On the Number of Cholesky Roots of the Zero Matrix over $\mathbb{F}_2$

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Abstract

A square, upper-triangular matrix $U$ is a Cholesky root of a matrix $M$ provided $U^*U = M$, where $^*$ represents the conjugate transpose. Over finite fields, as well as over the reals, it suffices for $U^TU = M$. In this paper, we investigate the number of such factorizations over the finite field with two elements, $\mathbb{F}_2$, and prove the existence of a rank-preserving bijection between the number of Cholesky roots of the zero matrix and the upper-triangular square roots the zero matrix.

1 Introduction

In this paper we will discuss enumerating distinct Cholesky factorizations of a (symmetric) matrix with entries in $\mathbb{F}_2$. We will give a count, by size and rank, for the number of Cholesky factorizations of the $\mathbb{F}_2$-zero matrix as well as prove a rank-preserving bijection between it and the set of upper-triangular square roots the zero matrix. Before doing so, we will briefly discuss Cholesky factorizations over the real and complex fields. Let $M$ be a matrix with complex (or real) entries. We say $M$ has a Cholesky factorization if it can be expressed as the product of a lower triangular matrix $L$ and its conjugate transpose $L^*$. Observe that in this case $M^* = (LL^*)^* = (L^*)^*L^* = LL^* = M$ so $M$ must be square and equal to its own conjugate transpose ($M$ is Hermitian). Over the reals, this just implies that $M$ must be symmetric. Let $n \geq 1$ and let $0_n^C, I_n^C$ denote the additive and multiplicative complex valued $n \times n$ identity matrices (respectively). Suppose $LL^*$ gives a Cholesky factorization for $0_n^C$, then for all $1 \leq i, j \leq n$ the dot product of the $i^{th}$ row of $L$ and the $j^{th}$ column of $L^*$ must equal zero. However, the $j^{th}$ column of $L^*$ is simply complex-conjugate of the $j^{th}$ row of $L$ so

$$\sum_{k=1}^{n} L[i,k]L[j,k]^* = 0 \text{ for all } 1 \leq i, j \leq n$$

So $L = 0_n^C$ and it follows that $0_n^C$ has a unique Cholesky factorization. Similarly, the identity matrix and every other Hermitian positive-definite matrix have
unique Cholesky factorizations if we insist the diagonal entries be non-negative. This uniqueness is lost for Hermitian positive-semidefinite matrices as well as over finite fields. In this paper we investigate the non-uniqueness of Cholesky factorizations over $\mathbb{F}_2$.

2 Cholesky Roots over $\mathbb{F}_2$

**Definition 1.** Let $M$ be a $n \times n$ symmetric matrix with entries in $\mathbb{F}_2$. We say $M$ has a Cholesky decomposition if there exists a lower-triangular matrix $L$ such that $LL^T = M$ or equivalently if there exists an upper-triangular matrix $U$ such that $U^T U = M$. In such case, we call $U$ a Cholesky root of $M$.

For all positive integer $n$, we let $I_n$ and $0_n$ denote the $n \times n$, $\mathbb{F}_2$ multiplicative and additive identity matrices (respectively). For $r \leq n$, we let $U_n(r)$ be the set of $n \times n$, rank $r$, upper-triangular matrices with entries from $\mathbb{F}_2$. For $n \geq 1$ and $r \leq n$ we define

$$A_n(r) = \{ U \in U_n(r) \mid U^2 = I_n \} \quad \text{and} \quad A_n = \bigcup_{0 \leq r \leq n} A_n(r);$$

$$B_n(r) = \{ U \in U_n(r) \mid U^2 = 0_n \} \quad \text{and} \quad B_n = \bigcup_{0 \leq r \leq n} B_n(r);$$

$$C_n(r) = \{ U \in U_n(r) \mid U^T U = 0_n \} \quad \text{and} \quad C_n = \bigcup_{0 \leq r \leq n} C_n(r).$$

**Observation 1.** For all $n \geq 1$:

$$|A_n| = |B_n|$$

**Proof.** Observe that $(X + I_n)^2 = X^2 + 2X + I_n = X^2 + I_n$. Hence, for all $X \in U_n$, $X^2 = 0$ if and only if $(X + I_n)^2 = I_n$. 

**Theorem 1.** For all $n \geq 1$ and $r \leq n$:

$$|B_n(r)| = |C_n(r)|$$

**Proof.** Observe that

$$B_1 = B_1(0) = \{[0]\} = C_1(0) = C_1.$$ 

We proceed by induction. Let $n > 1$ and assume that $|B_{n-1}(r)| = |C_{n-1}(r)|$ for all $r \leq n - 1$. Choose and fix a rank $r$, $n \times n$ upper-triangular matrix $B$. Observe that by Sylvester’s rank inequality $B_n(r) = C_n(r) = \emptyset$, so we may proceed with the assumption that $r < n$. Let $B'$ be the $n - 1 \times n - 1$ principal submatrix of $B$.

$$B^2 = \begin{bmatrix} B' & v \\ 0^T & b \end{bmatrix} \begin{bmatrix} B' & v \\ 0^T & b \end{bmatrix} = \begin{bmatrix} B'^2 & B'v + bv \\ 0^T & b^2 \end{bmatrix}.$$
Then $B \in \mathcal{B}_n$ if and only if $b = 0$ and $B'v = 0$ and $B' \in \mathcal{B}_{n-1}$. However $B'v = 0$ if and only if $v \in \text{Null}(B')$, the null space of $B'$. If $B' \in \mathcal{B}_{n-1}$ then the column space of $B'$, $\text{Col}(B')$, must be a subset of $\text{Null}(B')$. It follows that if $B \in \mathcal{B}_n$ then $v \in \text{Col}(B')$ or $v \in \text{Null}(B') \setminus \text{Col}(B')$. Hence, for each $r$:

\[
|B_n(r)| = |B_{n-1}(r)| \cdot 2^r + |B_{n-1}(r-1)| \cdot \left(2^\text{dim}(\text{Null}(B')) - 2^{r-1}\right)
\]

Choose and fix a rank $r$, $n \times n$ upper-triangular matrix $C$. Let $C'$ be the $n-1 \times n-1$ principal submatrix of $C$.

\[
C'^TC = \begin{bmatrix}
C'^T & 0 \\
0 & c
\end{bmatrix}
\begin{bmatrix}
C' \\
c
\end{bmatrix} = \begin{bmatrix}
C'^TC' & C'^Tw \\
C^Tw & c^2 + w^Tw + c^2
\end{bmatrix}.
\]

$C \in \mathcal{C}_n$ if and only if $w^Tw + c^2 = 0$ and $C'^TC = 0$ and $C' \in \mathcal{C}_{n-1}$. Equivalently $C \in \mathcal{C}_n$ if and only if $C' \in \mathcal{C}_{n-1}$ and

\[
\overline{CW} = \begin{bmatrix}
C'^T \\
c
\end{bmatrix}
\begin{bmatrix}
0 \\
1
\end{bmatrix} = 0.
\]

This occurs if and only if $\overline{w} \in \text{Null}(\overline{C})$. Observe that if $c = 0$ then $\overline{w} \in \text{Null}(\overline{C})$ exactly when $w \in \text{Row}(C') \cap \text{Null}(\overline{C})$ or $w \in \text{Null}(\overline{C}) \setminus \text{Row}(C')$. On the other hand if $c = 1$ then $\overline{w} \in \text{Null}(\overline{C})$ exactly when $w \in \text{Null}(\overline{C}) \setminus \text{Row}(C')$.

It follows that for each $r$:

\[
|C_n(r)| = |C_{n-1}(r)| \cdot 2^r + |C_{n-1}(r-1)| \cdot \left(2^\text{dim}(\text{Null}(\overline{C})) - 2^{r-1}\right)
\]

\[
|C_n(r)| = |C_{n-1}(r)| \cdot 2^r + |C_{n-1}(r-1)| \cdot \left(2^{n-r} - 2^{r-1}\right)
\]

As a consequence of the previous proof we get the following corollary without appealing to the rank-nullity theorem.

**Corollary 1.** For all $n \geq 1$, $\mathcal{B}_n(r) = \mathcal{C}_n(r) = \emptyset$ whenever $r \geq n/2$.

**Proof.** If $B \in \mathcal{B}_n(r)$ then $\text{Col}(U) \subset \text{Null}(U)$ where the inclusion is strict since $[0, \ldots, 0, 1]^T \in \text{Null}(U) \setminus \text{Col}(U)$. That is $r < n-r$, hence $r < n/2$.

In [3] the authors give a count for the number of upper-triangular matrices over $\mathbb{F}_q$ whose square is the zero matrix. By restricting to $q = 2$ we have the following result.
The number of distinct Cholesky factorizations for $A$ is $|B_{2n}| = \sum_j \left[\binom{2n}{n-3j} - \binom{2n}{n-3j - 1}\right] 2^{n^2 - 3j^2 - j}$

$|B_{2n+1}| = \sum_j \left[\binom{2n+1}{n-3j} - \binom{2n+1}{n-3j - 1}\right] 2^{n^2 + n - 3j^2 - 2j}$

**Corollary 2.** For all $n > 0$

$|A_n| = |B_n| = |C_n| = \sum_j \left[\binom{n}{\frac{n}{2} - 3j} - \binom{n}{\frac{n}{2} - 3j - 1}\right] 2^{\frac{n}{2} j^2 - 3j^2 - (\lfloor \frac{n}{2} \rfloor - \lfloor \frac{n}{2} \rfloor + 1)j}$

Given a $n \times n$ matrix $M$ with entries in $\mathbb{F}_2$, we let $M_k$ denote the $k^{th}$ leading principal submatrix of $M$, $1 \leq k \leq n$. We say $M$ is in leading principal non-singular (LPN) form if

$$\det_k(M) = \begin{cases} 1, & \text{if } k \leq \text{rank}(M) \\ 0, & \text{if } \text{rank}(M) < k \leq n \end{cases}$$

It was shown in [1] that if $M$ is a full-rank, symmetric matrix with entries in $\mathbb{F}_2$ then $M = U^T U$ from some upper-triangular matrix $U$ if and only if $M$ is in LPN form. Furthermore, this Cholesky decomposition is unique. In [2] it was demonstrated that uniqueness fails when $M$ is not full-rank, however, if $M$ is in LPN form then there exists a natural choice determined by the pressing instructions of a graph that has $M$ as its adjacency matrix.

**Corollary 3.** Let $A \in \mathbb{F}_2^{n \times n}$ of rank $r$ be in leading principal minors form. The number of distinct Cholesky factorizations for $A$ is $|C_n(n-r)|$

**Proof.** Let $A_{1,1}$ be the principal $r \times r$ submatrix of $A$ and suppose $B^T B = A$ is a Cholesky factorization of $A$. Then

$$B^T B = \begin{bmatrix} B_{1,1}^T & 0 \\ B_{1,2}^T & B_{2,2}^T \end{bmatrix} \begin{bmatrix} B_{1,1} & B_{1,2} \\ 0 & B_{2,2} \end{bmatrix} = \begin{bmatrix} B_{1,1}^T B_{1,1} & B_{1,1}^T B_{1,2} \\ B_{1,2}^T B_{1,1} & B_{1,2}^T B_{1,2} + B_{2,2}^T B_{2,2} \end{bmatrix}$$

where $B_{1,1}$ is an $r \times r$ matrix. However, [2] demonstrated that $A$ has an (instructonal) Cholesky decomposition of the form

$$V^T V = \begin{bmatrix} V_{1,1}^T \\ V_{1,2} \end{bmatrix} \begin{bmatrix} 0 & V_{1,1} \\ V_{1,2} & 0 \end{bmatrix} = \begin{bmatrix} V_{1,1}^T V_{1,1} & V_{1,1}^T V_{1,2} \\ V_{1,2}^T V_{1,1} & V_{1,2}^T V_{1,2} \end{bmatrix}$$

Since $A_{1,1}$ is a full-rank matrix it has a unique Cholesky decomposition over $\mathbb{F}_2$ (see proof in [1]). That is, $B_{1,1} = V_{1,1}$. Then by invertibility we have $B_{1,2} = (V_{1,1})^{-1} B_{1,1} B_{1,2} = (V_{1,1})^{-1} V_{1,1} V_{1,2} = V_{1,2}$ and hence

$$V_{1,2}^T V_{1,2} = B_{1,2}^T B_{1,2} + B_{2,2}^T B_{2,2} \Rightarrow B_{2,2}^T B_{2,2} = 0$$

□
3 Future Work

We have seen that for the special case that a $F_2$, square matrix is in leading principal minors form, then the number of Cholesky decompositions it yields is dictated by the count discussed in this paper (with rank parameter being replaced with corank). This fails to be the case when a matrix is not in leading principal minors form. For example

\[
\begin{bmatrix}
0 & 0 \\
0 & 1 \\
\end{bmatrix}^T \begin{bmatrix}
0 & 0 \\
0 & 1 \\
\end{bmatrix} = \begin{bmatrix}
0 & 1 \\
0 & 0 \\
\end{bmatrix}^T \begin{bmatrix}
0 & 1 \\
0 & 0 \\
\end{bmatrix}
\]

but the number of Cholesky roots of the $1 \times 1$ zero matrix (over $F_2$) is 1.

Another topic of interest would be to study the asymptotic behavior of

\[|C_n(r)| = \sum_j \left( \left( \left\lfloor \frac{n}{2} \right\rfloor - 3j \right) - \left( \left\lfloor \frac{n}{2} \right\rfloor - 3j - 1 \right) \right) 2^{\left\lfloor \frac{n}{2} \right\rfloor - 3j - (\left\lceil \frac{n}{2} \right\rceil - \left\lfloor \frac{n}{2} \right\rfloor + 1)j}
\]

Observe that $-\frac{n+3}{6} \leq j \leq \frac{n}{6}$ or the summand is zero. When $j = \left\lfloor -\frac{n+3}{6} \right\rfloor$ or $j = \left\lfloor \frac{n}{6} \right\rfloor$ the summand yields $2^{O(n^2)}$. At $j = 0$ the summand yields $(1 + o(1)) \frac{2^{n/\sqrt{2}n}(2e)^{n/2+o(1)}}{\sqrt{n}2^n} 2^{n^2/4}$. This however cannot be used as a lower bound since many of the terms in the summand can be negative.

Finally, it is worth mentioning that the bijection between the three sets (the Cholesky roots of zero, the upper-triangular roots of zero, and the upper-triangular roots of the identity) does not extend to other finite fields (in part because $(X + I)^2 = X^2 + I$ is unique to $F_2$). It follows that to count the number of Cholesky roots of a zero matrix over other finite fields one would need different techniques than the ones used in this paper, nevertheless it would be an interesting continuation of this work.
References

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[3] S. B. Ekhad and D. Zeilberger. The number of solutions of $x^2 = 0$ in triangular matrices over $gf(q)$. *Electron. J. Comb*, 3:R2, 1996.