s_{2k+1,2k-1}s_{2k-1,2k})}{s_{2k,2k-1}s_{2k-1,2k}}$$

$$= Cy(1,2k)\ \frac{c_{2k-1}}{b_{2k-1}} = \frac{c_1 c_2^t \cdots c_{2k-2}^t c_{2k-1}}{b_2 \cdots b_{2k-2} b_{2k-1}} \quad .$$

Hence, (6) is true for $m=k$, and therefore, true for all $m=2,3,\ldots[\frac{1}{2}n]$.

Clearly, we also have the formulas

$$\overset{t}{Cy}(1,2m) = \frac{\overset{t}{c_1}c_2\cdots\overset{t}{c}_{2m-3}c_{2m-2}}{b_2\cdots b_{2m-2}}$$

$$= \overset{t}{Cy}(1,2m-1)\,\frac{c_{2m-2}}{b_{2m-2}}$$

$$Cy^t(1,2m+1) = \frac{\overset{t}{c_1}c_2\cdots c_{2m-2}\overset{t}{c}_{2m-1}}{b_2\cdots b_{2m-1}} \tag{7}$$

$$= \overset{t}{Cy}(1,2m)\,\frac{\overset{t}{c}_{2m-1}}{b_{2m-1}}\;.$$

It is also clear that the index 1 can be replaced by an arbitrary number i in the expressions (6) and (7).

3. The Recursive Relation.

Let us denote $S\begin{pmatrix}1 & 2 & \ldots & k\\ 1 & 2 & \ldots & k\end{pmatrix}$ by d_k. Using a special case of a determinant formula of Maybee[1], we have that

$$d_n = a_n d_{n-1} - b_{n-1}d_{n-2} - \beta_{n-2} S\begin{pmatrix}1 & 2 & \ldots & n-3 & n-1\\ 1 & 2 & \ldots & n-3 & n-1\end{pmatrix}$$

$$+ \sum_{k=3}^{n} (-1)^{k+1} \left(\sum \mathcal{C}_\rho(n,k)\right) d_{n-k}\;, \tag{8}$$

where $\sum \mathcal{C}(n,k)$ is the sum of all cycles of length k containing the index n.

But, from the previous lemmas we know that there are exactly two non-zero cycles of length k with index n, hence

$$\sum \wp(n,k) = Cy(n-k+1,K) + \overset{t}{Cy}(n-k+1,k) \quad .$$

Let us write out the sum in (8) for n even, i.e. $n=2m$.

$$\sum_{k=3}^{n} \cdots = (c_{n-2} + \overset{t}{c}_{n-2})d_{n-3} - \left(\frac{c_{n-3}\overset{t}{c}_{n-2}}{b_{n-2}} + \frac{\overset{t}{c}_{n-3}c_{n-2}}{b_{n-2}}\right) d_{n-4}$$

$$+ \left(\frac{c_{n-4}\overset{t}{c}_{n-3}c_{n-2}}{b_{n-3}b_{n-2}} + \frac{\overset{t}{c}_{n-4}c_{n-3}\overset{t}{c}_{n-2}}{b_{n-3}b_{n-2}}\right) d_{n-5} - \cdots$$

$$- \left(\frac{c_1\overset{t}{c}_2\cdots c_{n-3}\overset{t}{c}_{n-2}}{} + \frac{\overset{t}{c}_1c_2\cdots \overset{t}{c}_{n-3}c_{n-2}}{b_2\cdots b_{n-2}}\right) d_0$$

$$= c_{n-2}\left[d_{n-3} - \frac{\overset{t}{c}_{n-3}}{b_{n-2}}d_{n-4} + \frac{\overset{t}{c}_{n-3}c_{n-4}}{b_{n-2}b_{n-3}}d_{n-5} - \cdots - \frac{\overset{t}{c}_1\cdots \overset{t}{c}_{n-3}}{b_2\cdots b_{n-2}}d_0\right]$$

$$+ \overset{t}{c}_{n-2}\left[d_{n-3} - \frac{c_{n-3}}{b_{n-2}}d_{n-4} + \frac{c_{n-3}\overset{t}{c}_{n-4}}{b_{n-2}b_{n-3}}d_{n-5} - \cdots - \frac{c_1\cdots c_{n-3}}{b_2\cdots b_{n-2}}d_0\right] \quad .$$

Denote the expression multiplying c_{n-2} by ϵ_{n-2} and the expression multiplying $\overset{t}{c}_{n-2}$ by e_{n-3}. Writing out the same sum for $n = 2m+1$, we get

$$\sum_{k=3}^{n} \cdots = c_{n-1}\left[d_{n-2} - \frac{c^t_{n-2}}{b_{n-1}}\left(d_{n-3} - \frac{c_{n-3}}{b_{n-2}} d_{n-4} + \cdots - \frac{c_1 c^t_2 \cdots c_{n-3}}{b_2 \cdots b_{n-2}} d_0\right)\right]$$

$$+ c^t_{n-1}\left[d_{n-2} - \frac{c_{n-2}}{b_{n-1}}\left(d_{n-3} - \frac{c^t_{n-3}}{b_{n-2}} d_{n-4} + \cdots - \frac{c^t_1 c_2 \cdots c^t_{n-3}}{b_2 \cdots b_{n-2}} d_0\right)\right] .$$

The expressions multiplying c_{n-1} and c^t_{n-1} respectively, are

$$\epsilon_{n-2} = d_{n-2} - \frac{c^t_{n-2}}{b_{n-1}} e_{n-3}$$

$$e_{n-2} = d_{n-2} - \frac{c_{n-2}}{b_{n-1}} \epsilon_{n-3} \quad . \tag{9}$$

These formulas hold in general. Considering the expansion (8) for $n = 2$, we see that we must have

$$\epsilon_{-1} = e_{-1} = 0 \quad .$$

The minor in (8) multiplying β_{n-2} can be written as

$$S\begin{pmatrix} 1 & 2 & \cdots & n-3 & n-1 \\ 1 & 2 & \cdots & n-3 & n-1 \end{pmatrix} = a_{n-1} d_{n-3} - \beta_{n-3} d_{n-4} \quad .$$

We can now state the algorithm:

Set $d_{-1} = 0,\ d_0 = 1,\ d_1 = a_1,\ d_2 = a_1 a_2 - b_1,\ \epsilon_{-1} = e_{-1} = 0$,

and compute

$$\delta_{k-2} = a_{k-1}d_{k-3} - \beta_{k-3}d_{k-4}$$

$$\epsilon_{k-3} = d_{k-3} - \frac{c^t_{k-3}}{b_{k-2}} e_{k-4}$$

$$e_{k-3} = d_{k-3} - \frac{c_{k-3}}{b_{k-2}} \epsilon_{k-4}$$

$$d_k = a_k d_{k-1} - b_{k-1}d_{k-2} - \beta_{k-2}\delta_{k-2} + c_{k-2}\epsilon_{k-3} + c^t_{k-2}e_{k-3}, \tag{10}$$

for $k = 3,4,\ldots,n$.

If S is cyclicly symmetric, i.e. $c_i = c^t_i$ $(i = 1,2,\ldots n-2)$, then the recursive relation can be simplified greatly. For, adding $\frac{c_{k-2}}{b_{k-2}} d_{k-1}$ to d_k and expanding, we eliminate the term containing e_{k-3} . We arrive at the 6-term recursive relation

$$d_k = \left(a_k - \frac{c_{k-2}}{b_{k-2}}\right) d_{k-1} - \left(b_{k-1} - \frac{a_{k-1}c_{k-2}}{b_{k-2}}\right) d_{k-2}$$

$$- \left(\beta_{k-2}a_{k-1} - c_{k-2}\right)d_{k-3} + \beta_{k-3}\left(\beta_{k-2} - \frac{a_{k-2}c_{k-2}}{b_{k-2}}\right)d_{k-4}$$

$$+ \frac{\beta_{k-3}\beta_{k-4}c_{k-2}}{b_{k-2}} d_{k-5} \tag{11}$$

If S is symmetric, then it is cyclicly symmetric, so (11) holds. Also, if S is tridiagonal, we have

$$\beta_k = c_k = c_k^t = 0 \qquad (k = 1,2,\ldots,n-2) \ ,$$

and the algorithm becomes the well-known three-term relation for computing the determinant of a tridiagonal matrix.

For S not cyclicly symmetric, a 7-term recursive relation may be derived which eliminates the factors ϵ_{k-3} and e_{k-3} from (10). It is very complicated and will not be given here.

4. An Example.

Consider finding the eigenvalues of the matrix of order 25

$$S = \begin{pmatrix} 5 & 4 & 1 & & & & \\ 4 & 6 & 4 & 1 & & & \\ 1 & 4 & 6 & 4 & 1 & & \\ & & \cdot & \cdot & \cdot & & \\ & & & & & 6 & 4 \\ & & & & & 4 & 5 \end{pmatrix} = J^2 \ ,$$

where $J = \text{tridiag}\{1,2,1\}$. The eigenvalues of J are

$$\lambda_i = 2 - 2 \cos \frac{i\pi}{26} \qquad (i = 1,2,\ldots,25) \ .$$

so the eigenvalues of S are just λ_i^2 . Differentiation of (11) gives a recursive relation for the derivative of the characteristic polynomial.

Newton's method was programmed in FORTRAN IV and using the IBM 360/50 the first 13 eigenvalues, $\tilde{\lambda}_i$, were computed. The results were

i	$\tilde{\lambda}_i$	$\lambda_i^2 - \tilde{\lambda}_i (\times 10^7)$
1	0.0002123	3.0
2	0.0033773	2.0
3	0.0168916	-1.0
4	0.0524811	2.0
5	0.1253387	0.0
6	0.2529873	0.0
7	0.4539454	-3.0
8	0.7462722	-1.0
9	1.1460857	-12.0
10	1.6661396	-5.0
11	2.3145628	-12.0
12	3.0938234	-11.0
13	4.0000000	0.0

All computation was done in double precision and required about 6 seconds of execution time.

REFERENCES

[1] Maybee, J. S. and Quirk, J. "Qualitative Problems in Matrix Theory," to appear in SIAM Review.