Maximal $j$-Simplices in the Real $d$-Dimensional Unit Cube

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For each positive even integer $j$ there is an infinite arithmetic sequence of dimensions $d$ for which we construct a $j$-simplex of maximum volume in the $d$-dimensional unit cube. For fixed $d$, all of these maximal $j$-simplices have the same Gram matrix, which is a multiple of $I + J$. For $j$ even, a new upper bound for the volume of a $j$-simplex in the $d$-dimensional unit cube is given.

1. INTRODUCTION

What is the maximal volume of a $j$-simplex spanned by $j$ vertices of the unit cube and the origin in real $d$-space? If $j = d$, then this is the celebrated Hadamard problem which has been studied extensively and is usually stated in terms of matrix theory. The translation into matrix theory is facilitated by the fact that the volume of the simplex spanned by the $j$ rows of the $j \times d$ matrix $A$ and the origin in real $d$-space is given by $(1/j!)(\det AA^T)^{1/2}$. Thus the problem of finding the volume of the largest $j$-simplex spanned by vertices of $C_j = [0, 1]^d$, the unit cube in real $d$-space, and the problem of finding the maximal determinant of $AA^T$, where $A \in M_{j,d}([0,1])$ is a $j \times d$ matrix whose entries are elements of $\{0, 1\}$, are equivalent.

The following upper bound for $\det AA^T$ was recently established:

THEOREM 1.1 [HKL Theorem 4.2]. For $A \in M_{j,d}([0,1])$,

$$\det AA^T \leq (j + 1)^{j/2} \left(\frac{j + 1}{j}\right)^{j} \left(\frac{d}{2}\right)^{j/2}.$$  \hspace{1cm} (1)

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Conditions for equality are also given in [HKL]. For \( j = 2k - 1 \) odd and \( d \) a multiple of the combinatorial coefficient \( C(j, k) \), [HKL] constructs a matrix \( A \in M_{j,d}(\{0, 1\}) \) for which equality holds in Eq. (1). These matrices are described in part 1 of Theorem 1.3.

However, equality in (1) is not attainable if \( j = 2k \) is even. Our first result is an improvement of inequality (1) for \( j \) even that is attainable for infinitely many values of \( d \).

**Theorem 1.2.** For \( j = 2k \) even and \( A \in M_{j,d}(\{0, 1\}) \),

\[
\det AA^T \leq (j+1) \left( \frac{j+2}{j+1} \right)^{d/2}. \tag{2}
\]

Equality holds in (2) if and only if \( AA^T = t(I+J) \), for some integer \( t \), and each column of \( A \) has either \( k \) or \( k+1 \) ones.

For each \( j = 2k \) even, equality is attained in (2) for dimensions \( d \) a multiple of \( C(j+1,k) \). The methods used in [HKL] to prove Theorem 1.1 are geometric and rely on the fact that the largest \( j \)-simplex inscribed in a given \( j \)-ball is regular [Fe]. This geometric argument does not seem to work for Theorem 1.2. We use a new matrix-theoretic argument to prove both Theorems 1.1 and 1.2 that gives additional information about the cases of equality.

In related matters, the article [GKL] deals with the more general situation of \( d \)-polytopes instead of the \( d \)-cube. Reference [NR] provides some new results when \( j = d \). The list of publications on this subject is extensive and the reader is referred to the excellent discussion and bibliography of [HKL] for further references.

Not surprisingly, this problem has close connection to design theory and has been studied under the concept of \( D \)-optimal designs (see [SS]).

In order to state the next result we introduce some notation. For \( 1 \leq k \leq j \), let \( G_k \in M_{j,k}(\{0, 1\}) \) be the matrix whose columns are formed by the \( C(j,k) \) distinct \( (0,1) \)-vectors with exactly \( k \) ones. If \( B \) is any matrix and \( m \) is a positive integer let \( m \cdot B = [B, B, \ldots, B] \) denote the matrix obtained by concatenating the matrix \( B \) \( m \) times.

**Theorem 1.3.** [HKL, Theorem 4.2 and 4.14]. Assume \( j = 2k - 1 \) is odd and \( d = mC(j,k) \) is a multiple of \( C(j,k) \). Let \( A_0 = m \cdot G_k = [G_k, G_k, \ldots, G_k] \). Then for all \( A \in M_{j,d}(\{0, 1\}) \),

\[
\det AA^T \leq \det A_0 A_0^T = (1+j)[mC(2k-3, k-1)]^j. \tag{3}
\]
2. Assume \( j = 2k \) is even and \( d = mC(j + 1, k) \) is a multiple of \( C(j + 1, k) \). Let \( A_0 = m \ast \{ G_k, G_{k+1}, G_k, G_{k+1}, \ldots, G_k, G_{k+1} \} \). Then for all \( A \in M_{j,d}(\{0,1\}) \),

\[
\det AA^T \leq \det A_0A_0^T = (1 + j)[mC(2k - 1, k)]^2.
\] (4)

Furthermore, equality occurs in (3) only if \( AA^T = A_0A_0^T \) and each column of \( A \) contains exactly \( k \) ones. Equality occurs in (4) only if \( AA^T = A_0A_0^T \) and each column of \( A \) contains either \( k \) or \( k + 1 \) ones.

In the following corollary, we restate Theorem 1.3 in the context of \( j \)-dimensional volumes. The proof follows immediately from the fact that the volume of a \( j \)-simplex defined by the rows of the \( j \times d \) matrix \( A \) and the origin is given by \((1/j!)(\det AA^T)^{1/2}\). Let \( V(j, d) \) denote the maximum volume of a \( j \)-simplex spanned by vertices of \( C_d \).

**Corollary 1.4.** 1. If \( j = 2k - 1 \) is odd and \( d = mC(j, k) \), then

\[
V(j, d) = \frac{1}{j!} (1 + j)^{1/2} \left[ mC(2k - 3, k) \right]^{1/2}. \tag{5}
\]

Thus, the volume of any \( j \)-simplex spanned by vertices of \( C_d \) is bounded by \((1/j!)(1 + j)^{1/2} (mC(2k - 3, k - 1))^{1/2}\).

2. If \( j = 2k \) is even and \( d = mC(j + 1, k) \), then

\[
V(j, d) = \frac{1}{j!} (1 + j)^{1/2} \left[ mC(2k - 1, k) \right]^{1/2}. \tag{6}
\]

Thus, the volume of any \( j \)-simplex spanned by vertices of \( C_d \) is bounded by \((1/j!)(1 + j)^{1/2} (mC(2k - 1, k - 1))^{1/2}\).

Theorem 1.3 also allows us to make a statement about the asymptotic behavior of the function \( V(j, d) \) for fixed values of \( j \).

**Corollary 1.5.** For fixed \( j \)

\[
\lim_{d \rightarrow \infty} V(j, d)^{d^{1/2}} = V(j), \tag{7}
\]

where \( V(j) = (1/j!)(1 + j)^{1/2} [(j + 1)/4j]^{1/2} \) if \( j = 2k - 1 \) is odd, and \( V(j) = (1/j!)(1 + j)^{1/2} [(j + 2)/4(j + 1)]^{1/2} \) if \( j = 2k \) is even.

This result can be viewed as an extension of the well-known fact that the maximum determinant of a \( d \times d \) \((0,1)\)-matrix is of order \((d + 1)^{(d+1)/2}\). The exact value of the quotient \( A((d + 1)^{(d+1)/2}) \) depends on the congruence class of \( d \) modulo 4. See [NR] for more details.
Proof. For fixed $j$, the function $V(j, d)$ is strictly increasing in $d$. Again it suffices to prove the corresponding fact for matrices. If $A \in M_{j,d}\{0, 1\}$ is maximal with respect to $\det AA^T$, then by the Cauchy–Binet Theorem at least one of the $j \times j$ submatrices of $A$ has a non-zero determinant. Let $u$ be any column of such a submatrix and form the $j \times (d+1)$ matrix $A_1 = (A, u)$ obtained from $A$ by adjoining the column vector $u$. Then by the Cauchy–Binet Theorem $\det AA^T < \det A_1A_1^T$.

If $j = 2k$ let $c = C(j + 1, k)$ and if $j = 2k - 1$ let $c = C(j, k)$. For any $d \geq c$ write $d = mc + r$ where $0 \leq r < c$. Then

$$V(j, mc) = V(j)(mc)^{j/2} \leq V(j, d)$$

$$\leq V(j, (m+1)c) = V(j)((m+1)c)^{j/2}.$$  

Hence

$$\frac{V(j, mc)}{d^{j/2}} \leq \frac{V(j, d)}{d^{j/2}} < \frac{V(j, (m+1)c)}{d^{j/2}}$$

and

$$\left(\frac{mc}{mc+r}\right)^{j/2} \leq \left(\frac{V(j, d)}{mc} \right)^{j/2} < \left(\frac{(m+1)c}{mc+r}\right)^{j/2}.$$  

Taking the limit as $d \to \infty$, i.e., $m \to \infty$, yields the result.  

2. PROOFS

Proof of Theorems 1.1 and 1.2. Let $A$ be a matrix in $M_{j,d}\{0, 1\}$. Instead of dealing directly with $\det AA^T$, we will establish an upper bound for $\det[((j+1)I-J)AA^T]$. Indeed, the core of the proof is to apply the arithmetic–geometric mean inequality to the eigenvalues of $((j+1)I-J)AA^T$. To do that, we must first show that the eigenvalues of $((j+1)I-J)AA^T$ are nonnegative. Note that $(j+1)I-J$ is positive semi-definite and the non-zero eigenvalues of $((j+1)I-J)AA^T$ are the equal of the non-zero eigenvalues of $AA^T((j+1)I-J)A$, which is positive semi-definite. Thus the eigenvalues of $AA^T((j+1)I-J)A$, and hence of $((j+1)I-J)AA^T$, are nonnegative.

Now we can apply the arithmetic–geometric mean inequality to these eigenvalues which yields

$$\det[((j+1)I-J)AA^T] \leq \left(\frac{1}{j}\text{trace}[(j+1)I-J)AA^T]\right)^j.$$

(12)
To evaluate $\text{trace}[((j+1) I - J) A A^T]$, we examine the diagonal entries of $A^T((j+1) I - J) A$, which has the same trace. Suppose the $i$th column $u$ of $A$ has $r$ ones and $j-r$ zeros. Then the $(i,i)$-entry of $A^T((j+1) I - J) A$ equals

$$u^T((j+1) I - J) u = (j+1) u^T u - u^T J u = (j+1) r - r^2 = r(j + 1 - r). \quad (13)$$

Thus if there are $n_r$ columns of $A$ with exactly $r$ ones, $r = 1, \ldots, j$, then

$$\text{trace}(A^T((j+1) I - J) A) = \sum_{r=1}^{j} r(j + 1 - r) n_r. \quad (14)$$

Now we consider the $j$ odd and $j$ even cases separately.

Case $j = 2k - 1$. The maximum value of $r(j + 1 - r)$ is $k^2$ and it occurs at $r = k$. Thus

$$\sum_{r=1}^{j} r(j + 1 - r) n_r \leq k^2 \sum_{r=1}^{j} n_r = k^2 d. \quad (15)$$

Combining (12), (14) and (15) we get

$$\det[(j+1) I - J] A A^T] \leq \left(\frac{k^2 d}{j}\right)^j \quad (16)$$

$$= \left(\frac{j+1}{j}\right)^{\frac{d}{4}} \quad (17)$$

But since $\det((j+1) I - J) = (j+1)^{j-1}$, inequality (1) follows.

Case $j = 2k$. The maximum value of $r(j + 1 - r)$ is $k(k+1)$ and occurs at $r = k$ and at $r = k + 1$. Thus

$$\sum_{r=1}^{j} r(j + 1 - r) n_r \leq k(k+1) \sum_{r=1}^{j} n_r = k(k+1) d. \quad (18)$$

Now by combining (12), (14) and (18) we get

$$\det[(j+1) I - J] A A^T] \leq \left(\frac{k(k+1) d}{j}\right)^j \quad (19)$$

$$= (j+2)^{\frac{d}{4}} \quad (20)$$

Inequality (2) follows.
To analyze the case of equality in Theorem 1.2, we must determine necessary and sufficient conditions on $A$ for equality to hold in inequalities (12) and (18). Equality holds in (18) if and only if each column of $A$ has either $k$ or $k+1$ ones. Equality holds in (12) if and only if the eigenvalues of $((j+1)I-J)AA^T$ are all equal. Notice that $((j+1)I-J)(I+J) = (j+1)I$. Thus, if $AA^T = t(I+J)$ for some integer $t$, then $((j+1)I-J)AA^T = t(j+1)I$ has equal eigenvalues. We finish the proof by showing that if $((j+1)I-J)AA^T$ has equal eigenvalues, then it is a scalar matrix.

Let $\lambda$ be the only eigenvalue of $((j+1)I-J)AA^T$. We prove that $((j+1)I-J)AA^T$ is a scalar matrix by showing that it has $j$ linearly independent eigenvectors. The eigenvalues of $A^T((j+1)I-J)A$ are $\lambda$ with multiplicity $j$, and 0 with multiplicity $d-j$. Since $A^T((j+1)I-J)A$ is symmetric, there exist linearly independent eigenvectors $v_1, ..., v_j$ in $R^d$ such that

$$A^T((j+1)I-J)Av_i = \lambda v_i,$$

for $i = 1, ..., j$. Then $v_i = A^Tu_i$, where $u_i = \lambda^{-1}((j+1)I-J)Av_i \in R^d$. So

$$A^T((j+1)I-J)AA^Tu_i = \lambda A^Tu_i$$

and then

$$AA^T((j+1)I-J)AA^Tu_i = \lambda AA^Tu_i$$

Since $AA^T$ is invertible, we have

$$((j+1)I-J)AA^Tu_i = \lambda^2 u_i,$$

for $i = 1, ..., j$. That $u_1, ..., u_j$ are linearly independent follows from the linear independence of $v_1, ..., v_j$.

A similar argument shows that equality holds in inequality (1) of Theorem 1.1 if and only if every column of $A$ contains exactly $k$ ones and $AA^T = t(I+J)$ for some integer $t$.

Proof of Theorem 1.3. We first observe that for any $1 \leq k \leq j$,

$$G_kG_k^T = C(j-2, k-1)I + C(j-2, k-2)J. \quad (21)$$

Assume $j = 2k$, $d = mC(j+1, k)$ and $A_0 = m \ast [G_k, G_{k+1}]$. Then

$$A_0A_0^T = mC(2k-1, k)(I+J). \quad (22)$$
Since \( \det(I + J) = j + 1 \), we have
\[
\det A_0A_0^T = [mC(2k - 1, k)]^j(j + 1)
\]
(23)
\[
= (j + 1) \left( \frac{j + 2}{j + 1} \right)^j \left( \frac{d}{4} \right)^j.
\]
(24)

So the upper bound in inequality (2) is attained at \( A_0 \) and inequality (4) is proved. By Theorem 1.2, equality holds in (4) for \( A \in M_{j,d}(\{0, 1\}) \) if and only if each column of \( A \) contains \( k \) or \( k + 1 \) ones and \( AA^T = t(I + J) \) for some integer \( t \). But then \( \det A_0A_0^T = \det AA^T = t^m(j + 1) \). From Eq. (23) we have \( t = mC(2k - 1, k) \) and so \( A_0A_0^T = AA^T \).

A similar argument proves the case where \( j = 2k - 1 \) is odd.

3. SIMPLICES WITH MAXIMAL VOLUME

3.1. Regularity

The \( j \)-simplex defined by the rows \( u_1, \ldots, u_j \) of the matrix \( A_0 \), in Theorem 1.3 is a highly regular object. In the proof of Theorem 1.3 we verified that the Gram matrix \( A_0A_0^T = r(I + J) \), where \( r \) is an integer that depends on \( j \) and \( d \). In terms of the vertices \( u_0 = 0, u_1, \ldots, u_t \) of the simplex, this means that for \( 1 \leq i, k \leq j \)
\[
u_i \cdot u_k = \begin{cases} 2r & \text{if } i = k \\ r & \text{if } i \neq k. \end{cases}
\]

Thus each side \( u_i - u_k \) (\( 0 \leq i \neq k \leq j \)) of the simplex has length \( \|u_i - u_k\| = \sqrt{2r} \), and the angle between any two adjacent sides is 60° since \( (u_i - u_k) \cdot (u_j - u_k) = r \), for \( 1 \leq i, k, l \leq j \) distinct. In particular, if \( j = d = 3 \) then the simplex is a regular tetrahedron in the unit cube \( C_3 \).

3.2. Uniqueness

For a given \( j \), let \( d \) and \( A_0 \) be defined as in Theorem 1.3. That is, \( d = mC(j, k) \) and \( A_0 = m \cdot G_k \) if \( j = 2k - 1 \) is odd, and \( d = mC(j + 1, k) \) and \( A_0 = m \cdot [G_k, G_{k+1}] \) if \( j = 2k \) is even. Are these \( j \times d \) \((0, 1)\)-matrices the only ones for which \( \det A_0A_0^T \) is maximal? In one sense the answer is no, because if \( A_1 \) is any \( j \times d \) matrix obtained by permuting the columns of \( A_0 \), then \( A_1A_1^T = A_0A_0^T \) and so \( A_1A_1^T \) is also maximal. But the converse is true only if \( j \leq 5 \). Indeed for \( j = 6, d = C(7, 3) = 35 \), there is a \( 6 \times 35 \) \((0, 1)\)-matrix \( A_1 \) for which \( \det A_1A_1^T = \det A_0A_0^T = 7 \cdot 10^6 \), but the columns of \( A_1 \) are not the same as the columns of \( A_0 = [G_3, G_4] \).
Example 3.1. Let $j = 6$, $A_0 = [G_3, G_4]$ and

$$R_0 = \begin{bmatrix}
1 & 1 & 1 & 1 \\
0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 \\
0 & 1 & 1 & 0
\end{bmatrix}, \quad R_1 = \begin{bmatrix}
1 & 1 & 1 & 1 \\
0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 1 & 1 \\
1 & 0 & 0 & 1
\end{bmatrix}.$$

The columns of $R_1$ are not a rearrangement of the columns of $R_0$, but

$$R_0R_0^T = R_1R_1^T.$$

The first two columns of $R_0$ appear in $G_3$ and the last two columns of $R_0$ appear in $G_4$. Remove these four columns from $A_0$ to obtain a $6 \times 31$ matrix $H$. Then

$$A_0A_0^T = H H^T + R_0R_0^T.$$

Let $A_1 = [H, R_1]$. The $6 \times 35$ matrix $A_1$ does not have the same columns as $A_0$, but

$$A_1A_1^T = H H^T + R_1R_1^T = H H^T + R_0R_0^T = A_0A_0^T.$$

Thus $A_1$ is also a maximal example.

Proposition 3.2. Let $j \leq 5$ and let $d$ and $A_0$ be defined as in Theorem 1.3. Suppose $A$ is a $j \times d$ $(0, 1)$-matrix for which $\det AA^T = \det A_0A_0^T$ is maximal. Then the columns of $A$ are the same as the columns of $A_0$.

Proof. We give the proof of the case $j = 4, d = 10m$. The proofs for $j = 2, 3, 5$ are similar.

Let $A$ be a $4 \times d$ $(0, 1)$-matrix satisfying $\det AA^T = \det A_0A_0^T = 5 \cdot (3m)^4$, where $A_0 = m \ast [G_2, G_3]$. Then from Theorem 1.3, each column of $A$ has either 2 or 3 ones. Suppose column $u_1 = (1, 1, 0, 0)^T$ occurs $k_1$ times, $u_2 = (1, 0, 1, 0)^T$ occurs $k_2$ times, $u_3 = (1, 0, 0, 1)^T$ occurs $k_3$ times, $u_4 = (0, 1, 1, 0)^T$ occurs $k_4$ times, $u_5 = (0, 1, 0, 1)^T$ occurs $k_5$ times, $u_6 = (0, 0, 1, 1)^T$ occurs $k_6$ times, $u_7 = (1, 1, 1, 0)^T$ occurs $k_7$ times, $u_8 = (1, 1, 0, 1)^T$ occurs $k_8$ times,
\(u_9 = (1, 0, 1, 1)^T\) occurs \(k_9\) times and \(u_{10} = (0, 1, 1, 1)^T\) occurs \(k_{10}\) times in \(A\). Then

\[AAT = \sum_{i=1}^{10} k_i u_i u_i^T.\]

But

\[A_0 A_0^T = \sum_{i=1}^{10} m u_i u_i^T,\]

and from Theorem 1.3 \(AAT = A_0 A_0^T\). Thus

\[\sum_{i=1}^{10} (m - k_i) u_i u_i^T = 0.\]

It is easy to show that the 4 \times 4 symmetric matrices \(u_1 u_1^T, \ldots, u_{10} u_{10}^T\) are linearly independent. (In fact they are a basis for the 10-dimensional space of symmetric 4 \times 4 matrices.) Thus \(k_i = m\) for \(i = 1, \ldots, 10\) and so \(A\) and \(A_0\) have the same columns, but possibly in a different order.

4. SMALL VALUES OF \(j\)

4.1. The Case \(j = 2\)

The case \(j = 2\) was dealt with in [HKL]. For all multiples of 3 it is also covered by Theorem 1.3 above. We give another proof of the following theorem from [HKL]:

**Proposition 4.1.** If \(d = 3k + i, i \in \{0, 1, 2\}\), then

\[V(2, d) = \begin{cases} 
\frac{1}{2} \sqrt{3k^2} & \text{if } i = 0, \\
\frac{1}{2} \sqrt{3k^2 + 2k} & \text{if } i = 1, \\
\frac{1}{2} \sqrt{3k^2 + 4k + 1} & \text{if } i = 2.
\end{cases}\]  

(25)

**Proof.** Assume \(A \in M_{k,d}(\{0, 1\})\) and that column \((1, 0)^T\) occurs \(k_1\) times, columns \((0, 1)^T\) occurs \(k_2\) times, and column \((1, 1)^T\) occurs \(k_3\) times. Then it is easy to see that

\[AAT = \begin{pmatrix} k_1 + k_3 & k_3 \\
k_3 & k_2 + k_3 \end{pmatrix}\]

(26)

and hence \(\det AAT = k_1 k_2 + k_1 k_3 + k_2 k_3 = E_2(k_1, k_2, k_3)\), the elementary symmetric function of degree 2 on \(k_1, k_2, k_3\). It is well-known (see [MO]).
that $E_d(k_1,k_2,k_3)$ subject to $k_1 + k_2 + k_3 = d$ and $k_i \in \mathbb{Z}^+$ is maximized when the $k_i$ are as equal as possible; i.e., $k_1 = k_2 = k_3 = k$ if $d = 3k$, $k_1 = k_2 = k_3 - 1 = k$ if $d = 3k + 1$, and $k_1 = k_3 - 1 = k_3 - 1 = k$ if $d = 3k + 2$. We call such an arrangement of the values of $k_i$, balanced. Thus if $A_0 \in M_{d, d}(\{0, 1\})$ has a balanced arrangement of columns, then

$$\det AA^T \leq \det A_0 A_0^T = \begin{cases} 3k^2 & \text{if } i = 0 \\ 3k^2 + 2k & \text{if } i = 1 \\ 3k^2 + 4k + 1 & \text{if } i = 2 \end{cases}$$

(27)

4.2. The Case $j = 3$

The case $j = 3$ was also dealt with in [HKL] and the following holds:

**Proposition 4.2.** If $d = 3k + i, i \in \{0, 1, 2\}$, then

$$V(3, d) = \frac{1}{3} \sqrt{k^2 - (k + 1)^2}.$$  

(28)

We give another proof here.

**Proof.** Let $A$ be a matrix in $M_{d, d}(\{0, 1\})$. Suppose column $(1, 0, 0)^T$ appears $k_1$ times, $(0, 1, 0)^T$ appears $k_2$ times, and $(0, 0, 1)^T$ appears $k_3$ times, $(1, 1, 0)^T$ appears $k_4$ times, $(1, 0, 1)^T$ appears $k_5$ times, $(0, 1, 1)^T$ appears $k_6$ times, and $(1, 1, 1)^T$ appears $k_7$ times in $A$, where $k_1 + k_2 + \cdots + k_7 = d$. Then

$$AA^T = \begin{bmatrix} k_1 + k_4 + k_5 + k_7 & k_4 + k_7 & k_5 + k_7 \\ k_4 + k_7 & k_2 + k_4 + k_6 + k_7 & k_6 + k_7 \\ k_5 + k_7 & k_6 + k_7 & k_3 + k_5 + k_6 + k_7 \end{bmatrix}.$$  

If $k_1 = k_2 = k_3 = k_7 = 0$, then $\det AA^T = 4k_4k_5k_6$. Thus $\det AA^T$ is maximized when $k_4, k_5, k_6$ are balanced. This yields the values of $V(3, d)$ of (28).

It remains to show that a maximal example in dimension $d \geq 3$ satisfies $k_1 = k_2 = k_3 = k_7 = 0$.

We proceed by induction $3 \leq d$. If $d = 3$, then it is well-known (see e.g., [NR]) that $k_4 = k_5 = k_6 = 1$ yields a maximal $3 \times 3$ matrix. This matrix is the incidence matrix of a symmetric Hadamard design.

Assume that the matrix $A$ is a maximal example in dimension $d + 1$ where $d = 3k + i, i \in \{0, 1, 2\}$ and assume $k_1 > 0$. Then we may assume without loss of generality that $A = (A_1, u)$ where $u^T = (1, 0, 0)$. Then

$$AA^T = A_1 A_1^T + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

(29)
and hence
\[
\det A A^T = \det A_1 A_1^T + \det A' A'^T,  \tag{30}
\]
where \( A' \in M_{2,d}(\{0,1\}) \) is the matrix obtained from \( A_1 \) by deleting its first row. By induction
\[
\det A_1 A_1^T \leq \begin{cases} 
4k^3 & \text{if } i = 0 \\
4k^2(k+1) & \text{if } i = 1 \\
4k(k+1)^2 & \text{if } i = 2.
\end{cases}
\]
Hence by (30) and inequality (27) applied to \( A' \), we have
\[
\det A A^T \leq \begin{cases} 
4k^3 + 3k^2 & \text{if } i = 0 \\
4k^2(k+1) + 3k^2 + 2k & \text{if } i = 1 \\
4k(k+1)^2 + 3k^2 + 4k + 1 & \text{if } i = 2
\end{cases}  \tag{31}
\]
\[
< \begin{cases} 
4k^2(k+1) & \text{if } i = 0 \\
4(k+1)^2 & \text{if } i = 1 \\
4(k+1)^3 & \text{if } i = 2
\end{cases}  \tag{32}
\]
\[
= \det A_0 A_0^T,  \tag{33}
\]
where \( A_0 \in M_{3,d+1}(\{0,1\}) \) is a balanced example with \( k_1 = k_2 = k_3 = k_7 = 0 \). This contradicts the assumption that \( A \) is a maximal example. Hence no maximal example contains \((1,0,0)^T\) as a column.

Similarly we can show that if \( k_2 > 0 \) or \( k_3 > 0 \), then \( A \) is not maximal.

If \( k_7 > 0 \), subtract the first row of \( A \) from rows 2 and 3, then multiply row 1 by \(-1\) and finally multiply all columns that contain \(-1\)s by \(-1\). The resulting matrix is a \((0,1)\)-matrix \( B \) satisfies \( \det B B^T = \det A A^T \) by the Cauchy–Binet Theorem. In addition it has a column \((1,0,0)^T\) and we can proceed as above.

We have shown that if \( A \) is a maximal example then \( k_1 = k_2 = k_3 = k_7 = 0 \) and we showed above that in this case the balanced examples as described above are maximal.

REFERENCES


