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A Note on Factoring 0-1 Matrices

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Nonnegative definite 0-1 matrices are shown to have a Cholesky factorization with the factors being 0-1 matrices. Conditions are derived for the existence of a "Cholesky" factorization of symmetric Boolean matrices. This condition is related to the structure of the graph associated with the matrix.

1. INTRODUCTION

Matrix factorizations are a paradigm for matrix theory and applied linear algebra and are intrinsic to many (perhaps most) important numerical algorithms in use today. Gilbert Strang [6] provides a nice summary of the basic factorizations in the interleaf of his linear algebra text. These basic factorizations now appear in nearly all of the recently published books in matrix theory and linear algebra.

Matrices with $\{0,1\}$ entries have been of interest in various contexts. See for example [1]. In this paper we investigate the possibilty of finding Cholesky factorizations for 0-1 matrices with ordinary arithmetic and with Boolean arithmetic. This work was initiated when we noted that with some slight modifications the proof of the existence of the Cholesky factorization in [5] leads to a proof for nonnegative definite 0-1 matrices. This prompted us then to also seek an analogue for Boolean matrices.

At several points we find it convenient to make use of some Matlab notaion. In particular $tril(A)$ for the lower triangular part of A and $ones(n,n)$ for an n by n matrix of all ones.

1.1 0-1 Matrices

THEOREM 1 *If A is a nonnegative definite 0-1 matrix, then A has Cholesky factorization $A = LL^T$, where L is a lower triangular 0-1 matrix.*

Proof Recall that if A is any nonnegative definite matrix, then the determinant of any principal submatrix of A is nonnegative. A consequence of this is that if $a_{ii} = 0$, then the i^{th} column and the i^{th} row of A are all zeros.

Assume that A is of order n. The proof is by induction on n. For $n = 1$ the result is obvious. Assume that every nonnegative definite 0-1 matrix of order less than n has a Cholesky factorization with the factors being 0-1 matrices. Let $A = \begin{bmatrix} a_{11} & \alpha^T \\ \alpha & A_1 \end{bmatrix}$

where A_1 is of order $n-1$ and $\alpha^T = [a_{12}\, a_{13}\ \ldots\ a_{1n}]$. First let us consider the case where $a_{11}=0$. Then as stated above it follows that $\alpha^T = [0\ldots0]$. Hence $A = \begin{bmatrix} 0 & 0 \\ 0 & A_1 \end{bmatrix}$ with A_1 being nonnegative definite. Hence by the induction hypothesis $A_1 = L_1 L_1^T$ with L_1 a lower triangular 0-1 matrix. Thus $A = \begin{bmatrix} 0 & 0 \\ 0 & L_1 \end{bmatrix}\begin{bmatrix} 0 & 0 \\ 0 & L_1^T \end{bmatrix}$.

Now suppose that $a_{11}=1$, *i.e.*, $A = \begin{bmatrix} 1 & \alpha^T \\ \alpha & A_1 \end{bmatrix}$. Let $B = A_1 - \alpha\alpha^T$, then B is nonnegative definite. This follows from the fact that B is the Schur complement of a nonnegative definite matrix (see e.g. [2]). To see this directly, let y be any $(n-1)$ vector and $x = \begin{bmatrix} -\alpha^T y \\ y \end{bmatrix}$. Then

$$\begin{aligned} 0 \le x^T A x &= [-\alpha^T y \quad y^T]\begin{bmatrix} 1 & \alpha^T \\ \alpha & A_1 \end{bmatrix}\begin{bmatrix} -\alpha^T y \\ y \end{bmatrix} \\ &= [-\alpha^T y \ \ y^T]\begin{bmatrix} 0 \\ -\alpha\alpha^T + A_1 y \end{bmatrix} \\ &= -y^T\alpha\alpha^T y + y^T A_1 y = y^T(A_1 - \alpha\alpha^T)y = y^T B y, \end{aligned}$$

so B is nonnegative definite. Also we'll see that B is a 0-1 matrix. Note that $b_{i-1,j-1} = a_{ij} - \alpha_{i-1}\alpha_{j-1} = a_{ij} - a_{i1}a_{j1}$. So, if $a_{ij}=1$, then $b_{i-1,j-1} = 0$ or 1. Suppose $a_{ij}=0$ and $a_{i1}a_{j1}=1$, then consider the principal submatrix $\begin{bmatrix} a_{11} & a_{1i} & a_{1j} \\ a_{i1} & a_{ii} & a_{ij} \\ a_{j1} & a_{ji} & a_{jj} \end{bmatrix}$ of A which would be $\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$, and which has determinant equal to -1, a contradiction. Consequently if $a_{ij}=0$, then $a_{i1}a_{j1}=0$ and thus $b_{ij}=0$.

Since B is a nonnegative definite 0-1 matrix of order $(n-1)$, by the induction hypothesis there is a lower triangular 0-1 matrix L_1 with $B = L_1 L_1^T = A_1 - \alpha\alpha^T$. That is, $A_1 = L_1 L_1^T + \alpha\alpha^T$, hence $A = \begin{bmatrix} 1 & 0 \\ \alpha & L_1 \end{bmatrix}\begin{bmatrix} 1 & \alpha^T \\ 0 & L_1^T \end{bmatrix}$. This completes the induction proof. ■

The next theorem leads to a characterization of the structure of nonnegative definite 0-1 matrices.

THEOREM 2 *If A is an irreducible, nonnegative definite* 0-1 *matrix of order n, then* $A = ones(n,n)$.

Proof Suppose that $a_{ij}=0$. Since A is irreducible, there is a path from i to j in the graph $\Gamma(A)$. Without loss of generality, we may assume that $i=1$ and that the path is given by the vertices $\{1,2,\ldots,j\}$. In this case the matrix $\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}$ is a leading principal submatrix of A and has determinant -1. It follows that every entry of A must be equal to one. ■

Note that it follows from this theorem that the graph associated with an irreducible, nonnegative definite 0-1 matrix is a complete graph. For an arbitrary nonnegative definite 0-1 matrix A we can find a permutation matrix P so that the Frobenius normal form PAP^T is a direct sum of irreducible matrices. Hence we have the following theorem.

THEOREM 3 *If A is any nonnegative definite 0-1 matrix, then A is cogredient to a direct sum of matrices $ones(k_i, k_i)$ and possibly a zero matrix.*

As a consequence of Theorem 3 we have the following.

COROLLARY 4 *For any $n \geq 1$, the only $n \times n$ positive definite 0-1 matrix is the identity matrix.*

Theorem 3 enables us to develop the following algorithm which finds the Cholesky factorization for a nonnegative definite 0-1 matrix A.

INPUT A, $n \times n$ nonnegative definite 0-1 matrix

OUTPUT L, $n \times n$ lower triangular 0-1 matrix such that $A = LL^T$

```
//initializations
for i = 1 to n
    d(i) = A(i,i)
    for j = 1 to n
        L(i,j) = 0
    end
//
for i = 1 to n
    if (d(i) = 1) then
        L(i,i) = 1
        for k = i + 1 to n
            if(A(k,i) = 1) then
                L(k,i) = 1
                d(k) = 0
            end
        end
    end
end
```

2. BOOLEAN MATRICES

We now turn our attention to 0-1 matrices using Boolean arithmetic which we'll refer to as Boolean matrices.

The classical definition for a symmetric matrix A to be positive definite is that $x^TAx > 0$ for all $x \neq 0$. For an $n \times n$ symmetric Boolean matrix A we will say that A is **positive definite** provided that $e_i^TAe_i > 0$, equivalently, $a_{ii} > 0$, for $i = 1, 2, \ldots, n$ where e_i denotes the vector with 1 in the *ith* entry and zeros elsewhere. With Boolean arithmetic this would of course imply that $x^TAx > 0$ for all $x \neq 0$.

A symmetric Boolean matrix is said to have a **Cholesky factorization** if there is a lower triangular Boolean matrix L such that $A = LL^T$.

First we give an example of a positive definite Boolean matrix which has no Cholesky factorization.

Example 5 Let $A = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}$. It can be shown by exhaustively checking all the possibilities that $A \neq LL^T$ for any lower triangular Boolean matrix L.

Remark 6 Let A be an $n \times n$ positive definite Boolean matrix and suppose $A = LL^T$, where L is a lower triangular Boolean matrix. Then some diagonal entry of L can be either 0 or 1 unless $A = I$, in which case $L = I$.

Proof Let $L = [l_{i,j}]$ and assume $A \neq I$. Let $i_0 = \max\{i : 1 \leq i \leq n, \sum_{k=1}^{i-1} l_{ik} = 1\}$. Then $i_0 \geq 2$ and if $i_0 < n$, then we would have $A = \begin{bmatrix} \tilde{A} & 0 \\ 0 & I \end{bmatrix}$, so the problem is reduced to considering $\tilde{A}$. Without loss of generality, we can assume that $\sum_{k=1}^{n-1} l_{nk} = 1$. Hence changing l_{nn} to zero still yields $A = LL^T$. ■

Note that for

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix},$$

it is possible to change $l_{33} = 0$, but changing $l_{22} = 0$ does not work. That is,

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \neq A.$$

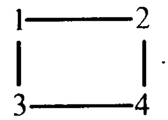
Since factorization of $A \neq I$ is not unique whenever it exits, we will characterize those matrices which allow a factorization of a particular form. That is, we consider the case where the positive definite Boolean matrix A can be factored as $A = LL^T$, with L equal to the lower triangular part of A or in Matlab notation, $L = tril(A)$. First we need some terminology and definitions.

Let i, j, and k denote vertices in the graph $\Gamma(A)$ associated with the matrix A.

DEFINITION We say that a vertex i of the graph $\Gamma(A)$ is **adjacent** to the vertex j if $a_{ij} = 1$.

DEFINITION We say that the graph $\Gamma(A)$ is **partially transitive** if for every i, j, k with $i < j < k, j$ is adjacent to k whenever i is adjacent to both j and k.

The graph for the matrix A in example 5 is



This graph is not partially transitive since 2 and 3 are both adjacent to 1 but 2 is not adjacent to 3, and partial transitivity of the graph is what is needed in order to be able to factor A as the product of its lower triangular part and its upper triangular part.

THEOREM 7 *Let A be a positive definite Boolean matrix. Then A has a Cholesky factorization of the form $A = LL^T$ with $L = tril(A)$ if and only if the graph $\Gamma(A)$ associated with the matrix is partially transitive.*

Proof Assume that $A = LL^T$ with $L = tril(A)$. If $i < j < k$ and $a_{ji} = 1, a_{ki} = 1$, then $a_{kj} = \sum_{m=1}^{j} l_{km}l_{jm} = \sum_{m=1}^{j} a_{km}a_{jm} \geq a_{ki}a_{ji} = 1$. Hence $\Gamma(A)$ is partially transitive.

Now assume $\Gamma(A)$ is partially transitive. We intend to show that for each pair (k,j) with $j < k$,

$$a_{kj} = \sum_{m=1}^{j} a_{km}a_{jm}. \tag{1}$$

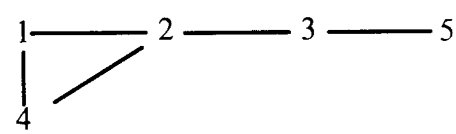
If $a_{kj} = 0$ then partial transitivity implies that $a_{km}a_{jm} = 0$ for all $m \leq j$. Hence the previous summation is also zero. If $a_{kj} = 1$ then the j^{th} term of the summation is one. Thus in either case we have (1). ■

There are some other results in the literature which establish relationships between existence of certain paths in the graph $\Gamma(A)$ and the LU factorization of A. For example, see [3] and [4].

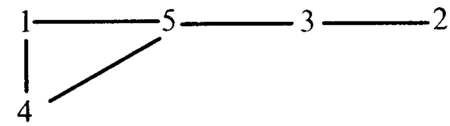
Next we consider an example where A has a factorization $A = L_1L_1^T$ with L_1 being a lower triangular matrix but $L_1 \neq tril(A)$.

Example 8 Let $A = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}$ and let $L_1 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}$

Then $A = L_1L_1^T$, but $A \neq LL^T$ with $L = tril(A)$ since the graph $\Gamma(A)$ is not partially transitive. The graph is the following



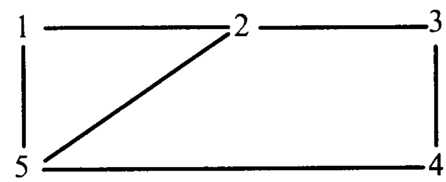
This graph fails to be partially transitive since 3 and 4 are not adjacent. However if we permute the vertices to get the following graph



then we obtain a graph that is partially transitive. The corresponding Boolean matrix is $B = PAP^T$ for some permutation matrix P and B can be factored as $B = LL^T$ with $L = tril(B)$. This example and many others led us to consider the possibility that a Boolean matarix A has a factorization as $A = L_1 L_1^T$, for some lower triangular Boolean matrix L_1 if and only if there is a permutation matrix P such that $\Gamma(B)$ is partially transitive for $B = PAP^T$. This is true for matrices of order less than or equal to 4. However as the following example shows, a matrix A can have a factorization and yet no permutation of the vertices of the graph $\Gamma(A)$ will yield a graph which is partially transitive.

Example 9 Let $L_1 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 \end{bmatrix}$ and $A = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \end{bmatrix} = L_1 L_1^T.$

The graph $\Gamma(A)$ is as follows:



Note (by Remark 6) that in each of examples 8 and 9, another Cholesky factorization of the respective matrices A is obtained by setting the $(5, 5)$ entry of L_1 to 0.

We conclude this paper with some remaining questions on the factorization of Boolean matrices. Suppose $A = L_1 L_1^T$ and $L_1 \neq tril(A)$. Find conditions on A such that for some permutation matrix $P, PAP^T = LL^T$ where $L = tril(PAP^T)$. Also find conditions on A such that $B = PAP^T$ is factorable as a product of a lower triangular matrix L with its transpose, L not necessarily equal to $tril(B)$.

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