METHODS OF INVERTING TRIDIAGONAL MATRICES*

B. BU~~K~~CHBERGER and G. A. EMEL'YANENKO

Innsbruck - Dubna

(*Received* 29 *March* 1971; *revised version* 21 *November* 1972)

EFFICIENT algorithms for the inversion of symmetric tridiagonal matrices are obtained. The results were published in [1].

Tridiagonal matrices are used not only in the application of finite difference methods to boundary value problems for second-order differential equations [2], but also in the solution of problems of nuclear physics [3]. Hence there is great interest in economical methods for the inversion of high-order band matrices by computer.

In this paper efficient algorithms for the inversion of symmetric tridiagonal matrices are obtained. The methods of inversion obtained are compared with other methods. The theorem proved is useful for the solution in analytic form of the problem of processing physical information about the motion of charged particles in bubble chambers [4].

Let A be a non-singular tridiagonal matrix

$$A = \begin{Vmatrix} b_1 & a_2 & & & & 0 \\ a_2 & b_2 & a_3 & & & \\ & a_3 & b_3 & a_4 & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ & & & & & a_n \\ & 0 & & & a_n & b_n \end{Vmatrix}, \qquad a_i, b_i \neq 0.$$

We find the matrix inverse to A. For this we use an expansion of A in the form [5]

(1) $$A = DQC,\ D = (d_{ij}),\ Q = (q_{ij}),\ C = (c_{ij}),$$

where

* *Zh. vȳchisl. Mat. mat. Fiz.*, 13, 3, 546-554, 1973.

$$d_{ij} = \begin{cases} b_i + C_i a_i, & i = j, \quad C_1 = 0, \\ 0, & i \neq j; \end{cases}$$

$$q_{ij} = \begin{cases} 1, & i = j, \\ \dfrac{a_i}{b_i + C_i a_i}, & i = j+1, \quad j = 1, 2, \ldots, n-1, \\ 0 & \text{otherwise} \end{cases}$$

From the condition of symmetry of the matrix A we obtain a recursive relation for the coefficients C_i:

(2) $$C_1 = 0, C_i = -\frac{a_i}{b_{i-1} + C_{i-1}a_{i-1}}, \; 2 \leqslant i \leqslant n.$$

We obtain the matrix inverse to A by using (1):

(3) $$A^{-1} = C^{-1}Q^{-1}D^{-1}.$$

The inversion of each of the cofactors in (3) presents no difficulty.

We introduce the notation: $A^{-1} = \|A_{ij}^{-1}\|_1^n$, $D^{-1} = \|d_{ij}^{-1}\|_1^n$, $C^{-1} = \|C_{ij}^{-1}\|_1^n$, $Q^{-1} = \|q_{ij}^{-1}\|_1^n$. Then the coefficients of the inverse matrices can be written in explicit form:

$$d_{ij}^{-1} = \begin{cases} b_1^{-1}, & i = j = 1, \\ -\dfrac{C_{i+1}}{a_{i+1}}, & 2 \leqslant i = j \leqslant n-1, \\ (b_n + C_n a_n)^{-1}, & i = j = n; \end{cases}$$

$$c_{ij}^{-1} = \begin{cases} 1 & i = j, \\ 0, & i > j, \\ \prod\limits_{i+1}^{k=j} C_k, & i < j; \end{cases}$$

$$q_{ij}^{-1} = \begin{cases} 1, & i=j, \\ 0, & j>i, \\ \dfrac{a_{j+1}}{a_{i+1}} \prod\limits_{k=j+2}^{i+1} C_k, & j<i\leqslant n-1, \\ -\dfrac{a_{j+1}}{b_n+C_na_n} \prod\limits_{k=j+2}^{n} C_k, & i=n, \quad 1\leqslant j\leqslant n-2, \\ -\dfrac{a_n}{b_n+C_na_n}, & i=n, \quad j=n-1. \end{cases}$$

We consider $Q^{-1}D^{-1} = F = \|f_{ij}\|_1^n$.

$$f_{11}=b_1^{-1}; \quad f_{ij}=0,\ i<j; \quad f_{ij}=-a_{i+1}^{-1}\prod_{k=j+1}^{i+1} C_k, \quad j\leqslant i,\ i=2,3,\ldots,\ n-1;$$

$$f_{nj}=(b_n+C_na_n)^{-1}\prod_{k=j+1}^{n} C_k, \quad 1\leqslant j\leqslant n-1; \quad f_{nn}=(b_n+C_na_n)^{-1}.$$

In order to determine the elements of the inverse matrix A^{-1} we multiply C^{-1} and F in such a way that the elements of the preceding column of A^{-1} will be functions of the elements of the succeeding column. Since A is symmetric, the recursive formulas are given below only for the elements of the upper triangle of A^{-1}:

$$A_{ij}^{-1}=C_{j+1}A_{ij+1}^{-1}-a_{j+1}^{-1}\prod_{k=i+1}^{j+1} C_k, \quad i\leqslant j, \quad j=n-1,\ n-2,\ldots,1;$$

$$(4) \qquad A_{in}^{-1}=\alpha\prod_{k=i+1}^{n} C_k, \quad i=n-1,\ n-2,\ldots,1;$$

$$A_{nn}^{-1}=\frac{1}{b_n+C_na_n}=\alpha, \qquad i=j=n.$$

In these formulas the C_i are the elements of the continued fraction (2). In the calculation of the elements of the matrix A^{-1} it is useful to use the following recommendations:

(a) the filling in of the inverse matrix must be begun from the diagonal upwards and the same holds for the last column, since it is especially simple to calculate;

$A^{-1}_{i-1,n} = C_i A_{in}^{-1}$, $i = n, n-1, \ldots, 2$;

(b) the calculation of preceding columns in terms of the succeeding ones (the natural order of numbering of the columns in the matrix is meant) is performed by 4 operations on each element of a column of the inverse matrix (two multiplications, a subtraction and a division).

The method enables the inverse matrix to be obtained directly in packed form, which is especially useful for setting up the calculations in algorithmic languages.

Often (see, for example, [4]) it is useful to know the explicit form of the elements of the inverse matrix A^{-1}, but this involves the use of rather unwieldy expressions with which it is difficult to work in practice. However, if in (4) we change from successive recursions to relations with the last column, it is easy to obtain a formula for the inverse elements in terms of C_k, which can be used if the matrix inverse to the tridiagonal matrix is an intermediate in a chain of unwieldy matrix expressions [4]. The form of this relation with the coefficients C_k is given below:

$$A_{ij}^{-1} = \alpha \prod_{k=i+1}^{n} C_k \prod_{\eta=j+1}^{n} C_\eta - a_{j+1}^{-1} \prod_{k=i+1}^{j+1} C_k -$$

$$(5)\qquad - \sum_{\mu=1}^{n-(j+1)} a_{n-\mu+1}^{-1} \prod_{k=i+1}^{n-\mu+1} C_k \prod_{\eta=\mu}^{n-(j+1)} C_{n-\eta}, \quad i \leqslant j, \quad 1 \leqslant j \leqslant n-1;$$

$$A_{nn}^{-1} = \alpha = \frac{1}{b_n + C_n a_n}, \qquad A_{in}^{-1} = \alpha \prod_{k=i+1}^{n} C_k, \quad 1 \leqslant i \leqslant n-1.$$

Here and later

$$\sum_{\mu=p}^{q} (\quad) = 0, \quad \prod_{k=p}^{q} C_k = 1, \quad \text{if} \quad q < p.$$

We represent the upper triangle of the inverse matrix A^{-1} as the sum of two upper non-triangular matrices: $\|A_{ij}^{-1}\| = \|B_{ij}\| + \|R_{ij}\|$, where

$$(6)\quad B_{ij}=\begin{cases}\Big(\prod\limits_{k=i+1}^{n} C_k\Big)\Big[\alpha\prod\limits_{\mu=j+1}^{n} C_\mu-\Big(a_{j+1}\prod\limits_{\mu=j+2}^{n} C_\mu\Big)^{-1}\Big], \\ \qquad i\leqslant j,\quad 1\leqslant j\leqslant n-1; \\ \alpha\prod\limits_{k=i+1}^{n} C_k, \qquad 1\leqslant i\leqslant n-1, \qquad j=n; \\ \alpha, \qquad i=j=n.\end{cases}$$

Therefore, in Equation (6) each element of the matrix B is written as the product of two cofactors. One of the cofactors depends on i, and the other only on j.

By means of fairly unwieldy transformations of the third term in Equation (5) the elements of the matrix R can be represented in a form similar to (6):

$$(7)\qquad R_{ij}=\begin{cases}\Big(\prod\limits_{k=i+1}^{n} C_k\Big)\Big(\prod\limits_{\eta=j+1}^{n} C_\eta\Big)\Big[\frac{1}{a_nC_n}+\sum\limits_{\tau=j+2}^{n-1}\frac{C_\tau}{a_\tau}\Big(\prod\limits_{\mu=\tau}^{n} C_\mu\Big)^{-2}\Big], \\ \qquad i\leqslant j,\quad 1\leqslant j\leqslant n-2; \\ 0\cdot\prod\limits_{k=i+1}^{n} C_k, \quad 1\leqslant i\leqslant n-1, \quad j=n-1; \\ 0\cdot\prod\limits_{k=i+1}^{n} C_k, \quad 1\leqslant i\leqslant n, \qquad j=n.\end{cases}$$

Since in Equations (6) and (7) the cofactors depending on i are the same, each element of the upper triangular matrix inverse to A can be written as the product of two elements, one of which depends only on i, and the other only on j.

We finally obtain $A_{ij}^{-1}=V_iW_j$, if $i\leqslant j$. After some simplifications of Equations (6) and (7) we obtain for the components of the column-vector V and of the row-vector W the expressions

$$(8)\quad V_i=\prod_{k=i+1}^{n} C_k,\quad 1\leqslant i\leqslant n;\qquad W_j=V_j\Big(\alpha-\sum_{k=j+1}^{n}\frac{C_k}{a_k}V_{k-1}^{-2}\Big),\quad 1\leqslant j\leqslant n,$$

where

$$\alpha=\frac{1}{b_n+C_na_n},\ C_1=0,\ C_k=-\frac{a_k}{b_{k-1}+C_{k-1}a_{k-1}},\ 2\leqslant k\leqslant n..$$

In order to construct the numerical procedure the following recursive formula for W_j must be used:

$$W_j = V_{j+1}^{-1}\left(V_j W_{j+1} - \frac{1}{a_{j+1}}\right), \qquad j = n-1, \dots, 1; \qquad W_n = \alpha.$$

In essence the first part of the following theorem has been proved above.

Theorem

If A is a non-singular tridiagonal matrix, all the elements of which are non-zero, the elements of the inverse matrix may be represented in the form

$$A_{ij}^{-1} = \begin{cases} V_i W_j, & i \leqslant j, \\ W_i V_j, & j \leqslant i. \end{cases} \tag{9}$$

The converse also holds, that is, the matrix inverse to (9) is tridiagonal.

The second part of the theorem is easily proved by the method of mathematical induction, it being useful for the inversion of a matrix representable in the form (9) to use the formulas of the bordering method [6]. Without giving a detailed proof of the second part of the theorem, we present the general form of the elements of the inverse matrix which is obtained by the method indicated above. The validity of the second part of the theorem is easily checked by direct multiplication of the direct and inverse matrices.

Therefore, let $M = \|M_{ij}\|_1^n$, $M^{-1} = \|M_{ij}^{-1}\|_1^n$ and

$$M_{ij} = \begin{cases} \alpha_i \beta_j, & i \leqslant j, \\ \beta_i \alpha_j, & j \leqslant i. \end{cases} \tag{10}$$

Then the elements of the inverse matrix M^{-1} are of the form

$$\begin{aligned}
&M_{11}^{-1} = \alpha_1^{-1}\left(\beta_1 - \frac{\alpha_1}{\alpha_2}\beta_2\right)^{-1}, \qquad i = j = 1;\\
&M_{22}^{-1} = \alpha_1\alpha_2^{-2}\left(\beta_1 - \frac{\alpha_1}{\alpha_2}\beta_2\right)^{-1} + \alpha_2^{-1}\left(\beta_2 - \frac{\alpha_2}{\alpha_3}\beta_3\right)^{-1}, \; i = j = 2;\\
&M_{33}^{-1} = \alpha_3^{-1}\beta_3^{-1} + \alpha_2\alpha_3^{-2}\left(\beta_2 - \frac{\alpha_2}{\alpha_3}\beta_3\right)^{-1} + \alpha_4^{-1}\frac{\beta_4}{\beta_3}\left(\beta_3 - \frac{\alpha_3}{\alpha_4}\beta_4\right)^{-1},\\
&i = j = 3;\\
&M_{ii}^{-1} = \alpha_i^{-1}\frac{\beta_{i-1}}{\beta_i}\left(\beta_{i-1} - \frac{\alpha_{i-1}}{\alpha_i}\beta_i\right)^{-1} + \alpha_{i+1}^{-1}\frac{\beta_{i+1}}{\beta_i}\left(\beta_i - \frac{\alpha_i}{\alpha_{i+1}}\beta_{i+1}\right)^{-1},
\end{aligned} \tag{11}$$

$$3 < i = j \leqslant n-1;$$

$$M_{nn} = \alpha_n^{-1} \frac{\beta_{n-1}}{\beta_n} \left(\beta_{n-1} - \frac{\alpha_{n-1}}{\alpha_n} \beta_n \right)^{-1}, \qquad i = j = n;$$

$$M_{ij} = 0, \qquad |i-j| > 1;$$

$$M_{i,i+1} = -\alpha_j^{-1} \left(\beta_i - \frac{\alpha_i}{\alpha_j} \beta_j \right)^{-1}, \qquad 2 \leqslant j = i+1 \leqslant n;$$

$$M_{i,i-1} = -\alpha_i^{-1} \left(\beta_j - \frac{\alpha_j}{\alpha_i} \beta_i \right)^{-1}, \qquad 2 \leqslant i = j+1 \leqslant n,$$

that is, as follows from (11), M^{-1} is triangular. The relations (11) may be used for the inversion of matrices of the form (10). Therefore, the theorem is proved.

The representation (9) is convenient in analytic transformations. In what follows we will call the representation (8) $VW1$. A comparison of the numerical procedure $VW1$ with other methods will be given below.

Below we give another proof of the first part of the theorem which enables us to obtain no less efficient an algorithm for the inversion of tridiagonal matrices. A minor of the matrix obtained from A by the deletion of the i-th row and j-th column, will be of the form

$$\alpha_{ij} = \left| \begin{array}{c:c:c} \begin{matrix} b_1 a_2 & & \\ a_2 b_2 a_3 & & \\ & \ddots & \\ & & a_{i-1} \\ & & a_{i-1} b_{i-1} \end{matrix} & \begin{matrix} \\ \\ \\ \\ a_i \end{matrix} & 0 \\ \hdashline & \begin{matrix} a_{i+1} b_{i+1} a_{i+2} & & \\ & \ddots & \\ & & a_j \end{matrix} & a_{j+1} \\ \hdashline 0 & & \begin{matrix} b_{j+1} a_{j+2} & & \\ a_{j+2} b_{j+2} a_{j+3} & & \\ & \ddots & \\ & & a_n \\ & & a_n b_n \end{matrix} \end{array} \right|$$

By a theorem on block matrices [7], the determinant is equal to the product of the determinants of three blocks in the diagonal, the left upper and right lower blocks being tridiagonal, and the middle block being upper triangular. We agree to write

$$\det{}_n(\beta_1,\beta_2,\ldots,\beta_n;\ \alpha_2,\alpha_3,\ldots,\alpha_n)=\begin{vmatrix}\beta_1\alpha_2 & & 0\\ \alpha_2\beta_2\alpha_3 & & \\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot & & \cdot\\ & & \alpha_n\\ 0 & & \alpha_n\beta_n\end{vmatrix},\quad \det{}_0=1.$$

en for the elements of the upper triangular inverse matrix $A_{ij}^{-1}=(-1)^{i+j}a_{ij}$ $^{-1}$, $i\leqslant j$, we can write

$$A_{ij}^{-1}=\frac{(-1)^{i+j}}{\det_n(b_1,\ldots,b_n;a_2,\ldots,a_n)}\det{}_{i-1}(b_1,\ldots,b_{i-1};a_2,\ldots,a_{i-1})\times$$

$$\times\left(\prod_{k=i+1}^{j}a_k\right)\det{}_{n-j}(b_{j+1},\ldots,b_n;a_{j+2},\ldots,a_n).$$

et $a_k\neq 0$, $k=2,\ldots,n$, then

$$\prod_{k=i+1}^{j}a_k=\prod_{k=2}^{n}a_k\left(\prod_{k=2}^{i}a_k\prod_{k=j+1}^{n}a_k\right)^{-1}.$$

f we introduce the notation

(12) $$V_i=\text{const}(-1)^i\det{}_{i-1}(b_1,\ldots,b_{i-1};a_2,\ldots,a_{i-1})\left(\prod_{k=2}^{i}a_k\right)^{-1}$$

$$W_j=(-1)^j\det{}_{n-j}(b_{j+1},\ldots,b_n;\ a_{j+2},\ldots,a_n)\left(\prod_{k=j+1}\qquad\right)^{-1}$$

$$\text{const}=[\det{}_n(b_1,\ldots,b_n;a_2,a_3,\ldots,a_n)]^{-1}\prod_{k=2}^{n}a_k,$$

the formula for the elements of the upper triangular matrix assumes the form

$$A_{ij}^{-1}=V_iW_j,\ i\leqslant j.$$

By this we have demonstrated the validity of the first statement of the theorem for $i\leqslant j$. The validity of the statement of the theorem for the lower triangle follows from the condition of symmetry of the matrix A.

The determinants in (12) are easily expressed recursively, namely:

$$\begin{aligned}
&\det_0 = 1, \quad \det_1(b_1) = b_1,\\
&\det_i(b_1, \ldots, b_i; a_2, \ldots, a_i) = b_i \det_{i-1}(b_1, \ldots, b_{i-1}; a_2, \ldots, a_{i-1}) -\\
(13)\ &- a_i^2 \det_{i-2}(b_1, \ldots, b_{i-2}; a_2, \ldots, a_{i-2}), \quad i = 2, 3, \ldots, n;\\
&\det_1(b_n) = b_n,\\
&\det_l(b_{n-l+1}, \ldots, b_n; a_{n-l+2}, \ldots, a_n) =\\
&= b_{n-l+1} \det_{l-1}(b_{n-l+2}, \ldots, b_n; a_{n-l+3}, \ldots, a_n) -\\
&- a_{n-l+2}^2 \det_{l-2}(b_{n-l+3}, \ldots, b_n; a_{n-l+4}, \ldots, a_n), \quad l = 2, 3, \ldots, n.
\end{aligned}$$

Formulas (13) are easily obtained if the determinant of the symmetric tridiagonal matrix is expanded twice in succession: the first time by the elements of the first (last) row, and the second time, in one of the terms obtained, by the elements of the first (last) column.

From (12), (13) it is easy to obtain the following algorithm (VW2) for calculating the quantities V_i, W_j, where $a_1 = a_{n+1} = 1$:

$$W_{n+1} = 0, \quad W_n = (-1)^n, \quad W_{j-2} = -\frac{b_{j-1}W_{j-1} + a_j W_j}{a_{j-1}},$$

$$j = n+1, \ldots, 2,$$

$$V_0 = 0, \quad V_1 = -1/W_0, \quad V_{i+2} = -\frac{b_{i+1}V_{i+1} + a_{i+1}V_i}{a_{i+2}},$$

$$i = 0, \ldots, n-2.$$

The possibility of representing the elements of a matrix inverse to a tridiagonal matrix in the form $A_{ij}^{-1} = V_i W_j$ has a number of practical advantages. Firstly, the storage of the inverse matrix in the memory of the computer requires $2n$ locations instead of n^2, since we store only V, W. This enables us to solve the linear system

(14) $\qquad AX = B$

by the direct method (that is, $X = A^{-1}B$, where A is tridiagonal). The absence of the representation (9) led many authors to avoid the direct method of solving the linear systems (14) and to develop special methods [5]. Secondly, the calculation of only one component $x_i \in X$ (the solution of system (14)) does not require the calculation of all the elements of the inverse matrix, but only that of the other components of the solution vector. This advantage is obtained in [4] by a fairly complicated method.

The method of storing the matrix A^{-1} in the computer memory in the form of two vectors is also convenient in the case where it is necessary to retrieve its elements from the memory many times in succession (for example, to solve (14) ith many right sides). In principle it is then necessary to perform two reading operations via index registers and one multiplication $V_i W_j$. But if the whole inverse matrix A^{-1} is stored in the computer memory, it is usually necessary to calculate $i * n + j$ in order to determine the position of the element A_{ij}^{-1} in the computer memory. Therefore, one multiplication and several index operations are also required. This implies that economy of the memory does not slow the speed of computation, and this is a great advantage over the pivotal condensation method [8], where B in (14) is a matrix.

In conclusion we mention that the inversion of a tridiagonal matrix by the $VW1$ method requires $9n + n(n+1)/2$ operations, and by the $VW2$ method only $8n + n(n+1)/2$ operations, which is considerably less than the time spent in using, for example, the Jordan, bordering and square-root methods [9].

The advantages of the proposed methods of inverting tridiagonal matrices indicated above are essentially valid for the QR-expansions [10] of the matrix A, since more than $11n$ multiplicative operations are necessary to obtain only the unitary (orthogonal) matrix Q.

To obtain the upper non-triangular three-layer matrix R at least as great a number of multiplicative operations is required. Therefore, it is obvious that not only is there an advantage in the volume of the memory required for the storage of A^{-1} in the form VW instead of QR, but also in the expenditure of computer time on obtaining the upper triangle of A^{-1}. Also the solution of (14) taking into account the QR-expansion of the matrix A leads either to the solution of two simple systems of linear equations

$$RX = Y, \; QY = B,$$

or to the solution of the system

$$RX = Q^{T}B,$$

which once more requires more than the $10n + n^2/2$ operations necessary for the solution by the proposed VW method.

The author is obliged to N. N. Govorun, E. P. Zhidkov and I. N. Silin for useful discussions.

Translated by J. Berry

REFERENCES

1. BUKHBERGER, B. and EMEL'YANENKO, G. A. Methods of inverting tridiag... matrices. Preprint OIYaI, P11-5686, Dubna, 1971.

2. HENRICI, P. *Discrete Variable Methods in Ordinary Differential Equations.* J. Wiley and Sons, Inc., New York–London, 1962.

3. MANYUKOV, B. A. and SHLYAPINKOV, P. V. A function of the distribution of random migrations of points of a track due to multiple Coulomb scattering. Preprint OIYaI, P10-4256, Dubna, 1969.

4. EMEL'YANOV, G. A. A complete probability function for processing cloud chamber photographs. Preprint OIYaI. P10-5278, Dubna, 1970.

5. THOMAS, T. A method of solving a system of linear equations whose coeffici... form a tridiagonal matrix. *Quart. Appl. Math.*, 22, 2, 105–106, 1964.

6. FADDEEV, D. K. and FADDEEVA, V. N. *Computational Methods of Linear Algebra* (Vychislitel'nye metody lineinoi algebry) Fizmatgiz, Moscow, 1960

7. RUBLEV, A. N. *Linear Algebra* (Lineinaya algebra), "Vysshaya shkola", Mos... 1968.

8. DEMIDOVICH, B. N., MARON, I. A. and SHUVALOVA, E. Z. *Numerical Metho... Analysis* (Chislennye metody analiza), Fizmatgiz, Moscow, 1962.

9. VOEVODIN, V. V. *Numerical Methods of Algebra (Theory and Algorithms)* (Chislennye metody algebry (teoriya i algoritmy)), Fizmatgiz, Moscow, 1966.

10. WILKINSON, J. H. *The Algebraic Eigenvalue Problem* (Algebraicheskaya probl... sobstvennykh znachenii), "Nauka", Moscow, 1970.