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NOTES ON LINEAR SYSTEMS WITH POSITIVE DEFINITE TRI-DIAGONAL COEFFICIENT MATRICES

MOAWWAD E. A. EL-MIKKAWY

Mansoura University, Faculty of Science, Mansoura, 35516, Egypt
e-mail:mikkawy@yahoo.com

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In this article the author shows that under certain conditions a three-term recurrence for a tri-diagonal matrix becomes a two-term recurrence. Using this new recurrence, the possibility of the LU factorization of any tri-diagonal matrix is now easy to investigate. The positive definiteness of any real symmetric tri-diagonal matrix of any positive definite tri-diagonal is given. Some numerical examples are also given.

Key Words : Tri-diagonal Matrix; Positive Definite Matrix; Determinants; LU Factorization; Dot Product

1. INTRODUCTION

The linear system of equations whose coefficient matrix is of tri-diagonal type of the form

$$\begin{bmatrix} d_1 & a_1 & 0 & \dots & \dots & 0 \\ b_2 & d_2 & a_2 & \ddots & & \vdots \\ 0 & b_3 & d_3 & \ddots & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & & 0 \\ \vdots & & 0 & \ddots & & a_{n-1} \\ 0 & \dots & \dots & 0 & b_n & d_n \end{bmatrix} \quad \dots (1.1)$$

is of special importance in many scientific and engineering applications. For example in parallel computing and in solving differential equations using finite differences. The motivation of the current paper is therefore to show the role of the n quantities β_i, $i = 1\ (1)\ n$ associated with matrices of the form (1.1) and given by :

$$\beta_i = \begin{cases} d_1 & \text{if } i = 1 \\ d_i - \dfrac{b_i}{\beta_{i-1}} a_{i-1} & \text{if } i = 2\,(1)\,n \end{cases} \qquad \ldots (1.2)$$

2. THE MAIN RESULTS

In this section we are going to give some important results concerning tri-diagonal matrices of the form (1.1). To do this let us denote by

$$f_1 = |d_1| = d_1, f_i = \begin{vmatrix} d_1 & a_1 & 0 & \ldots & 0 \\ b_2 & d_2 & a_2 & & \vdots \\ 0 & b_3 & d_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & a_{i-1} \\ 0 & \ldots & 0 & b_i & d_i \end{vmatrix}, \; i = 2(1)\; n \qquad \ldots (2.1)$$

As stated correctly in[1], the determinants in (2.1) satisfy a three-term recurrence

$$f_i = d_i f_{i-1} - b_i a_{i-1} f_{i-2} \qquad \ldots (2.2)$$

in which the initial values for the minors f_i are $f_0 = 1$ and $f_{-1} = 0$.

We may now formulate the following results :

Theorem 2.1 — *The LU factorization of the tri-diagonal matrix A given by (1.1) is possible if* $\beta_i \neq 0$ *for each i = 1 (1) n. In this case at least the following two LU factorizations*

$$A = L_1 U_1 = L_2 U_2 \qquad \ldots (2.3)$$

where

$$L_1 = \begin{vmatrix} 1 & 0 & 0 & \ldots & \ldots & 0 \\ \dfrac{b_2}{\beta_1} & 1 & 0 & & & \vdots \\ 0 & \dfrac{b_3}{\beta_2} & 1 & & 0 & \vdots \\ \vdots & 0 & & & & 0 \\ \vdots & & & & & 0 \\ 0 & \ldots & \ldots & 0 & \dfrac{b_n}{\beta_{n-1}} & 1 \end{vmatrix}$$

$$U_1 = \begin{vmatrix} \beta_1 & a_1 & 0 & \dots & \dots & 0 \\ 0 & \beta_2 & a_2 & & & \vdots \\ 0 & 0 & \beta_3 & & 0 & \vdots \\ \vdots & & & & & 0 \\ \vdots & & & 0 & & a_{n-1} \\ 0 & \dots & & \dots & 0 \; 0 & \beta_n \end{vmatrix} \qquad \dots (2.4)$$

$$L_2 = \begin{bmatrix} \beta_1 & 0 & 0 & \dots & \dots & 0 \\ b_2 & \beta_2 & 0 & & & \vdots \\ 0 & b_3 & & & 0 & \vdots \\ \vdots & 0 & & & & 0 \\ \vdots & & & & & 0 \\ 0 & \dots & & \dots & 0 \; b_n & \beta_n \end{bmatrix}$$

and

$$U_2 = \begin{bmatrix} 1 & \frac{a_1}{\beta_1} & 0 & \dots & \dots & 0 \\ 0 & 1 & \frac{a_2}{\beta_2} & & & \vdots \\ 0 & 0 & 1 & & 0 & \vdots \\ \vdots & & & & & 0 \\ \vdots & & & 0 & & \frac{a_{n-1}}{\beta_{n-1}} \\ 0 & \dots & & \dots & 0 \; 0 & 1 \end{bmatrix} \qquad \dots (2.5)$$

are available.

PROOF : See [2].

Corollary 2.1 — The matrices L_1, L_2, U_1 and U_2 in (2.4) and (2.5) are related by :

$$L_2 = L_1 D \qquad \dots (2.6)$$

and

$$U_2 = D^{-1} U_1 \qquad \dots (2.7)$$

where
$$D = diag\ (\beta_1, \beta_2, \ldots, \beta_n) = \begin{bmatrix} \beta_1 & 0 & 0 & \ldots & \ldots & 0 \\ 0 & \beta_2 & 0 & & & \vdots \\ & & & & & \\ 0 & 0 & & & 0 & \vdots \\ & & & & & \\ \vdots & & & & & 0 \\ & & & & & \\ 0 & \ldots & \ldots & 0 & 0 & \beta_n \end{bmatrix} \quad \ldots (2.8)$$

and D^{-1} is its inverse.

PROOF : Easy.

Note 2.1 — The two factorizations $L_1 U_1$ and $L_2 U_2$ in Theorem 2.1 are called the Doolittle and the Crout factorization[3] respectively.

Note 2.2 — If $\beta_i \neq 0$ for each $i = 1\ (1)\ n-1$, then both the Doolittle and the Crout factorizations will be possible but the relations (2.6) and (2.7) may or may not be satisfied depending on the value of β_n. However, if $\beta_i = 0$ for some $i \leq n-1$, then no LU factorization will be available for the matrix A. In this case $f_i, f_{i+1}, \ldots, f_n$ may be calculated, if required, by using the three-term recurrence (2.2). It is well known that the matrix A given in (1.1) is positive definite if and only if all its principal minors $f_1, f_2, \ldots, f_n$ are all positive. Computing the determinants using minors is a notoriously expensive method. The following useful result is straightforward and should be used in evaluating determinants.

Corollary 2.2 — For the matrix A given in (1.1) if $\beta_i \neq 0$ for each $i = 1\ (1)\ n-1$, then we have

$$\det\ (A) = \beta_1 \times \beta_2 \times \ldots \times \beta_n. \quad \ldots (2.9)$$

PROOF : Obvious.

Theorem 2.2 — *If $\beta_i \neq 0$ for each $i = 1\ (1)\ n-1$, then the three-term recurrence (2.2) reduces to the two-term recurrence*

$$f_i = \beta_i f_{i-1} \text{ for each } i = 1\ (1)\ n \quad \ldots (2.10)$$

PROOF : By using (1.2) in (2.2) we obtain

$$f_i = (f_{i-1} - \beta_{i-1} f_{i-2})\, d_i + \beta_i \beta_{i-1} f_{i-2},\ i = 1\ (1)\ n \quad \ldots (2.11)$$

For $i = 2$, the recurrence (2.11) gives :

$$f_2 = \beta_2 f_1 \quad \ldots (2.12)$$

For $i = 3$, the recurrence (2.11) gives :

$$f_3 = \beta_3 f_2 \quad \ldots (2.13)$$

having used (2.12). Similarly for $i = 4$, the recurrence (2.11) gives $f_4 = \beta_4 f_3$, for $i = 5$, it gives $f_5 = \beta_5 f_4$, ..., and for $i = n$ we obtain $f_n = \beta_n f_{n-1}$. This completes the proof.

As a direct consequence of theorem 2.2 we see that minors $f_1, f_2, \ldots, f_n$ are all positive if and only if $\beta_1, \beta_2, \ldots, \beta_n$ are positive. Thus we have proved the following interesting result.

Theorem 2.3 — *Any real symmetric tri-diagonal matrix of the form :*

$$\begin{bmatrix} d_1 & a_1 & 0 & \cdots & \cdots & 0 \\ a_1 & d_2 & a_2 & & & \vdots \\ 0 & a_2 & d_3 & & 0 & \vdots \\ \vdots & & 0 & & & a_{n-1} \\ 0 & \cdots & \cdots & 0 & a_{n-1} & d_n \end{bmatrix} \quad \ldots (2.14)$$

is positive definite if and only if $\beta_1, \beta_2, \ldots, \beta_n$ are all positive.

Note 2.3 — For the symmetric tri-diagonal matrix given by (2.14), if $\beta_i > 0$ for each $i = 1(1)\ n$, then an additional LU factorization of the form $L L^t$ is always possible for this matrix. This factorization is called the Choleski factorization[3].

3. AN APPLICATION

In this section we are going to give an algorithm for solving linear systems of the form :

$$AX = C \quad \ldots (3.1)$$

where $A = \begin{bmatrix} d_1 & a_1 & 0 & \cdots & \cdots & 0 \\ a_1 & d_2 & a_2 & & & \vdots \\ 0 & a_2 & d_3 & & 0 & \vdots \\ \vdots & & 0 & & & a_{n-1} \\ 0 & \cdots & \cdots & 0 & a_{n-1} & d_n \end{bmatrix}$, $C = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}$ and $X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$ ... (3.2)

are called the coefficient matrix, the constant matrix and the solution vector of the system (3.1) respectively.

The LU factorization in[2] gives us the following result for positive definite tri-diagonal matrices.

Algorithm 3.1 — Assume the matrix A in (3.2) is positive definite tri-diagonal, then we have $A = LL^t$ where the matrix $L = (l_{ij})_{n \times n}$ is given by :

$$l_{ij}=\begin{cases}\sqrt{\beta_i} & j=i\\ \dfrac{a_{i-1}}{\sqrt{\beta_{i-1}}} & j=i-1\\ 0 & \text{otherwise}\end{cases} \qquad \ldots (3.3)$$

where $\beta_i, i=1\,(1)\,n$ are given by (1.2) (with $b_i=a_{i-1}, i=2\,(1)\,n$)

The algorithm will be referred to as *LPDT* as an abbreviation for Lower triangular matrix for a Positive Definite Tri-diagonal matrix. Thus for any $n\times n$ PDT matrix, the LPDT algorithm requires $(2n-1)$ square roots, $(3n-3)$ multiplications/divisions and $(n-1)$ additions/subtractions. Thus the cost is $O(n)$.

Now $A=LL^t$ gives

$$A^{-1}=(L^t)^{-1}L^{-1}=(L^{-1})^tL^{-1} \qquad \ldots (3.4)$$

From (3.4) we see that the inverse matrix A^{-1} of the matrix A may be obtained once the inverse matrix L^{-1} is available. To find the inverse matrix L^{-1} one can use the following method whose proof is obtained by mathematical induction.

Algorithm 3.2 — Assume the matrix A in (3.2) is positive definite tri-diagonal and $A=LL^t$, where the matrix L is obtained by using the LPDT algorithm, then the inverse matrix $L^{-1}=M=(m_{ij})_{n\times n}$ is the lower triangular matrix given by :

$$m_{ii}=\frac{1}{l_{ii}},\ i=1\ (1)\ n$$

$$m_{i+1,i}=\frac{-l_{i+1,i}}{\sqrt{\beta_i\,\beta_{i+1}}},\ i=1\ (1)\ n-1 \qquad \ldots (3.5)$$

$$m_{i+j,i}=\frac{m_{i+j,i+j-1}\,m_{i+j-1,i}}{m_{i+j-1,i+j-1}},\quad j=2\,(1)\,n-1,\ i=1\,(1)\,n-j.$$

This algorithm will be referred to as LI as an abbreviation for Lower triangular matrix Inverse. For any $n\times n$ PDT algorithm, the cost of the LI algorithm is $O(n^2)$.

It should be mentioned that if the matrix A is positive definite then A^{-1} is also positive definite. Moreover this inverse is given by

Algorithm 3.3 — If $A^{-1}=(\alpha_{ij})_{n\times n}$ is the inverse of the coefficient matrix of the system (3.2), then the elements of this matrix are given by :

$$\alpha_{ij}=\sum_{k=\max(i,j)}^{n} m_{ki}\ m_{kj},\ i,j=1\,(1)\,n. \qquad \ldots (3.6)$$

where $m_{ij}, i,j=1\,(1)\,n$ are the elements of the matrix $M=L^{-1}$ obtained by using the *LI* algorithm. In other words, for specific integers i and j, the element α_{ij} in A^{-1} is the dot product of column i and column j of the matrix L^{-1}.

This algorithm will be referred to as PDTI as an abbreviation for Positive Definite Tri-diagonal Inverse. For any $n \times n$ PDT algorithm, the cost of the PDTI algorithm is $O(n^2)$. Thus the PDTI algorithm has considerable computational advantage over the methods that do not consider the PDT property of the matrix especially for large values of n. For example the cost for the Gauss-Jordan method is $O(n^3)$.

4. NUMERICAL EXAMPLES

In this section we are going to give some illustrative numerical examples:

Example 4.1 — For the matrix

$$A = \begin{bmatrix} 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix} \quad \ldots (4.1)$$

the three *LU* factorizations mentioned above in section 2 are possible since $\beta_k = \frac{k+1}{k} > 0$ for k = 1, 2, ..., 10. Also A is positive definite and det $(A) = \beta_1 \times \beta_2 \times \ldots \times \beta_{10} = 11$.

Example 4.2 — For the matrix

$$B = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \quad \ldots (4.2)$$

the *LU* factorization is not possible in any form although the matrix is non-singular (its determinant is equal to $-1 \neq 0$). This is because $\beta_2 = 0$.

Example 4.3 — Consider the singular matrix

$$C = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix} \quad \ldots (4.3)$$

For this matrix we have $\beta_1 = \beta_2 = 1$ but $\beta_3 = 0$. Both the Doolittle and the Crout factorizations are possible but the Choleski factorization is impossible. In this case the relations (2.6) and (2.7) can't be satisfied.

Example 4.4 — Solve the following system for x_1, x_2, x_3 and x_4 by matrix inversion method.

$$C=\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}=\begin{bmatrix} -3 \\ 6 \\ -1 \\ 1 \end{bmatrix} \qquad \ldots (4.4)$$

Solution

Using (1.2) we obtain :

$$\beta_1 = 2 > 0, \beta_2 = \frac{3}{2} > 0, \beta_3 = \frac{4}{3} > 0, \beta_4 = \frac{5}{4} > 0, \qquad \ldots (4.5)$$

$$\det(A) = f_4 = 2 \times \frac{3}{2} \times \frac{4}{3} \times \frac{5}{4} = 5 > 0.$$

Thus A is positive definite and the LPDT algorithm gives :

$$L=\begin{bmatrix} \sqrt{2} & 0 & 0 & 0 \\ \frac{-\sqrt{2}}{2} & \frac{\sqrt{6}}{2} & 0 & 0 \\ 0 & \frac{-\sqrt{6}}{3} & \frac{2\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{-\sqrt{3}}{2} & \frac{\sqrt{5}}{2} \end{bmatrix} \qquad \ldots (4.6)$$

At this stage, the LI algorithm yields :

$$L^{-1}=\begin{bmatrix} \frac{1}{2}\sqrt{2} & 0 & 0 & 0 \\ \frac{1}{6}\sqrt{6} & \frac{1}{3}\sqrt{6} & 0 & 0 \\ \frac{1}{6}\sqrt{3} & \frac{1}{3}\sqrt{3} & \frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{10}\sqrt{5} & \frac{1}{5}\sqrt{5} & \frac{3}{10}\sqrt{5} & \frac{2}{5}\sqrt{5} \end{bmatrix} \qquad \ldots (4.7)$$

Finally the PDTI algorithm gives the inverse A^{-1} of the coefficient matrix A of the system (4.4). This inverse is

$$A^{-1}=\begin{bmatrix} \frac{4}{5} & \frac{3}{5} & \frac{2}{5} & \frac{1}{5} \\ \frac{3}{5} & \frac{6}{5} & \frac{4}{5} & \frac{2}{5} \\ \frac{2}{5} & \frac{4}{5} & \frac{6}{5} & \frac{3}{5} \\ \frac{1}{5} & \frac{2}{5} & \frac{3}{5} & \frac{4}{5} \end{bmatrix} \qquad \ldots (4.8)$$

Thus the solution vector X of the system (4.4) is

$$X = \begin{bmatrix} \frac{4}{5} & \frac{3}{5} & \frac{2}{5} & \frac{1}{5} \\ \frac{3}{5} & \frac{6}{5} & \frac{4}{5} & \frac{2}{5} \\ \frac{2}{5} & \frac{4}{5} & \frac{6}{5} & \frac{3}{5} \\ \frac{1}{5} & \frac{2}{5} & \frac{3}{5} & \frac{4}{5} \end{bmatrix} \begin{bmatrix} -3 \\ 6 \\ -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 5 \\ 3 \\ 2 \end{bmatrix}. \quad \ldots (4.9)$$

Therefore $x_1 = 1, x_2 = 5, x_3 = 3$ and $x_4 = 2$.

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