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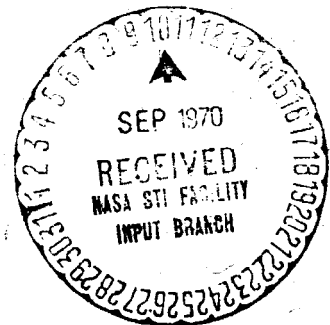
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TRIANGULAR DECOMPOSITION AS AN AID IN DETERMINING EIGENVALUES OF LARGE-ORDER BANDED SYMMETRIC MATRICES

EDWARD F. PUCCINELLI

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**TRIANGULAR DECOMPOSITION
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REPORT STATUS

This report shows how to use a little-known theorem as an aid in the determination of the eigenvalues in an interval of the real axis for large-order real symmetric matrices.

AUTHORIZATION

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Edward F. Puccinelli
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SUMMARY

In determining a subset of eigenvalues of the eigenspectrum of a real symmetric matrix one can not always be sure that all the eigenvalues in a certain region of the real axis have been found.

This report describes how triangular decomposition, an essential step in many eigenvalue solution methods, can form a Sturm sequence. By forming two Sturm sequences the number of eigenvalues in any region of the real axis can be determined.

First, matrix decomposition is discussed followed by a description of how a symmetric matrix decomposition (i.e. a decomposition which preserves eigenvalues) can always be made. Next it is shown how the diagonal terms of the U matrix in a symmetric LU decomposition form a Sturm sequence and finally how this information can be used in conjunction with the determinant method of eigenvalue solution

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TRIANGULAR DECOMPOSITION
AS AN AID IN DETERMINING EIGENVALUES
OF LARGE-ORDER BANDED SYMMETRIC MATRICES

INTRODUCTION

In finding a subset of the eigenvalues of real symmetric matrices, determining that all eigenvalues in a certain interval have been found is often a problem.

The most obvious solution to this problem is to determine the complete eigenspectrum. However, depending upon the order of the matrix, this approach may not be feasible economically.

Another solution to the problem is use of the Sturm sequence method (Reference 2, p. 245) for finding eigenvalues. This method determines one eigenvalue at a time and simultaneously reveals how many eigenvalues occur in a given interval. However, for large-order matrices, most of the computational work used by this method involves tri-diagonalizing the matrix. Tri-diagonalization requires about as many computations for a banded matrix as it does for a full matrix, so analysts frequently use methods which require fewer computations for banded matrices.

Examples of simpler methods are the determinant and the inverse power with shifts methods (Reference 3, Section 10). Both of these methods use triangular decomposition rather than tri-diagonalization. Dependent upon the number of eigenvalues sought and the order and bandwidth of the matrix, these two methods may prove faster because the triangular decomposition procedure takes advantage of the bandedness of the matrix. That is, fewer computations are required to decompose a banded matrix than to tri-diagonalize it.

Although for banded matrices such procedures may prove to be less expensive computationally, these procedures do not include determination of the number of eigenvalues in any given interval of interest.

This report shows how a little-known consequence of symmetric matrix decomposition can reveal the number of eigenvalues in any given region. The determinant method of eigenvalue solution included in this report may serve as a model for application to other single-extraction algorithms.

The decomposition algorithm is a relatively simple tool for gathering information for finding the eigenvalues of a matrix. For matrices which are small enough to allow calculation by hand, triangular decomposition is an easy method not only of

determining the number of positive and negative eigenvalues of a matrix, but also of determining the multiplicity of an already known eigenvalue.

In the rest of this report, all matrices referred to are assumed to be real and symmetric unless otherwise specified.

TRIANGULAR DECOMPOSITION OF MATRICES

Definition

A lower triangular matrix is a square matrix $C = (c_{ij})$ such that $c_{ij} = 0$ for $i < j$.

If $c_{ij} = 0$ for $i > j$ then C is called upper triangular.

If $c_{ii} = 1$, $c_{ij} = 0$ for $i < j$ (for $i > j$) then C is lower (upper) unit triangular.

Theorem 1

Given a real symmetric matrix A of order n , none of whose principal minor matrices A_k composed of the first k columns and rows ($k = 1, 2, \dots, n - 1$) has a zero determinant, a unique lower-unit triangular matrix $L = (\ell_{ij})$ and a diagonal matrix $D = (d_{ij})$ exist such that $LDL^T = A$. Moreover:

$$\det(A) = \prod_{i=1}^n d_{ii}^*$$

Theorem 1 establishes the existence of the matrices L and D when A does not have any singular principal minors. Theorem 1 also reveals a simple means of finding the determinant of A .

The elements of D and L are given by:

$$d_{ii} = a_{ii} - \sum_{k=1}^{i-1} \ell_{ik}^2 d_{kk} \quad (1)$$

*Proof of this theorem is in Reference 1, p. 27.

$$\ell_{ij} = \left[a_{ij} - \sum_{k=1}^{j-1} \ell_{ik} d_{kk} \ell_{jk} \right] / d_{jj} \quad i > j \quad (2)$$

The d_{ii} 's are called pivots. The procedure described by Equations (1) and (2) is analogous to Gaussian elimination. If at some stage i , a d_{ii} is equal to zero, Equation (2) cannot be computed. To solve this problem, interchange row i with some row t , ($t > i$), where $a_{ti} \neq 0$. Such a row must exist because theorem 1 ensures decomposability.

ENSURING DECOMPOSABILITY WHILE PRESERVING EIGENVALUES

The decomposition procedure breaks down when the A_k principal minor has a zero determinant, because Equation (1) yields $d_{kk} = 0$ and Equation (2) requires division by d_{kk} .

Because the results included in the following sections apply to decomposable matrices, a useful tool would be a process which could alter the given matrix (while preserving its eigenvalues) and permit a decomposition.

In decomposition procedures, interchanging the rows of a matrix when a zero pivot is encountered permits continuation of the decomposition procedure. However, row interchanges alone generally alter the eigenvalues of the original matrix.

Interchanging the corresponding two columns in addition to interchanging two rows is effectively a similarity transformation on the original matrix and, therefore, does not change its eigenvalues. This method also preserves the symmetry of the original matrix, which is crucial in the proofs of the following sections.

Theorem 2

Given a real symmetric matrix A of order n , at least one of whose principal minor matrices A_k composed of the first k columns and rows ($k = 1, 2, \dots, n-1$) has a zero determinant, a procedure exists for forming a similarity transformation of that matrix such that this similar matrix may be expressed as the product of a lower-unit triangular matrix L and an upper triangular matrix U .

Proof

Let P_{ij} be an elementary matrix which interchanges rows (columns) i and j when A is multiplied on the left (right) by P_{ij} . Then $P_{ij} A P_{ij}$ is similar to A

and differs from A only in that rows i and j are interchanged and columns i and j are interchanged.

Applying this proof to the decomposition procedure, when a zero pivot exists in position i, ($d_{i,i} = 0$), interchange columns and rows i and j, which puts a zero in position $a_{j,j}$. Choose the number j, so that $a_{j,j}$ is the last non-zero term on the diagonal of A. In general $j = n$, even if several similarity transformations must be made.

However, a string of zeroes can occur in positions (i, i) , $(i + 1, i + 1)$, ..., (n, n) in the final D matrix.

In this case the $U = DL^T$ matrix would have the form shown in Figure 1 at some stage of the decomposition.

If this should occur, do not interchange rows and columns but use a different type of similarity transformation. A feasible type of similarity transformation to use would be the 45-degree plane rotation in the $(i + 1, j)$ plane, where j is such that element $(i + 1, j) \neq 0$.

$$\begin{bmatrix}
 u_{11} & u_{12} & \dots & u_{1i} & & u_{1,i+1} & & & u_{1n} \\
 & u_{22} & \dots & u_{2i} & & u_{2,i+1} & & & u_{2n} \\
 & & & & & & & & \\
 & & & & & & & & \\
 & & & & & & & & \\
 & & & & u_{ii} & & & & \\
 & & & & & & u_{i,i+1} & & u_{i,n} \\
 & & & & & & & & \\
 & & & & & & 0 & X & X & \dots & X \\
 & & & & & & X & 0 & X & \dots & X \\
 & & & & & & X & X & 0 & \dots & X \\
 & & & & & & \dots & \dots & \dots & \dots & \dots \\
 & & & & & & \dots & \dots & \dots & \dots & \dots \\
 & & & & & & X & X & X & \dots & 0
 \end{bmatrix}$$

Figure 1. A Possible Decomposition Form

The $(i + 1, i + 1)$ pivot is now non-zero and the decomposition algorithm can proceed. If zero pivots occur again, reapply the similarity transformation logic already described (row-column interchanges first and then plane rotations, if necessary). Figure 2 is a simple flowchart of the procedure.

Therefore, in determining the eigenvalues of a matrix, that particular matrix or a similar one is always decomposable.

DETERMINING THE SIGNS OF EIGENVALUES

Lemma 1

Given an $n \times n$ real symmetric matrix A which has a zero eigenvalue of multiplicity m , if A is decomposable into the product of a lower-unit triangular matrix L and an upper triangular matrix U , the number of zeroes on the diagonal of U is m .

Proof

Because of its form L is non-singular, and therefore the rank of U is equal to the rank of A . By the hypothesis, the rank of A is $n - m$. Therefore, the rank of U is $n - m$, and the matrix U must have m zero eigenvalues. But the eigenvalues of U are simply its diagonal elements because of its form. Therefore U has m zero diagonal elements.

Lemma 1 provides the means for determining the multiplicity of any known eigenvalue λ of A , if the decomposition of $A - \lambda I$ is possible. The previous section shows that such a decomposition (or at least an identical decomposition of a similar matrix) is always possible.

Theorem 3

If an $n \times n$ real symmetric matrix A is decomposable into the product of a lower triangular matrix L with unit diagonal and an upper triangular matrix U , the number of positive terms on the diagonal of U is equal to the number of eigenvalues of A which are greater than zero. Furthermore, the number of zero terms on the diagonal of U is equal to the number of zero eigenvalues of A . (Note that this implies that the diagonal terms of the matrix U form a Sturm sequence.)

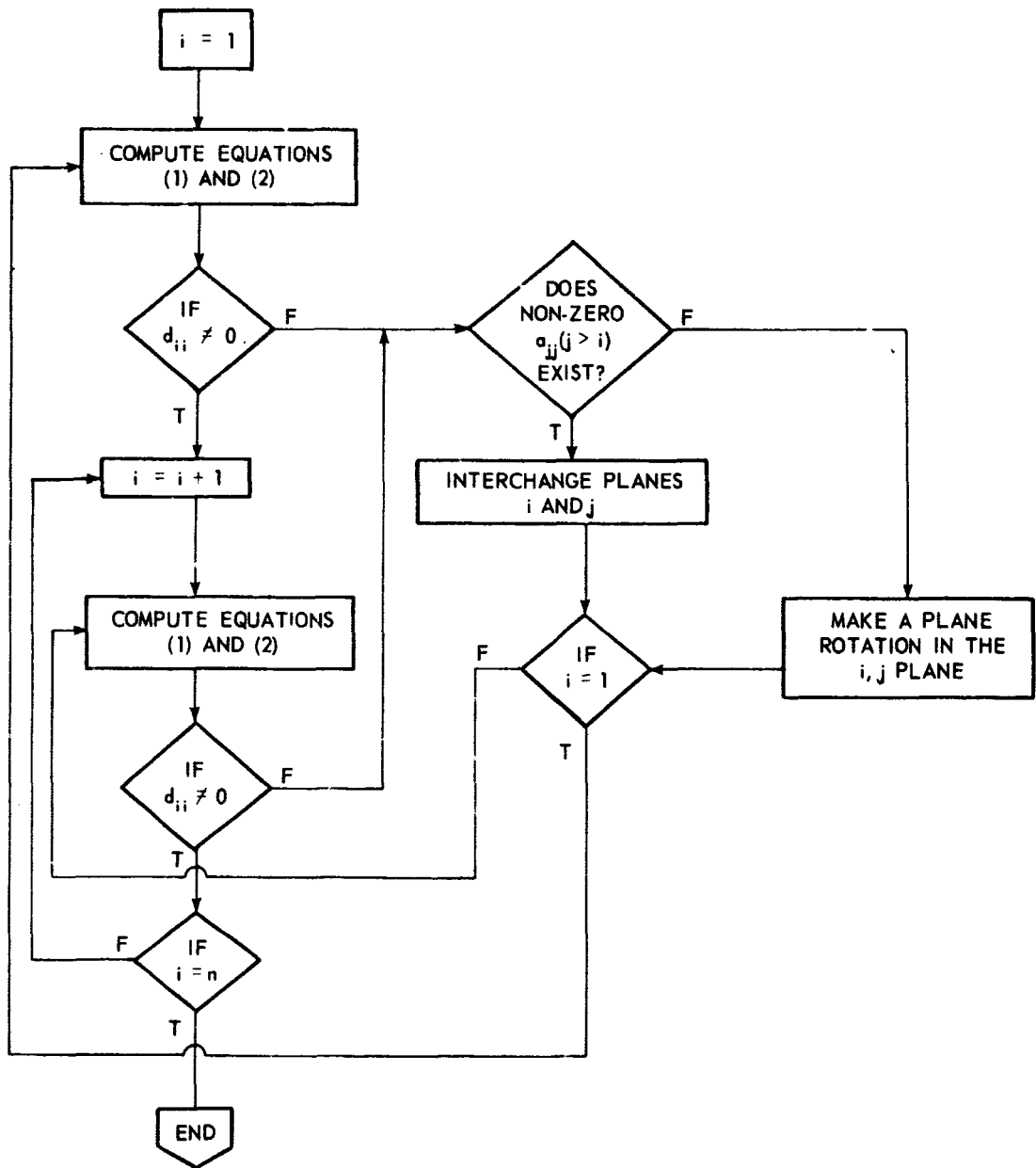


Figure 2. Decomposition Procedure Flow Chart

Proof

The proof* follows by induction on the order of A.

For $n = 1$, the theorem is trivially true.

Assume the theorem is true for A_{k-1} where $k - 1 = n$, and let $\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_{k-1}$ be its eigenvalues.

Let

$$A_k = \left[\begin{array}{ccc|c} & & & a_{1,k} \\ & & & \cdot \\ & & & \cdot \\ & & & \cdot \\ & & & a_{k-1,k} \\ \hline a_{k,1} & \dots & a_{k,k-1} & a_{kk} \end{array} \right]$$

and

$$U_k = \left[\begin{array}{ccc|c} & & & u_{1,k} \\ & & & \cdot \\ & & & \cdot \\ & & & \cdot \\ & & & u_{k-1,k} \\ \hline 0 & \dots & 0 & u_{kk} \end{array} \right]$$

Let $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_k$ be the eigenvalues of A_k .

*The author developed this proof for another proof, see Reference 4.

By the bordering property (Reference 2, p. 244), $\lambda_i \leq \alpha_i \leq \lambda_{i+1}$ for $i = 1, 2, \dots, k - 1$. By assumption, the number of α_i 's greater than zero is equal to the number of u_{ii} 's greater than zero.

Case 1—Suppose p of the α_i 's are greater than zero and none of the α_i 's equal zero, as in Figure 3. The problem is to determine where λ_{k-p+1} falls (is λ_{k-p+1} greater than, equal to, or less than zero).

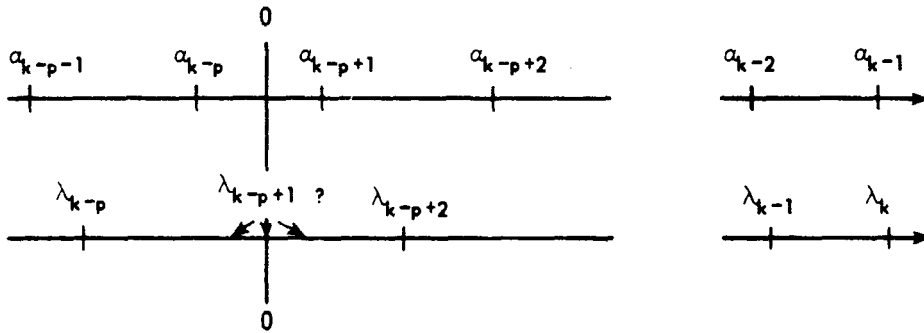


Figure 3. Eigenspectra of A_k and A_{k-1}

By Lemma 1, if $u_{kk} = 0$ then $\lambda_{k-p+1} = 0$. Suppose $u_{kk} > 0$. Since $\det(U_k) = \det(U_{k-1}) \times u_{kk}$, then $\text{sign } \det(U_k) = \text{sign } \det(U_{k-1})$. Now

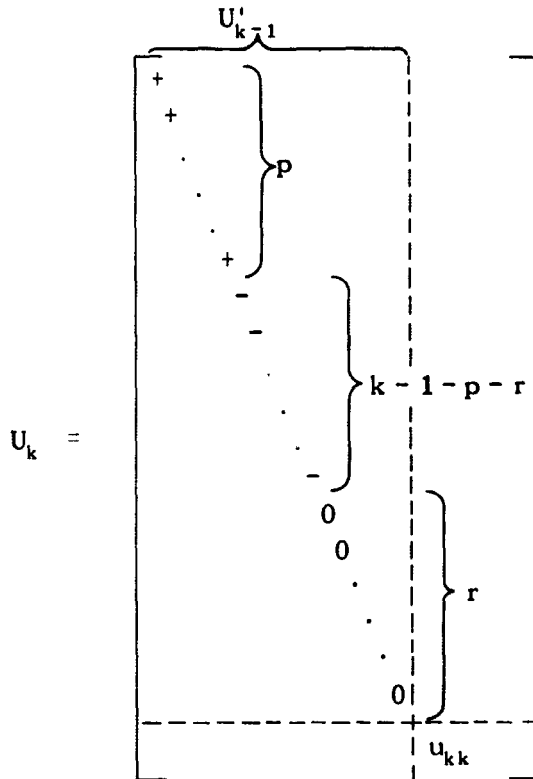
$$\det(U_{k-1}) = \prod_{i=1}^{k-1} \alpha_i$$

$$\det(U_k) = \prod_{i=1}^k \lambda_i$$

Because the signs are the same, λ_{k-p+1} must be greater than zero. Similarly, if u_{kk} is less than zero, the signs must be opposite; hence, λ_{k-p+1} must be less than zero.

Case 2—Suppose p of the α_i 's are greater than zero and r of the α_i 's equal zero ($r = 1, \dots, n - p$). If $u_{kk} = 0$, then by Lemma 1, $\lambda_{k-p+1} = 0$.

Suppose $u_{kk} \neq 0$, then



with $u_{kk} > 0$ or $u_{kk} < 0$.

Note that the terms on the diagonal of U_{k-1} can be arranged as in Figure 3 by similarity transformations on A_k which interchange appropriate rows and columns. U_k may not be upper triangular (nor will L_k be lower triangular), but the characteristic that $\det(A_j) = \det(U_j)$ is preserved because matrices P used for interchanging rows and columns have a determinant of minus 1.

Next, interchange one more row and column so that u_{kk} is in position $(k-r, k-r)$ and the zero which was in that position goes to position (k, k) . Hence:

$$A'_k = P A_k P = (P L_k P) (P U_k P) = L'_k U'_k$$

$$\prod_{i=1}^{k-r} \gamma_i = \prod_{i=1}^{k-r-1} \beta_i \cdot u_{kk}$$

The bordering property shows that:

$$\gamma_i \leq \beta_i \leq \gamma_{i+1} \quad i = 1, \dots, k-r-1$$

Hence, at least as many negative (positive) eigenvalues exist in A'_{k-r} as the number of negative (positive) eigenvalues existing in A'_{k-r-1} . If u_{kk} is greater (less) than zero, the extra eigenvalue of A'_{k-r} is also greater (less) than zero.

Let $\zeta_i^{(k-r-j)}$ be the eigenvalues of A'_{k-r-j} . In particular,

$$\zeta_i^{(k)} = \lambda_i$$

$$\zeta_i^{(k-r-1)} = \beta_i$$

$$\zeta_i^{(k-r)} = \gamma_i$$

Consider A'_{k-r+1} . The U'_{k-r+1} matrix shows* that the addition of the row and column to A'_{k-r} which forms A'_{k-r+1} introduces a zero eigenvalue to the eigenspectrum of A'_{k-r+1} . By the separation theorem, as many positive and negative eigenvalues still exist in A'_{k-r+1} as the number existing in the A'_{k-r} matrix. That is, the number of $\zeta_i^{(k-r+1)} > 0$ (< 0) is equal to the number of $\zeta_i^{(k-r)} > 0$ (< 0). The logic is the same for each row and column added until the original is formed.

Figure 4 is a pictorial description of this phenomenon where e is positive or negative depending on the sign of u_{kk} . Hence, by lemma 1, A_k has r zero eigenvalues and by the above argument, if $u_{kk} > 0$, then A_k has $p + 1$ positive eigenvalues. If $u_{kk} < 0$, then A_k has $k - p - r$ negative eigenvalues.

*By lemma 1

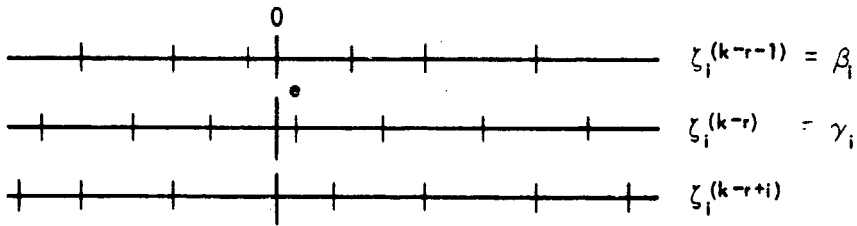


Figure 4. Eigenspectra of Principal Minors

This theorem provides a simple means of determining the number of eigenvalues of the matrix A in any interval $[a, b]$ of the real axis. First, translate the eigenspectrum of A , using a and b as shift values. Then decompose the two matrices $A - aI$ and $A - bI$ (or similar matrices) into the product of triangular matrices $L_a U_a$ and $L_b U_b$ respectively. As indicated in theorem 2, observe the signs of the terms on the diagonal of U_a and then of U_b to determine how many eigenvalues occur in (a, b) . For instance, if U_a has r positive terms on its diagonal and U_b has s positive terms on its diagonal, then $|r - s|$ eigenvalues exist in (a, b) . The number of zeroes on the diagonal of U_a indicate the number of eigenvalues at point a , and the number of zeroes on the diagonal of U_b indicate the number of eigenvalues at point b .

For example, consider the matrix

$$A = \begin{bmatrix} 5 & 2 & 4 & 7 \\ 2 & 1 & 3 & 8 \\ 4 & 3 & 8 & 5 \\ 7 & 8 & 5 & 3 \end{bmatrix}$$

To determine the number of eigenvalues between -2 and $+4$, decompose the following:

$$A + 2I = \begin{bmatrix} 7 & 2 & 4 & 7 \\ 2 & 3 & 3 & 8 \\ 4 & 3 & 10 & 5 \\ 7 & 8 & 5 & 5 \end{bmatrix}$$

Its U matrix is:

$$U_{-2} = \begin{bmatrix} 7 & 2 & 4 & 7 \\ 0 & 17/7 & 13/7 & 6 \\ 0 & 0 & 107/17 & -61/17 \\ 0 & 0 & 0 & \frac{-15,712}{1819} \end{bmatrix}$$

Next decompose:

$$A - 4I = \begin{bmatrix} 1 & 2 & 4 & 7 \\ 2 & -3 & 3 & 8 \\ 4 & 3 & 4 & 5 \\ 7 & 8 & 5 & -1 \end{bmatrix}$$

Its U matrix is:

$$U_4 = \begin{bmatrix} 1 & 2 & 4 & 7 \\ 0 & -7 & -5 & -6 \\ 0 & 0 & -59/7 & -131/7 \\ 0 & 0 & 0 & -1365/413 \end{bmatrix}$$

U_{-2} has three positive diagonal terms, and U_4 has one positive diagonal term indicating two eigenvalues in $(-2, 4)$. Because no zeroes appear on the diagonal of either U matrix, only two eigenvalues occur in $[-2, 4]$.

The eigenvalues of A, to two decimal places, are:

$$\begin{array}{r} -7.10 \text{-----} -2 \\ 1.36 \\ 3.56 \text{-----} +4 \\ 19.18 \end{array}$$

If a zero had occurred on the diagonal of U_a or U_b , -2 or +4 would had to have been an eigenvalue.

DETERMINANT METHOD OF EIGENVALUE SOLUTION

The determinant method of eigenvalue solution is based on the concept of finding the roots of the characteristic polynomial of a given matrix. The characteristic polynomial of A may be expressed as:

$$\det (A - \lambda I) = (\lambda - \lambda_1) (\lambda - \lambda_2) \dots (\lambda - \lambda_n),$$

where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of A .

To determine an eigenvalue, evaluate the determinant of $A - \lambda I$ for various values of λ . The value which yields a zero value for the determinant must be an eigenvalue.

The most practical method for evaluating the determinant of a matrix is to use the result of the decomposition theorem (make the triangular decomposition $A = LDL^T = LU$). The determinant of A is simply the product of the diagonal terms of U .

Several polynomial curve fitting schemes exist for tracking the roots of a determinant. Wilkinson⁵ shows that little is to be gained by using polynomials higher than the second degree.

The following is Muller's quadratic method from Wilkinson's text (p. 435).

Choose three points $(p_{k-2}, f(p_{k-2}))$, $(p_{k-1}, f(p_{k-1}))$, and $(p_k, f(p_k))$ on the characteristic polynomial $f(\lambda) = \det (A - \lambda I)$. Interpolate these three points and determine the zeroes of the resulting quadratic equation. Use the zero closest to p_k as a p_{k+1} , and repeat the process until a satisfactory zero of the characteristic polynomial is computed (Figure 5).

A fault in this method appears when A has some very close or multiple roots. The following graph (Figure 6) of the characteristic equation of such a matrix shows such a fault. If p_{k-2} , p_{k-1} , and p_k are as shown in the graph, the process converges to λ_3 rather than λ_1 .

In calculating the determinants of $A - (p_{k-2})I$, $A - (p_{k-1})I$, and $A - (p_k)I$ by using triangular decomposition as described in theorem 2, the results of

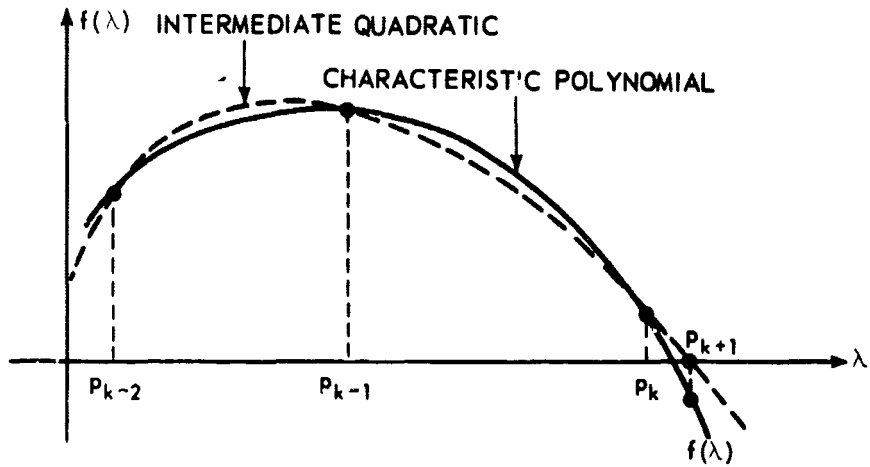


Figure 5. Local Plot of a Characteristic Polynomial

theorem 3 reveals how many positive, negative, and zero eigenvalues each of the matrices have. Taking the difference of the answers shows exactly how many eigenvalues occur between the points p_{k-2} , p_{k-1} , and p_k . An example of how this information may be useful is given in the problem described by Figure 6 where instead of the procedure predicting p_{k+1} on the right of p_k , a modified algorithm can force p_{k+1} to be between p_{k-2} and p_k .

However, the search logic does not need extra tests at this stage. Suppose in a search for all of the eigenvalues in region $[a, b]$, the characteristic equation

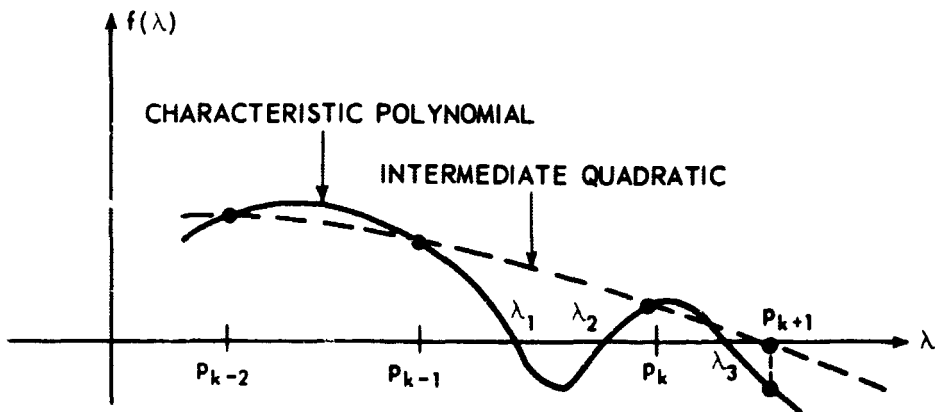


Figure 6. Example of a Possible Failure With Muller's Method

$f(\lambda) = \prod (\lambda - \lambda_i) g(\lambda)$ (where i is such that $a \leq \lambda_i \leq b$) looks like Figure 7.

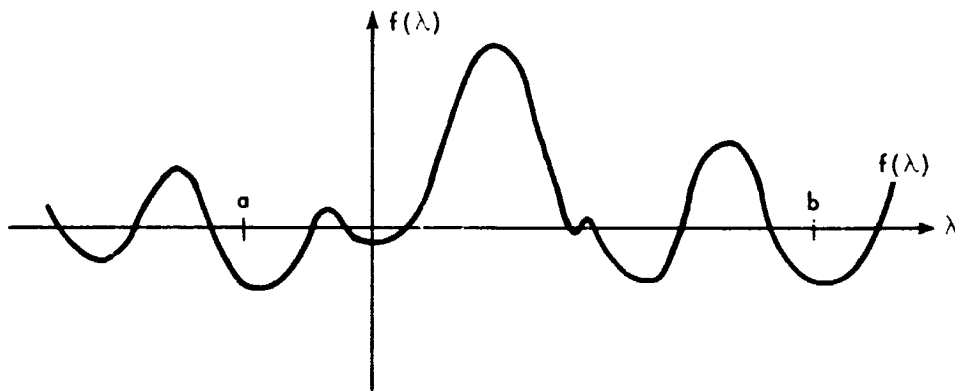


Figure 7. Characteristic Polynomial Over Interval $[a, b]$

Suppose the search logic proceeds from left to right beginning at point a and sweeping out eigenvalues as it proceeds. If the method ran to completion and found all the eigenvalues, the resulting graph might appear as Figure 8.

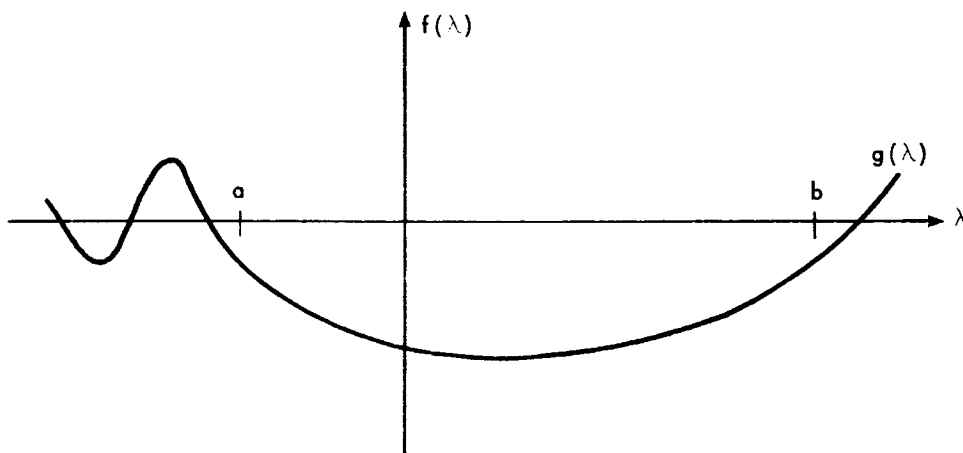


Figure 8. Deflated Polynomial $g(\lambda)$ When All Eigenvalues in $[a, b]$ Have Been Found

However, if some eigenvalues had been missed, the curve of the deflated polynomial $g(\lambda)$ might appear as Figure 9.

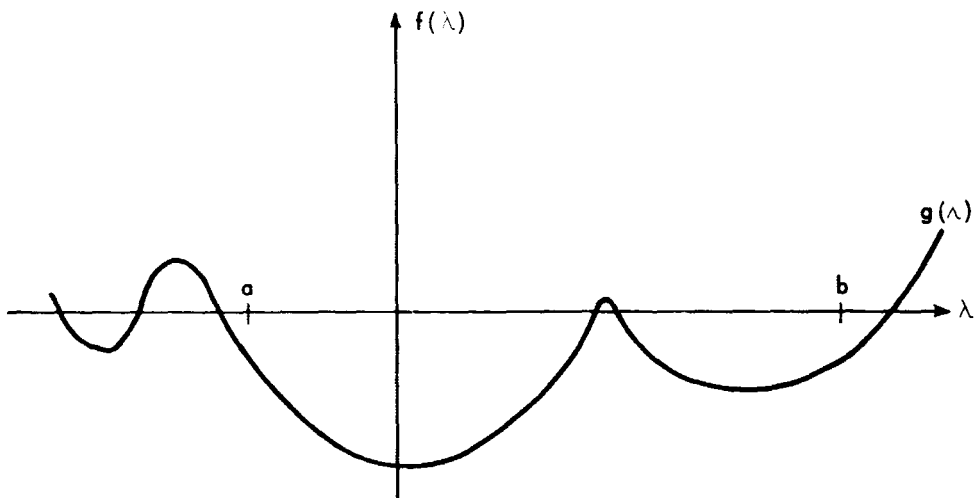


Figure 9. Deflated Polynomial $g(\lambda)$ When Two Eigenvalues in $[a, b]$ Were Missed

In any event, the decomposition of $A - aI$ and $A - bI$ determines the number of eigenvalues between a and b . If that number equals the number found, then all the eigenvalues have been found. If the number is not equal to the number found, then some of the eigenvalues have not been found. If the number of negative eigenvalues for each of the decompositions of $A - p_k I$ was recorded, the record could be searched to determine approximately where the missing roots occur.

Figure 10 is a flow chart of the proposed method for ensuring that all eigenvalues in an interval have been found.

CONCLUSIONS

Therefore, by theorem 3, the exact number of eigenvalues that fall within a given interval of interest can be determined without using the Sturm sequence method. Hence solution methods more efficient than the Sturm sequence method can be used without the risk of missing some eigenvalues in a certain range. Information about the eigenvalues of a matrix may already be present in a solution method which uses triangular decomposition. In this case only a few alterations to the method are necessary to ensure that all eigenvalues are found in a given range.

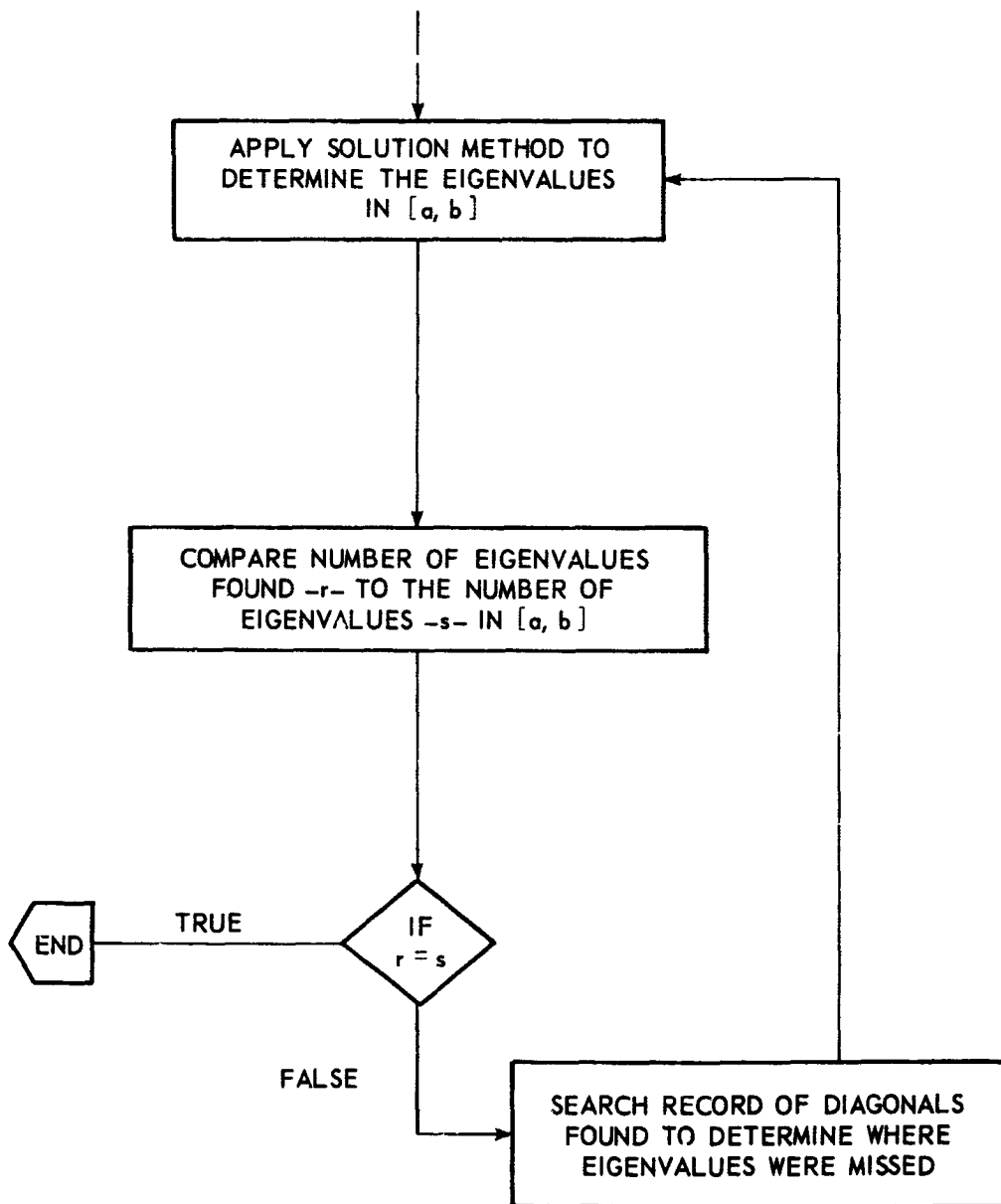


Figure 10. Flow Chart of Proposed Method for Ensuring That All Eigenvalues in an Interval Have Been Found

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