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D-OPTIMAL WEIGHING DESIGNS FOR FOUR AND FIVE OBJECTS*

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Abstract. For $j = 4$ and $j = 5$ and all $d \geq j$, the maximum value of $\det XX^T$, where X runs through all $j \times d$ (0,1)-matrices, is determined along with a matrix X_0 for which the maximum determinant is attained. In the theory of statistical designs, X_0 is called a D-optimal design matrix. Design matrices that were previously thought to be D-optimal, are shown here to be D-optimal.

Key words. D-optimal design, weighing design

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1. Introduction. Let $M_{j,d}(0,1)$ be the set of all $j \times d$ (0,1)-matrices. Our problem is to find

$$G(j,d) = \max\{\det AA^T : A \in M_{j,d}(0,1)\},$$

and matrices for which the maximum is attained. Since $\det AA^T = 0$ if $j > d$, we assume throughout that $j \leq d$. This is an old problem that arises in two contexts. The first is statistical and begins with the work of Hotelling [Ho] in 1944 and Mood [Mo] 1946. They were interested in estimating the weights of j objects with d weighings on an inaccurate scale. Each matrix A in $M_{j,d}(0,1)$ corresponds to a weighing design. Namely, for the kth weighing ($1 \leq k \leq d$), weigh all objects i ($1 \leq i \leq j$) for which $a_{i,k} = 1$. If $a_{i,k} = 0$, leave object i off the scale. In this context, A is called a *design matrix* and we will use this terminology throughout. Under certain assumptions about the distribution of errors for the scale, the smallest confidence region (an ellipsoid) is obtained at the design matrix A for which $\det AA^T$ is maximal among all $j \times d$ design matrices. For details see [SS].

Definition 1.1. A matrix $A \in M_{j,d}(0,1)$ is a *D-optimal (design) matrix* if $\det AA^T = G(j,d)$.

The second context for the problem is geometric. The volume of the j-simplex generated by the origin and the rows (in $\mathbb{R}^d$) of a $j \times d$ matrix A is $(1/j!)(\det AA^T)^{\frac{1}{2}}$. Thus the problem of maximizing the volume of a j-simplex in the d-dimensional cube $[0,1]^d$ is equivalent to finding $G(j,d)$.

The maximum $G(j,d)$ is not known in general. But for each j, infinite families of D-optimal matrices A exist for which $\det AA^T = G(j,d)$ [HKL], [NWZ1], [NWZ2]. And for $j = 2,3$, $G(j,d)$ is known for all $d \geq j$ [HKL]. We summarize the results for $j = 2,3$ in the following result.

Proposition 1.2 ([HKL]). *Let $d = 3t + r \geq 2$, where $0 \leq r < 3$. Then*

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1.

$$G(2,d)=\begin{cases} 3t^2 & \textit{if } r=0 \\ 3t^2+2t & \textit{if } r=1 \\ 3t^2+4t+1 & \textit{if } r=2, \end{cases}$$

and the maximum value $G(2,d)$ is attained at the D-optimal matrix whose kth column is the $(k \bmod 3)$ column of

$$B_2=\begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}.$$

2.

$$G(3,d)=4t^{3-r}(t+1)^r$$

and the maximum value $G(3,d)$ is attained at the D-optimal matrix whose kth column is the $(k \bmod 3)$ column of

$$B_3=\begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

As an example, A_1 is a 2×4 D-optimal matrix and A_2 is a 2×5 D-optimal matrix, where

$$A_1=\begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}, \text{ and } A_2=\begin{bmatrix} 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{bmatrix}.$$

As a part of their of results on D-optimal matrices, Hudelson, Klee and Larman[HKL] give lower bounds for values of $G(j,d)$ for $4\le j\le 8$ and all $d\ge j$ and they list design matrices for which lower bounds for these matrices are attained. As noted earlier, $G(j,d)$ is known for $j=2,3$ and all $d\ge j$. The purpose of this paper is to settle the question for $j=4,5$ and all $d\ge j$. Indeed we show here that for $j=4,5$, the lower bounds on $G(j,d)$ given in [HKL] are infact equal to $G(j,d)$, which proves that the design matrices given in [HKL] are D-optimal.

Before presenting the results for $j=4,5$, we note that in general each column of a $j\times d$ D-optimal matrix contains about $j/2$ ones and $j/2$ zeros provided d is sufficiently large in relation to j. To be precise:

THEOREM 1.3 ([NWZ2]). *1. For every $j=2k-1$ odd, there exists a d_0 such that for all $d\ge d_0$ all columns of all D-optimal $A\in M_{j,d}(0,1)$ have exactly k ones.*
2. For every $j=2k$ even, there exists a d_0 such that for all $d\ge d_0$ all columns of all D-optimal $A\in M_{j,d}(0,1)$ have exactly k or $k+1$ ones.

That is, for fixed j and d sufficiently large, all $j\times d$ D-optimal matrices are in the set

$$S_{j,d}(0,1)=\begin{cases} \{A\in M_{j,d}(0,1): e_jA=ke_d\} & \text{if } j=2k-1 \\ \{A\in M_{j,d}(0,1): e_jA=ke_d \text{ or } (k+1)e_d\} & \text{if } j=2k, \end{cases}$$

where e_n is the all-ones vector of length n. Thus for large d, $G(j,d) = F(j,d)$ where

$$F(j,d) = \max\{\det AA^T | A \in S_{j,d}(0,1)\}.$$

Of course it is always true that $F(j,d) \leq G(j,d)$ and in Section 4 we will encounter cases of strict inequality for $j = 5$ and small values of d. In the analysis for $j = 4, 5$, we use an inequality by Cohn [Co1], which is discussed and proved in Section 6.

2. D-optimal $4 \times d$ designs. In this section we show that the lower bounds on $G(4,d)$ given in [HKL, Theorem 6.2] are in fact equal to $G(4,d)$ and that all $4 \times d$ D-optimal matrices are in $S_{4,d}(0,1)$ so that $G(4,d) = F(4,d)$ for all $d \geq 4$. We begin with some notation to describe certain design matrices in $S_{4,d}(0,1)$. Let $v_1, ..., v_{10}$ be the 10 distinct $(0,1)$-vectors of length 4 which contain exactly 2 ones or exactly 3 ones, i.e. $v_1, ..., v_{10}$ are, in order, the columns of the matrix

$$A_0 = \begin{bmatrix} 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

For non-negative integers $b_1, ..., b_{10}$, let $A = [b_1 * v_1, b_2 * v_2, ..., b_{10} * v_{10}]$ denote the $(0,1)$-matrix where the column v_i is repeated b_i times. Then $AA^T = A_0 \operatorname{diag}(b_1, \ldots, b_{10}) A_0^T$.

Now suppose $d = 10t + r$, where $0 \leq r \leq 9$. For $b = (b_1, \ldots, b_{10})$, define $a = (a_1, \ldots, a_{10})$ so that $b = te_{10} + a = (t + a_1, \ldots, t + a_{10})$. The vector a is integral and $a_1 + \ldots + a_{10} = r$, but some of the a_i may be negative.

For an integral vector a, there is a family of design matrices, $A(t) = [(t + a_1) * v_1, \ldots, (t + a_{10}) * v_{10}]$, where t must be large enough so that $t + a_i \geq 0$, for all i. Now since

$$A(t)A(t)^T = A_0 \operatorname{diag}(t + a_1, \ldots, t + a_{10}) A_0^T,$$

it is clear that $\det A(t)A(t)^T$ is a polynomial of degree 4 in t.

For each $r = 0, \ldots, 9$, [HKL] exhibits a family of design matrices $A_r(t)$ in $S_{4,10t+r}(0,1)$ $(10t + r \geq 0)$ and a 4^{th} degree polynomial $K_r(t)$ for which

$$\det A_r(t)A_r(t)^T = K_r(t).$$

The families $A_r(t)$ and the polynomial $K_r(t)$ are given below:

$$A_r(t) = (b_1 * v_1, \ldots, b_{10} * v_{10}),$$

where $b = te_{10} + a$ and $a = (a_1, ..., a_{10})$ is

$$(1)\qquad \begin{array}{lll} (0,0,0,0,0,0,0,0,0,0) & \text{if} & r=0 \\ (1,0,0,0,0,0,0,0,0,0) & \text{if} & r=1 \\ (0,0,0,-1,0,0,0,1,1,1) & \text{if} & r=2 \\ (0,0,0,0,0,0,0,1,1,1) & \text{if} & r=3 \\ (1,1,1,1,0,0,0,0,0,0) & \text{if} & r=4 \\ (1,1,1,1,1,0,0,0,0,0) & \text{if} & r=5 \\ (0,0,0,0,1,1,1,1,1,1) & \text{if} & r=6 \\ (1,1,1,1,1,1,1,0,0,0) & \text{if} & r=7 \\ (1,1,1,2,1,1,1,0,0,0) & \text{if} & r=8 \\ (0,1,1,1,1,1,1,1,1,1) & \text{if} & r=9, \end{array}$$

and

$$(2)\qquad \begin{array}{ll} K_0(t) = 405t^4 & \text{if } r=0 \\ K_1(t) = 405t^4 + 162t^3 & \text{if } r=1 \\ K_2(t) = 405t^4 + 324t^3 + 81t^2 + 9t & \text{if } r=2 \\ K_3(t) = 405t^4 + 486t^3 + 189t^2 + 24t & \text{if } r=3 \\ K_4(t) = 405t^4 + 648t^3 + 378t^2 + 96t + 9 & \text{if } r=4 \\ K_5(t) = 405t^4 + 810t^3 + 576t^2 + 174t + 19 & \text{if } r=5 \\ K_6(t) = 405t^4 + 972t^3 + 864t^2 + 336t + 48 & \text{if } r=6 \\ K_7(t) = 405t^4 + 1134t^3 + 1161t^2 + 516t + 84 & \text{if } r=7 \\ K_8(t) = 405t^4 + 1296t^3 + 1539t^2 + 804t + 156 & \text{if } r=8 \\ K_9(t) = 405t^4 + 1458t^3 + 1944t^2 + 1134t + 243 & \text{if } r=9. \end{array}$$

Since $K_r(t)$ is achievable as $\det A_r(t)A_r(t)^T$, $K_r(t)$ is a lower bound for $G(4, 10t+r)$. In this section we prove that $G(4, 10t + r) = K_r(t)$ for all $0 \le r \le 9$. In other words we prove that

$$\det AA^T \le K_r(t),$$

for all $A \in M_{4,10t+r}(0, 1)$.

THEOREM 2.1. *Let $j = 4$, $d = 10t + r \ge 4$ and $K_r(t)$ be as in (2) above. Then*
1. $F(4, 10t + r) = K_r(t)$, for all $t \ge 0$ and $0 \le r \le 9$.
2. For all $d \ge 4$, every D-optimal matrix is in $S_{4,d}(0, 1)$.
3. For all $d \ge 4$, $G(4, d) = F(4, d)$.

It follows from Theorem 2.1 that the matrices from [HKL], exhibited in (1) are D-optimal. Although all D-optimal matrices are in $S_{4,d}(0, 1)$, they are not unique. For example, a matrix obtained from a D-optimal matrix by permuting rows is also D-optimal.

Proof of Theorem 2.1, Part 1. Let $A = (b_1 * v_1, ..., b_{10} * v_{10}) \in S_{4,d}(0, 1)$ with $d = 10t + r$, where $0 \le r \le 9$. Let $a = b - te_{10}$. We begin by using the inequality in Corollary 6.3 to obtain an upper bound $U_r(t, ||a||^2)$ for $\det AA^T$ for which $U_r(t, ||a||^2) \le K_r(t)$ for all $t \ge 0$ and $||a||^2$ sufficiently large. Actually it is easier to apply the inequality in Corollary 6.3 to the matrix $N = PAA^TP^T$, where P is the symmetric matrix with $P^2 = 5I_4 - J_4$. ($P = \sqrt{5}I + \alpha J$, with α chosen so that $P^2 = 5I - J$.)

The upper bound on $\det N$ depends on $\operatorname{trace} N$ and $||N||$, which we now compute.

$$\begin{aligned}
\operatorname{trace} N &= \operatorname{trace} PAA^TP^T \\
&= \operatorname{trace} A^TP^2A \\
&= \operatorname{trace} A^T(5I - J)A \\
&= \sum_{i=1}^{d} (5A^TA - A^TJA)_{ii} \\
&= 6\sum_{i}^{10} b_i \\
&= 6d.
\end{aligned}$$

(Since each column of A has either 2 or 3 ones, $(5A^TA - A^TJA)_{ii} = 6$ for all i.) Next we compute $||N||^2$.

$$\begin{aligned}
||N||^2 &= \operatorname{trace} NN^T = \operatorname{trace} NN \\
&= \operatorname{trace} PAA^TP^2AA^TP^T \\
&= \operatorname{trace} A^TP^2AA^TP^2A \\
&= \operatorname{trace} (A^T(5I - J)A)^2 \\
&= ||A^T(5I - J)A||^2 \\
&= \sum_{1 \le i,j \le d} b_ib_j[v_i^T(5I - J)v_j]^2 \\
&= b^TQb,
\end{aligned}$$

where

$$Q = \begin{bmatrix}
36 & 1 & 1 & 1 & 16 & 16 & 1 & 16 & 1 & 1 \\
1 & 36 & 1 & 1 & 16 & 1 & 16 & 1 & 16 & 1 \\
1 & 1 & 36 & 1 & 1 & 16 & 16 & 1 & 1 & 16 \\
1 & 1 & 1 & 36 & 1 & 1 & 1 & 16 & 16 & 16 \\
16 & 16 & 1 & 1 & 36 & 1 & 1 & 1 & 1 & 16 \\
16 & 1 & 16 & 1 & 1 & 36 & 1 & 1 & 16 & 1 \\
1 & 16 & 16 & 1 & 1 & 1 & 36 & 16 & 1 & 1 \\
16 & 1 & 1 & 16 & 1 & 1 & 16 & 36 & 1 & 1 \\
1 & 16 & 1 & 16 & 1 & 16 & 1 & 1 & 36 & 1 \\
1 & 1 & 16 & 16 & 16 & 1 & 1 & 1 & 1 & 36
\end{bmatrix}$$

is the 10×10 symmetric matrix of the quadratic form above, i.e. $Q = (A_0^T(5I - J)A_0)^{(2)} = ((A_0(5I - J)A_0)_{ij}^2)$, the Schur square of $A_0^T(5I - J)A_0$. From a computer calculation, we obtain the characteristic polynomial of Q: $(x - 90)(x - 5)^4(x - 50)^5$. The eigenspace for $\lambda_1 = 90$ is spanned by e_{10}. Thus $Q = 90P_1 + 5P_4 + 50P_5$, where

$P_1 = \frac{1}{10}J_{10}$ is the symmetric projection of $\mathbb{R}^{10}$ onto the 1-dimensional eigenspace, spanned by $< e_{10} >$, for the eigenvalue $\lambda_1 = 90$, P_4 is the symmetric projection onto the 4-dimensional eigenspace for the eigenvalue $\lambda_2 = 5$, and P_5 is the symmetric projection onto the 5-dimensional eigenspace for the eigenvalue $\lambda_3 = 50$. Thus

$$\begin{aligned} b^TQb &= 90||P_1b||^2 + 5||P_4b||^2 + 50||P_5b||^2 \\ &\geq 85||P_1b||^2 + 5||b||^2 \\ &= 8.5d^2 + 5||b||^2, \end{aligned}$$

which yields

$$||N||^2 \geq 8.5d^2 + 5||b||^2.$$

We now obtain a lower bound for the quantity c of Corollary 6.3 for the positive semidefinite matrix N:

$$\begin{aligned} c^2 &= \frac{4}{3}\left(-4 + \frac{16||N||^2}{36d^2}\right) \\ &\geq \frac{4}{3}\left(-4 + \frac{16(8.5d^2 + 5||b||^2)}{36d^2}\right) \\ &= \frac{8}{27d^2}(10||b||^2 - d^2). \end{aligned}$$

Since $d = 10t + r$ and $b = te_{10} + a$, we have $10||b||^2 - d^2 = 10||a||^2 - r^2$. Thus

$$c^2 \geq \frac{8}{27d^2}(10||a||^2 - r^2).$$

Note that $\det(5I - J) = 5^3$ and that the Cauchy-Schwartz inequality implies $10||a||^2 - r^2 \geq 0$.

Now Corollary 6.3 yields

$$\begin{aligned} &\det AA^T = \frac{1}{5^3}\det N \\ &\leq \frac{1}{5^3}\left(\frac{3d}{2}\right)^4\left(1 + \frac{3c}{4}\right)\left(1 - \frac{c}{4}\right)^3 \\ &\leq \frac{1}{5^3}\left(\frac{3}{2}\right)^4\left(d + \frac{3}{4}\sqrt{\frac{8(10||a||^2 - r^2)}{27}}\right)\left(d - \frac{1}{4}\sqrt{\frac{8(10||a||^2 - r^2)}{27}}\right)^3 \\ &= 405t^4 + 162rt^3 + \frac{9(11r^2 - 2||a||^2)}{4}t^2 \\ &\quad + \left(\frac{171r^3 - 90r||a||^2}{100} - \frac{(10||a||^2 - r^2)^{\frac{3}{2}}}{50\sqrt{6}}\right)t \\ &\quad + \left(\frac{1079r^4 - 1060r^2||a||^2 - 100||a||^4}{24000} + \frac{r(10||a||^2 - r^2)^{\frac{3}{2}}}{500\sqrt{6}}\right) \\ &:= U_r(t, ||a||^2). \end{aligned}$$

The second inequality follows from the fact that $\left(1+\frac{3c}{4}\right)\left(1-\frac{c}{4}\right)^3$ is a decreasing function of c. For the same reason, $U_r(t,||a||^2)$ is a decreasing function of $||a||^2$. Now we can determine a lower bound m_r on $||a||^2$ for each $1 \leq r \leq 9$ such that $U_r(t,||a||^2) < K_r(t)$ for all $t \geq 0$ and $||a||^2 \geq m_r$. Notice that the leading coefficients of $U_r(t,||a||^2)$, 405 and $162r$, do not depend on $||a||^2$ and are the same as the leading coefficients of $K_r(t)$. Thus the degree of $K_r(t) - U_r(t,||a||^2)$ does not exceed 2.

For example, if $r = 3$ and $||a||^2 = 9$, then

$$K_3(t) - U_3(t,||a||^2) = 6.75t^2 - 3.82t - 1.51 > 0$$

for $t \geq 1$. But if $||a||^2 = 8$

$$K_3(t) - U_3(t,||a||^2) = 2.25t^2 - 5.45t - 1.66,$$

which is negative at $t = 1, 2$. Thus $m_3 = 9$. The values of m_r for the other r are computed in a similar way and appear in Table 1. To summarize, if $||a||^2 \geq m_r$, then $U_r(t,||a||^2) < K_r(t)$.

r	1	2	3	4	5	6	7	8	9
m_r	6	5	9	5	11	7	13	12	16

TABLE 1

It is now an easy task to check, with the help of a computer, all possible a with $||a||^2 < m_r$ and the corresponding values for $\det AA^T$. In all cases, $\det AA^T \leq K_r(t)$. Thus $F(4, 10t + r) \leq K_r(t)$ and so $F(10t + r, d) = K_r(t)$. □

Before the proofs of Parts 2 and 3 of Theorem 2.1, we state and prove a necessary lemma. This lemma can be found in the proof of [NWZ2, Lemma 4.2], but it is not explicitly stated there.

LEMMA 2.2. *Let A be a $j \times d$ design matrix and let n_s be the number of columns in A with exactly s ones. Then*

$$\det AA^T \leq (j+1)\left(\frac{1}{j(j+1)}\sum_{s=0}^{j} s(j+1-s)n_s\right)^j. \tag{3}$$

The quantity $s(j + 1 - s)$ is largest when $s = (j + 1)/2$ if j is odd and when $s = j/2$ and $s = (j + 2)/2$ if j is even. This proves the following corollary which is Lemma 4.2 in [NWZ2].

COROLLARY 2.3. *Let A be a $j \times d$ design matrix. If A is not in $S_{j,d}(0, 1)$, then*

$$\det AA^T \leq \begin{cases} (j+1)\left(\frac{1}{j(j+1)}\right)^j\left(\frac{(d(j+1)^2}{4}-1\right)^j, & \textit{if } j \textit{ is odd} \\ (j+1)\left(\frac{1}{j(j+1)}\right)^j\left(\frac{dj(j+2)}{4}-2\right)^j, & \textit{if } j \textit{ is even} \end{cases} \tag{4}$$

Proof of Lemma 2.2. Let A be as in the statement of the lemma. To prove inequality (4), we use the arithmetic-geometric mean inequality on the eigenvalues of the matrix $((j+1)I_j - J_j)AA^T$. The nonzero eigenvalues of $((j+1)I_j - J_j)AA^T$ are nonnegative since they are the same as the nonzero eigenvalues of the positive semidefinite matrix $A^T((j+1)I_j - J_j)A$. Thus by the arithmetic-geometric mean inequality, we have

$$\det((j+1)I_j - J_j)AA^T \leq \left(\frac{1}{j}\mathrm{tr}((j+1)I_j - J_j)AA^T\right)^j. \tag{5}$$

But $\det((j+1)I_j - J_j) = (j+1)^{j-1}$. So the left side of (5) is $(j+1)^{j-1}\det AA^T$. From the right side of (5), we compute

$$\mathrm{tr}((j+1)I - J)AA^T = \mathrm{tr}A^T((j+1)I - J)A.$$

Now let u be the ith column of A and assume that u has exactly s ones. Then

$$\begin{aligned}(A^T((j+1)I - J)A)_{ii} &= u^T((j+1)I - J)u\\ &= (j+1)s - s^2\\ &= s(j+1-s).\end{aligned}$$

It follows that

$$\mathrm{tr}((j+1)I - J)AA^T = \sum_{s=0}^{j} s(j+1-s)n_s.$$

From inequality (5), we have

$$(j+1)^{j-1}\det AA^T \leq \left(\frac{1}{j}\sum_{s=0}^{j} s(j+1-s)n_s\right)^j. \ \square$$

Proof of Theorem 2.1, Parts 2 and 3. We must show that $\det AA^T < K_r(t)$ for all $4\times d$ design matrices $A \notin S_{4,d}(0,1)$. From Corollary 2.3, if $A \notin S_{4,d}(0,1)$, then

$$\det AA^T \leq 5\left(\frac{3(10t+r)-1}{10}\right)^4 := V_r(t). \tag{6}$$

We can now compare the upper bound of $V_r(t)$, defined in (6), with the lower bound $K_r(t)$ on $G(4,d)$. For each r and all values t such that $d = 10t+r \geq 4$ we have that $V_r(t) < K_r(t)$.For example, if $r = 3$

$$K_r(t) - V_r(t) = 54t^3 + \frac{81}{5}t^2 - \frac{168}{25}t - \frac{256}{125} \geq 0,$$

for $t \geq 1$. A similar calculation shows that K_r dominates V_r, for all other values of r. Thus every D-optimal matrix is in $S_{4,d}$ and $F(4,10t+r) = G(4,10t+r)$. By part 1 of Theorem 2.1, $G(4,10t+r) = K_r(t)$. $\square$

3. D-optimal $5 \times d$ designs for large d. In this section we obtain the values of $F(5,d)$ for all $d \geq 5$, and of $G(5,d)$ for all but 29 values of d. As in the analysis for $j=4$, let $d = 10t + r$, where $0 \leq r \leq 9$. For each r, [HKL] gives a family of design matrices $A_r(t) \in S_{5,10t+r}(0,1)$ and a polynomial $L_r(t)$ such that $\det A_r(t)A_r(t)^T = L_r(t)$ for all t. As before, we describe design matrices in $S_{5,10t+r}(0,1)$ in terms of the columns $v_1, \ldots, v_{10}$ of the 5×10 matrix

$$A_0 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \end{bmatrix}. \tag{7}$$

Now let $A_r(t) = [b_1 * v_1, ..., b_{10} * v_{10}]$ where $b = (b_1, ..., b_{10}) = (t + a_1, ..., t + a_{10})$ and $a = (a_1, ..., a_{10})$ is

$$\begin{aligned} &(0,0,0,0,0,0,0,0,0,0)\text{if } r = 0 \\ &(1,0,0,0,0,0,0,0,0,0)\text{if } r = 1 \\ &(1,1,0,0,0,0,0,0,0,0)\text{if } r = 2 \\ &(1,1,1,0,0,0,0,0,0,0)\text{if } r = 3 \\ &(1,1,0,1,0,0,1,0,0,0)\text{if } r = 4 \\ &(0,0,0,0,0,1,1,1,1,1)\text{if } r = 5 \\ &(1,1,1,0,1,0,0,1,0,1)\text{if } r = 6 \\ &(1,1,0,0,0,1,1,1,1,1)\text{if } r = 7 \\ &(1,1,1,1,1,1,1,1,0,0)\text{if } r = 8 \\ &(1,1,1,1,1,1,1,1,1,0)\text{if } r = 9. \end{aligned} \tag{8}$$

Then $\det A_r(t)A_r(t)^T = L_r(t)$ where

(9) $L_r(t) =$

$$\begin{cases} L_0(t) = 1458t^5 & \text{if } r = 0 \\ L_1(t) = 1458t^5 + 729t^4 & \text{if } r = 1 \\ L_2(t) = 1458t^5 + 1458t^4 + 324t^3 & \text{if } r = 2 \\ L_3(t) = 1458t^5 + 2187t^4 + 972t^3 + 135t^2 & \text{if } r = 3 \\ L_4(t) = 1458t^5 + 2916t^4 + 1944t^3 + 540t^2 + 54t & \text{if } r = 4 \\ L_5(t) = 1458t^5 + 3645t^4 + 3240t^3 + 1242t^2 + 198t + 9 & \text{if } r = 5 \\ L_6(t) = 1458t^5 + 4374t^4 + 4860t^3 + 2484t^2 + 594t + 54 & \text{if } r = 6 \\ L_7(t) = 1458t^5 + 5103t^4 + 6804t^3 + 4266t^2 + 1242t + 135 & \text{if } r = 7 \\ L_8(t) = 1458t^5 + 5832t^4 + 9072t^3 + 6804t^2 + 2430t + 324 & \text{if } r = 8 \\ L_9(t) = 1458t^5 + 6561t^4 + 11664t^3 + 10206t^2 + 4374t + 729. & \text{if } r = 9. \end{cases}$$

(These formulas can be computed directly using the observation that $A(t)A(t)^T = A_0 \mathrm{diag}(t + a_0, \ldots, t + a_{10})A_0^T$, where $A(t)$ is the family of design matrices defined by $A(t) = [(t + a_0) * v_0, \ldots, (t + a_{10}) * v_{10}]$.) Thus

$$L_r(t) \leq F(5, 10t + r) \leq G(5, 10t + r),$$

for all t. In this section we show that $F(5,10t+r) = L_r(t)$ for all t and $G(5,10t+r) = L_r(t)$ for sufficiently large t. However for some small t, $G(5,10t+r) > L_r(t)$. In fact for $d = 10t+r = 5,6,7,8,15,16,17,27$, there is a $5 \times d$ design matrix A such that $\det AA^T > L_r(t)$. [HKL] noted these exceptional cases and, without presenting the actual design matrices, gave the values of $\det AA^T$ for these exceptional cases. In the next section, we show that the exceptional d listed above are the only cases where $G(5,d) > L_r(t)$ and that the lower bounds for $G(5,d)$, given in [HKL], for the exceptional values of d are in fact equal to $G(5,d)$.

We now state the main result of this section.

THEOREM 3.1. *Let $j = 5$, $d = 10t+r$ and $A \in M_{j,d}(0,1)$. Let $L_r(t)$ be as in* (9) *above. Then*
1. $F(5,10t+r) = L_r(t)$, for all $10t+r \geq 5$.
2. If $r = 1,9$ and $t \geq 2$, or $r = 2,8$ and $t \geq 3$, or $r = 3,7$ and $t \geq 4$, or $r = 4,5,6$ and $t \geq 5$, then

$$\det AA^T \leq L_r(t) = G(5,10t+r).$$

Furthermore, equality occurs for the design matrices $A_r(t)$ defined in (8).

We remark here that the D-optimal design matrices listed above are not unique. Obviously, a row or column interchange of A does not change the value of $\det AA^T$. Furthermore, if we subtract any row from all the other rows and then change any resulting entries -1 back to 1 by multiplying appropriate columns and rows of A by -1 the value of $\det AA^T$ remains the same. (See Section 5 for details.)

Proof of Theorem 3.1, Part 1. Assume that $A \in S_{5,d}(0,1)$ and $A = (b_1 * v_1, \ldots, b_{10} * v_{10})$. Let α be chosen such that $(I_5 + \alpha J_5)^2 = I - \frac{1}{6}J$. Set $N = (I+\alpha J)AA^T(I+\alpha J)$. We compute $\operatorname{trace} N$ and $||N||^2$ and apply Corollary 6.3 to the matrix N.

$$\begin{aligned}
\operatorname{trace} N &= \operatorname{trace}(I+\alpha J)AA^T(I+\alpha J)\\
&= \operatorname{trace} A^T(I+\alpha J)^2 A\\
&= \operatorname{trace} A^T(I - \frac{1}{6}J)A.
\end{aligned}$$

But $A^T(I-\frac{1}{6}J)A = A^TA - \frac{3}{2}J_d$ since every column of A has exactly 3 ones. Furthermore, each diagonal entry of $A^T(I-\frac{1}{6}J)A$ is $\frac{3}{2}$. Thus,

$$\operatorname{trace} N = \frac{3d}{2}.$$

Next we compute $||N||^2$.

$$\begin{aligned}
||N||^2 &= \operatorname{trace} NN^T = \operatorname{trace} NN\\
&= \operatorname{trace}(I+\alpha J)AA^T(I+\alpha J)^2AA^T(I+\alpha J)\\
&= \operatorname{trace} A^T(I+\alpha J)^2AA^T(I+\alpha J)^2A\\
&= \operatorname{trace}(A^T(I-\frac{1}{6}J)A)^2\\
&= ||A^T(I-\frac{1}{6}J)A||^2
\end{aligned}$$

ELA

$$\begin{aligned} &= ||A^T A - \frac{3}{2} J_d||^2 \\ &= \sum_{1 \le i,j \le d} [(A^T A - \frac{3}{2} J_d)_{ij}]^2 \\ &= \sum_{1 \le i,j \le 10} b_i b_j [(A_0^T A_0 - \frac{3}{2} J_{10})_{ij}]^2. \end{aligned}$$

Since each column of A has exactly 3 ones, each diagonal entry of $A_0 A_0^T$ equals 3 and the off-diagonal entries equal 1 or 2. Thus the diagonal entries of $A_0 A_0^T - \frac{3}{2} J_{10}$ are equal to $\frac{3}{2}$ and the off-diagonal entries are $\pm\frac{1}{2}$. It follows that $(A_0 A_0^T - \frac{3}{2} J_{10})^{(2)} = 2I_{10} + \frac{1}{4} J_{10}$. So

$$\begin{aligned} ||N||^2 &= b^T (2I_{10} + \frac{1}{4} J_{10}) b \\ &= 2||b||^2 + \frac{d^2}{4}. \end{aligned}$$

Before we apply Corollary 6.3 to the matrix N, we compute the quantity c of Corollary 6.3.

$$\begin{aligned} c^2 &= \frac{25}{4} \left(-1 + \frac{5(2||b||^2 + \frac{d^2}{4})}{\frac{9d^2}{4}} \right) \\ &= \frac{25}{9d^2} (-d^2 + 10||b||^2). \end{aligned}$$

Setting $d = 10t + r$, $b_i = t + a_i$ and $a = (a_1, ..., a_{10})^T$ we have

$$c^2 = \left(\frac{5}{3d} \right)^2 (10||a||^2 - r^2).$$

Note that by the Cauchy-Schwartz inequality $10||a||^2 - r^2 \ge 0$.

Now Corollary 6.3 yields

$$\begin{aligned} &\det AA^T \\ &= 6 \det N \\ &\le 6 \left(\frac{3d}{10} \right)^5 \left(1 + \frac{4c}{5} \right) \left(1 - \frac{c}{5} \right)^4 \\ &\le 6 \left(\frac{3}{10} \right)^5 \left(d + \frac{4(\sqrt{10||a||^2 - r^2}}{3} \right) \left(d - \frac{\sqrt{10||a||^2 - r^2}}{3} \right)^4 \\ &= 1458t^5 + 729rt^4 + 162(r^2 - ||a||^2)t^3 + \gamma_2 t^2 + \gamma_1 t + \gamma_0 \\ &:= U_r(t, ||a||^2). \end{aligned}$$

The coefficients $\gamma_0, \gamma_1, \gamma_2$ are functions of r and $||a||^2$. Observe that the coefficients of t^5 and t^4 in $U_r(t, ||a||^2)$ and in $L_r(t)$ agree. Furthermore, the coefficient of t^3 in $L_r(t)$

is given by $162(r^2-r)$. Thus if $||a||^2>r$, then $U_r(t,||a||^2)<L_r(t)$ for large t. Since $\left(1+\frac{4c}{5}\right)\left(1-\frac{c}{5}\right)^4$ is a decreasing function of c, $U_r(t,||a||^2)$ is decreasing in $||a||^2$. A direct calculation of $U_r(t,||a||^2)$, with $||a||^2=r+1$ reveals that $U_r(t,r+1)<L_r(t)$ for all $t>0$. Thus $U_r(t,||a||^2)<L_r(t)$ for all t whenever $||a||^2>r$. Thus for A to be D-optimal it is necessary that $||a||^2=r$. Since $||a||^2=\sum_{i=1}^{10}a_i^2$ and $\sum_{i=1}^{10}a_i=r$, a must have exactly r ones and $10-r$ zeros, whenever A is D-optimal. Using Mathematica [M], we calculated $\det AA^T$ where

$$\begin{aligned} A &= [b_1 * v_1, \ldots, b_{10} * v_{10}] \\ &= [(t+a_1)v_1, \ldots, (t+a_{10}) * v_{10})], \end{aligned}$$

and $a=(a_1,\ldots,a_{10})$ runs through all vectors with exactly r ones and $10-r$ zeros. In every case, $\det AA^T \le K_r(t)$ with equality occurring for the choices of a in Theorem 3.1. □

Proof of Theorem 3.1, Part 2. From Corollary 2.3, if $A \notin S_{5,d}(0,1)$, then

$$\det AA^T \le 6\left(\frac{9(10t+r)-1}{30}\right)^5 := V_r(t). \tag{10}$$

For each remainder r modulo 10, a computer was used to calculate $L_r(t)-V_r(t)$ and the smallest value t_0 of t for which $L_r(t)-V_r(t)>0$, for all $t\ge t_0$. The results are listed in Table 2.

r	0	1	2	3	4	5	6	7	8	9
t_0	1	2	3	4	5	5	5	4	3	2

TABLE 2

Thus, we have shown that for all values of d, except possibly for the 29 values 5, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 22, 23, 24, 25, 26, 27, 28, 33, 34, 35, 36, 37, 44, 45, 46, of d, $G(5,d)=F(5,d)=L_r(t)$, where $d=10t+r$. □

4. D-optimal $5\times d$ designs for small d. In this section we analyze the 29 values of d not covered by Theorem 3.1, Part 2. In all but eight cases, $d=5,6,7,8,15,16,17,27$, $G(5,d)=F(5,d)$, but $G(5,d)>F(5,d)$ for these eight values of d. In all 29 cases the values for $G(5,d)$ listed in Table 3 are the same as the lower bounds for $G(5,d)$ given in [HKL]. The additional information contained in columns 3 -7 of Table 3 will be explained below.

In this section we show that the values given in column 2 of Table 3 are in fact equal to the maximum value $G(5,d)$ of $\det AA^T$. This is established by proving that $\det AA^T$ cannot exceed the proposed value of $G(5,d)$ in Table 3 and by providing a design matrix A for which that value of $\det AA^T$ is attained. For all but the eight exceptional values of d, the D-optimal design matrices were given in the previous section.

We begin with a result that restricts the number of columns (in a $5\times d$, D-optimal matrix) that do not have exactly 3 ones. Let $A\in M_{5,d}(0,1)$, $d=10t+r$. Recall that

d	$G(5,d)$	δ_{max}	s_{min}	$H(d,s_{min})$	$H(d,s_{min}+1)$	possible s
*5	25					
*6	64	6				
*7	192	7				
*8	384	5				
9	729	2	10	711		
11	2187	1	14	2106		
12	3240	2	17	3193		
13	4752	3	20	4760	4520	20
14	6912	3	23	6961	6655	23
*15	9880	3	26	9991	9602	26
*16	13975	2	29	14087	13591	29
*17	19500	1	32	19535	18903	32
18	25920	1	36	25879		
19	34992	1	40	33982		
22	72576	1	53	71414		
23	89964	1	58	88980		
24	111132	1	63	110256		
25	136269	1	68	135850		
26	166698	1	73	166451		
*27	202752	1	78	202843	200080	78
28	244944	1	84	242697		
33	558900	1	116	533010		
34	648000	1	123	642315		
35	748800	1	130	744046		
36	864000	1	137	859578		
37	993600	1	144	990436		
44	2372760	1	203	2353522		
45	2654145	1	212	2636477		
46	2965950	1	221	2948829		

TABLE 3

* *denotes the eight values of d for which $G(5,d) > F(5,d)$*

n_s is the number of columns of A with exactly s ones. Applying Lemma 2.2 to the case $j = 5$ we get the following inequality

$$\begin{aligned} \det AA^T &\leq 6\left(\frac{9n_3 + 8(n_2+n_4) + 5(n_1+n_5)}{30}\right)^5 \\ &= 6\left(\frac{9d - (n_2+n_4) - 4(n_1+n_5)}{30}\right)^5 \qquad (11) \\ &= 6\left(\frac{9d-\delta}{30}\right)^5, \end{aligned}$$

where $\delta = \delta(A) = (n_2 + n_4) + 4(n_1 + n_5)$. If $\delta(A)$ is too large, then the upper bound

(11) on $\det AA^T$ is less than the value of $G(5,d)$ in Table 3. And thus, A cannot be D-optimal. More precisely, we have the following result.

LEMMA 4.1. *Let A be a $5 \times d$ design matrix and let δ_{max} be as in Table 3. If $\delta(A) > \delta_{max}$, then $\det AA^T$ is less than the value of $G(5,d)$ in Table 3, and hence A is not D-optimal.*

Proof. The upper bounds δ_{max} on $\delta(A)$ for a D-optimal matrix A, are established by comparing the upper bound (11) on $\det AA^T$ with the value of $G(5,d)$ in Table 3. We illustrate the method by proving that $\delta_{max} = 3$ for $d = 14$. Suppose $\delta(A) \geq 4$. Then

$$\det AA^T \leq 6\left(\frac{9\cdot 14 - 4}{30}\right)^5 = 6673.5 < G(5,14) = 6912 = L_4(1).$$

So A is not D-optimal. But

$$\det AA^T \leq 6\left(\frac{9\cdot 14 - 3}{30}\right)^5 = 6951.4 > G(5,14) = 6912,$$

so $\delta(A) = 3$ cannot be ruled out for a D-optimal matrix A using inequality (11). (As we shall see shortly, however, $\delta(A) \neq 3$, if A is D-optimal.) The computation of δ_{max} for the other 28 values of d is similar. □

From now on we restrict our attention to the cases $d \geq 9$ and we deal with the cases $d = 5, 6, 7$ and 8 at the end of this section.

Next we apply Cohn's inequality, Corollary 6.3 to show that $\delta(A)$ cannot be 2 or 3, if A is D-optimal. We note that the entries of AA^T are non-negative integers and that the bound in Corollary 6.3, with $R = AA^T$, is a decreasing function of $||AA^T||^2$. Thus we can obtain an upper bound on $\det AA^T$ by minimizing $||AA^T||^2$ subject to certain constraints forced by the column structure of A.

LEMMA 4.2. *If $d \geq 9$ and $A \in M_{5,d}(0,1)$ with $\delta(A) = 3$, then A is not D-optimal.*

Proof. From Lemma 4.1, the result is clear for all d except $d = 13, 14$ and 15. First consider the case $d = 13$ and let $R = AA^T$. Suppose $\delta(A) = n_2 + n_4 + 4(n_1 + n_5) = 3$. Then $n_1 = n_5 = 0$. There are four cases: $n_2 = 0$ and $n_4 = 3$, $n_2 = 1$ and $n_4 = 2$, $n_2 = 2$ and $n_4 = 1$, and $n_2 = 3$ and $n_4 = 0$. In the last case, for example,

$$\begin{aligned}\operatorname{trace} R &= 3\cdot 2 + 10\cdot 3\\ &= 36,\end{aligned}$$

and

$$\begin{aligned}\sum_{i\neq j} R_{i,j} &= 3\cdot 2^2 + 10\cdot 3^2 - \operatorname{trace} R\\ &= 66.\end{aligned}$$

(Notice that $\operatorname{trace} R$ equals the sum of the row sums of A and that $\sum R_{i,j}$ equals the sum of the squared row sums of A.) The quantity $||R||^2$ is thus minimized if and only if the entries on the diagonal of R are 7,7,7,7,8 while 6 off-diagonal entries of R are

4 and 14 off-diagonal entries are 3. This yields the minimal for $||R||^2$ of 482. Now Corollary 6.3 applied to $R = AA^T$ with $n = 5$, $\operatorname{trace} R = 36$ and $||R||^2 = 482$ yields

$$\det AA^T = \det R \leq 4573.26 < 4752 = G(5, 13).$$

Thus A is not a D-optimal matrix. The other cases for $d = 13$ follow similarly and the analysis for $d = 14$ and $d = 15$ is analogous. □

The case $\delta = 2$ follows the same pattern as the case $\delta = 3$ except that for $d = 13, 14$ and 15, some additional arguments are needed.

LEMMA 4.3. *If $d \geq 9$ and $A \in M_{5,d}(0, 1)$ with $\delta(A) = 2$, then A is not D-optimal.*

Proof. From Lemma 4.1, the result is clear for all d except $d = 9, 12, 13, 14, 15, 16$. Since $\delta(A) = n_2 + n_4 + 4(n_1 + n_5)$ we conclude that $n_1 = n_5 = 0$ and $n_2 + n_4 = 2$. By the results of Section 5 we may assume that $n_2 = 2$ and $n_4 = 0$. (See the last example at the end of Section 5.)

For $d = 9, 12$ and 16. The proof follows the steps of the previous lemma and is straightforward.

For $d = 13$, let A be a 5×13 design matrix with $\delta(A) = 2$, $n_1 = n_4 = n_5 = 0$, $n_2 = 2$ and $n_3 = 11$. Set $R = AA^T$. Then

$$\begin{aligned} \operatorname{trace} R &= 2 \cdot 2 + 11 \cdot 3 \\ &= 37, \end{aligned}$$

and

$$\begin{aligned} \sum_{i \neq j} R_{i,j} &= 2 \cdot 2^2 + 11 \cdot 3^2 - \operatorname{trace} R \\ &= 70. \end{aligned} \tag{12}$$

Subject to the constraints (12) on R, $||R||^2 \geq 525$ and the minimum value 525 is attained if and only if the diagonal entries of R are 7,7,7,8,8; 10 of the off-diagonal entries are 3; and the rest are 4.

However, Corollary 6.3 implies that if $||R||^2 \geq 527$, then $\det R < 4752$ so A is not D-optimal. But the parity of $||R||^2$ is the same as the parity of $\sum R_{i,j} = 107$, which is odd. Thus we need to search for D-optimal matrices A only from among those for which $||R||^2 = 525$ and (12) holds for $R = AA^T$. A computer search reveals that $\det R < 4752 = G(5, 13)$ whenever the diagonal entries of R are 7,7,7,8,8; 10 of the off-diagonal entries are 3; and the rest are 4, i.e. whenever R satisfies (12) and $||R||^2 = 525$. It follows that there is no D-optimal matrix A with $\delta(A) = 2$. This proves the result for $d = 13$.

Up to a point, the argument for $d = 14$ is similar to that for $d = 13$. Let A be a 5×14 design matrix with $n_1 = n_4 = n_5 = 0, n_2 = 2$, and $n_3 - 12$, and $R = AA^T$. Then

$$\operatorname{trace} R = 40, \tag{13}$$

and

$$\sum_{i \neq j} R_{i,j} = 76. \tag{14}$$

Since the sum of all entries in R is 116, $||R||^2$ is also an even integer and by Corollary 6.3, A is not D-optimal whenever $||R||^2 \geq 618$. But $||R||^2 \geq 612$ and attains its minimum of 612 if and only if the diagonal entries of R are 8,8,8,8,8, and the off-diagonal entries are 3 (4 times) and 4 (16 times).

Thus we need to search for D-optimal matrices only from among those satisfying (13) and (14) with $||R||^2$ equal to 612, 614, or 616.

The only 5×5 integral, symmetric matrices R satisfying equations (13) and (14) with nonnegative entries and $||R||^2 = 612$, are described above. Computer calculations show that $\det R < 6912 = G(5,14)$, for each such R.

Now suppose $||R||^2 = 614$. An easy argument shows that the main diagonal entries of R are 7,8,8,8,9, and the off-diagonal entries are 3 (4 times) and 4(16 times). Again computer calculations show that $\det R < 6912$, for all such R.

There are only three ways $||R||^2$ can be 616:
1. diagonal of R: 8,8,8,8,8
off-diagonal of R: 2 (2 times), 4 (18 times)
2. diagonal of R: 8,8,8,8,8
off-diagonal of R: 3 (6 times), 4 (12 times), 5 (2 times)
3. diagonal of R: 7,7,8,9,9
off-diagonal of R: 3 (4 times), 4(16 times).

Each of these possibilities was checked by a computer program which showed that $\det R < 6912$ in each case. Thus there are no 5×14 D-optimal matrices with $||R||^2 = 612$, 614, or 616, and hence, no D-optimal matrices A with $\delta(A) = 2$. This proves the result for $d = 14$.

For $d = 15$, the analysis is very similar to the case $d = 14$ and no D-optimal matrices with $\delta(A) = 2$ exist. ☐

This leaves us with the case $\delta(A) = 1$. By the results form Section 5 we may assume that $n_2 = 1, n_4 = 0$ and that the first column of A is $(1,1,0,0,0)^T$ while all other columns of A have exactly 3 ones. The next lemma, which is a special case of Corollary 6.3, is the critical ingredient.

LEMMA 4.4. *Assume that $A \in M_{5,d}(0,1)$ contains the column $w = (1,1,0,0,0)^T$ while all other columns have exactly 3 ones, i.e. $A = [w, b_1 * v_1, ..., b_{10} * v_{10}]$ with $\sum_{i=1}^{10} b_i = d-1$. Then*

$$\det AA^T \leq H(d,s) := \frac{1}{6^4}\left(\frac{9d-1}{5}\right)^5 \left(1+\frac{4c}{5}\right)\left(1-\frac{c}{5}\right)^4, \tag{15}$$

where $b(A) = b = (b_1, \ldots, b_{10})$,

$$c = c(s(b)) = \frac{5}{2}\left(-1+5\frac{64+72s(b)+9(d-1)^2}{(9d-1)^2}\right)^{\frac{1}{2}}$$

and $s(b) = b_1 + b_2 + b_3 + b_{10} + \sum_{i=1}^{10} b_i^2$.

Proof. The proof uses Corollary 6.3 and is similar to the argument for Theorem 2.1: Choose a 5×5 symmetric matrix P such that $P^2 = 6I - J$ and set $N = PAA^TP$.

Then,

$$\operatorname{trace} N = \operatorname{trace} A^T(6I - J)A = 9d - 1,$$

and

$$\begin{aligned} ||N||^2 &= \operatorname{trace} N^2 \\ &= \operatorname{trace} (A^T(6I - J)A)^2 \\ &= ||A^T(6I - J)A||^2 \\ &= [1, b^T]Q \begin{bmatrix} 1 \\ b \end{bmatrix} \\ &= 64 + 72s(b) + 9(d-1)^2, \end{aligned}$$

where

$$Q = \begin{bmatrix} 64 & 36 & 36 & 36 & 0 & 0 & 0 & 0 & 0 & 0 & 36 \\ 36 & 81 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 9 \\ 36 & 9 & 81 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 9 \\ 36 & 9 & 9 & 81 & 9 & 9 & 9 & 9 & 9 & 9 & 9 \\ 0 & 9 & 9 & 9 & 81 & 9 & 9 & 9 & 9 & 9 & 9 \\ 0 & 9 & 9 & 9 & 9 & 81 & 9 & 9 & 9 & 9 & 9 \\ 0 & 9 & 9 & 9 & 9 & 9 & 81 & 9 & 9 & 9 & 9 \\ 0 & 9 & 9 & 9 & 9 & 9 & 9 & 81 & 9 & 9 & 9 \\ 0 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 81 & 9 & 9 \\ 0 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 81 & 9 \\ 36 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 9 & 81 \end{bmatrix}. \square$$

We now apply Lemma 4.4 to all 25 values of $d \geq 9$. The results are in Table 3. To explain the last four columns of Table 3, we consider the case $d = 22$. If there is a 5×22 D-optimal matrix A with $\delta(A) = 1$, then there is a D-optimal matrix A with the form in Lemma 4.4. (See Section 5.) Using the notation of Lemma 4.4, we have $b_1 + \cdots + b_{10} = 21$. (The other column of A is w.) It is clear that the minimum value s_{min} of $s(b)$ is 53 and is attained at $b = (2, 2, 2, 3, 2, 2, 2, 2, 2, 2)$ and at any other b having one $b_i = 3$ with $4 \leq i \leq 9$ and all other $b_j = 2$. The function $H(d, s)$ is decreasing in s and $s_{min} = 53$, so from Lemma 4.4 (15) we obtain

$$\det AA^T \leq H(22, s(b)) \leq H(22, 53) = 71414,$$

rounded to the nearest integer. Thus $\det AA^T < 72576 = F(5, 22)$, the maximum value of $\det AA^T$ for matrices A with $\delta(A) = 0$. Thus there are no 5×22 D-optimal matrices A with $\delta(A) = 1$. But $\delta_{max} = 1$ for $d = 22$, so there are no D-optimal matrices with $\delta(A) > 1$. It follows that $\delta(A) = 0$ for all D-optimal matrices A, that is all D-optimal matrices are in $S_{22}(0, 1)$. Thus $G(5, 22) = F(5, 22) = 72576$.

The same argument works for 17 other values of d and we summarize the results.

LEMMA 4.5. *If $d = 11, 18, 19, 22, 23, 24, 25, 26, 28, 33, 34, 35, 36, 37, 44, 45$, or 46, all $5 \times d$ D-optimal matrices are in $S_d(0, 1)$ and thus $G(5, d) = F(5, d)$.*

This leaves only the cases $d = 5, 6, 7, 8, 9, 12, 13, 14, 15, 16, 17$ and 27.

First consider the case $d = 13$. As before, if there is a D-optimal matrix A with $\delta(A) = 1$, then we may assume there is a D-optimal matrix A with the form in Lemma 4.4. Now $s_{min} = 20$ is attained at $b = (1, 1, 1, 2, 2, 1, 1, 1, 1, 1)$ or any other of the fifteen 10-tuples b having two $b_i = 2$ with $4 \le i \le 9$ and the other eight $b_j = 1$. For each of the 15 corresponding design matrices A, $\det AA^T = 4680$, which is less than $F(5, 13) = 4752$. So there are no D-optimal matrices A with $s(b(A)) = 20$. But if $s(b(A)) \ge 21$, then

$$\det AA^T \le H(13, s(b(A))) \le H(13, 21) = 4520 < 4752.$$

Thus there are no D-optimal matrices A with $s(b(A)) \ge 21$. It follows that there are no D-optimal matrices A with $\delta(A) = 1$.

The same argument works for $d = 14$ with $\delta = 1$. In this case $s_{min} = 23$ is attained for twenty 10-tuples b including $b = (1, 1, 1, 2, 2, 2, 1, 1, 1, 1)$. For the 20 possible b and corresponding design matrices A, $\det AA^T = 6825$ or $6864 < 6912 = F(5, 13)$. The arguments for $d = 9$ and $d = 12$ are similar. To summarize:

LEMMA 4.6. *If d =9, 12,13 or 14 and A is a D-optimal matrix, then $\delta(A) = 0$. Thus for these values of d, all $5 \times d$ D-optimal matrices are in $S_{5,d}(0, 1)$ and $G(5, d) = F(5, d)$.*

Now consider the case $d = 15$. Let A be a D-optimal matrix with $\delta(A) = 1$. We may assume that A has the form in Lemma 4.4. The minimum $s_{min} = 26$ is attained at $b = (1, 1, 1, 2, 2, 2, 2, 1, 1, 1)$ and fourteen other b. For each of the fourteen corresponding matrices A, $\det AA^T = 9750$ or 9880, which is greater than $F(5, 15) = 9792$. If $s(A) > 26$, then $\det AA^T \le H(15, 27) < 9880$. (See Table 3.) thus $G(5, 15) = 9880$.

Next consider the case $d = 16$. Let A be a D-optimal matrix with $\delta(A) = 1$. We may assume that A has the form in Lemma 4.4. The minimum $s_{min} = 29$ is attained for $b = (1, 1, 1, 1, 2, 2, 2, 2, 2, 1)$ or any of the six 10-tuples b having 5 twos and 1 one in coordinates 4,5,6,7,8,9 and ones in coordinates 1,2,3,10. For each of the six corresponding design matrices A,

$$\det AA^T = 13975 > 13824 = F(5, 16).$$

But if $s(b(A)) \ge 30$, then

$$\det AA^T \le H(16, s(b)) \le H(16, 30) = 13591 < 13975.$$

LEMMA 4.7. *1. If $d = 15$ and A is a D-optimal matrix, then $\delta(A) = 1$. The maximum value of $\det AA^T$ equals 9880 and is attained at the design matrix A with $b(A) = (1, 1, 1, 2, 2, 2, 2, 1, 1, 1)$.*
2. If $d = 16$ and A is a D-optimal matrix, then $\delta(A) = 1$. The maximum value of $\det AA^T$ equals 13975 and is attained at the design matrix A with $b(A) = (1, 1, 1, 1, 2, 2, 2, 2, 2, 1)$.

Now consider the case $d = 17$. If there is a D-optimal matrix A with $\delta(A) = 1$, we may assume A has the form in Lemma 4.4. The minimum value of $s(b)$ for $d = 17$

is $s_{min} = 32$ and is attained only at $b = (1,1,1,2,2,2,2,2,2,1)$. Let A be the design matrix with $b(A) = (1,1,1,2,2,2,2,2,2,1)$. Then

$$\det AA^T = 19500 > 19008 = F(5,17).$$

But if $s(b(A)) \geq 33$, for a design matrix A with $\delta(A) = 1$, then

$$\det AA^T \leq H(17, s(b)) \leq H(17,33) = 18903 \leq 19500.$$

Since $\delta_{max} = 1$, we have $G(5,17) = 19500$. The argument for $d = 27$ is the same.

LEMMA 4.8. *If $d = 17, 27$ and A is D-optimal, then $\delta(A) = 1$. Furthermore,*

$G(5,17) = 19500$ *is attained at* $b(A) = (1,1,1,2,2,2,2,2,2,1)$

and

$G(5,27) = 202752$ *is attained at* $b(A) = (2,2,2,3,3,3,3,3,3,2)$.

Thus we are left only with the cases $d = 5, 6, 7$ and 8. In dealing with the cases $d = 6, 7$ and 8 we make use of the following observation. If A is a $5 \times d$ design matrix with $n_1 + n_5 > 0$, then by Section 5, there is a matrix $A_1 = (v|A')$ where $v = (1,0,0,0,0)^T$ such that $\det AA^T = \det A_1A_1^T$. Then by the Cauchy-Binet Theorem $\det AA^T = \det A'A'^T + \det A''A''^T$ where A'' is the matrix obtained by deleting row 1 from A'. It follows that $\det AA^T \leq G(j, d-1) + G(j-1, d-1)$.

The case d=5. The D-optimal 5×5 design matrices have been known for a long time. One of them is

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

and $\det AA^T = (\det A)^2 = 25$. In the square case the problem of finding D-optimal $j \times j$ $(0,1)$-matrices is equivalent to finding D-optimal $(j+1) \times (j+1)$ (± 1)-matrices and the theory of D-optimal (± 1)-matrices has been much better understood. For recent results see [NR]. In the non-square case there is no connection between the two problems in general. In [NWZ2] a connection between the two problems was established in the restricted setting where all columns of $M_{j,d}(0,1)$ have the same number of 1s. This approach produced the D-optimal matrices given in Theorem 3.1 for $r = 1$ and 9.

The case d=6. The following is an example of a D-optimal $A \in M_{5,6}(0,1)$,

$$B_6 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

Note that $\det B_6B_6^T = 64$. To show B_6 is D-optimal we let $A \in M_{5,6}(0,1)$. If $n_1+n_5 \geq 1$, then $\det AA^T \leq G(5,5)+G(4,5) = 25+19 = 44 < 64 = \det B_6B_6^T$. Thus if A is D-optimal $n_1+n_5=0$, and by Table 3, $0 \leq n_2+n_4 \leq 6$. If $n_2+n_4=0$, then $\det AA^T \leq F(5,6) = 54 < 64 = \det B_6B_6^T$ and A is not D-optimal. So we consider the six cases $1 \leq n_2+n_4 \leq 6$. This reduces the number of computations to a manageable size. The exhaustive search produced the above matrix as one of many possible D-optimal design matrices. Note that for B_6, $n_2+n_4=1$. But D-optimal design matrices also occur when $n_2+n_4 = 2,4$.

The case d=7. The following is an example of a D-optimal $A \in M_{5,7}(0,1)$,

$$B_7 = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}.$$

Note that $B_7B_7^T = 2(I+J)$ and hence $\det B_7B_7^T = 192$. To show B_7 is D-optimal, let $A \in M_{5,7}(0,1)$. If $n_1+n_5 \geq 1$, then $\det AA^T \leq G(5,6)+G(4,6) = 64+48 = 132 < 192 = \det B_7B_7^T$. Thus if A is D-optimal, $n_1+n_5=0$. By Table 3, $0 \leq n_2+n_4 \leq 7$. If $n_2+n_4=0$, then $\det AA^T \leq F(5,7) = 135 < 192 = \det B_7B_7^T$. So we consider the seven cases $1 \leq n_2+n_4 \leq 7$. This reduces the number of computations to a manageable size. The exhaustive search produced the above matrix as one of many possible D-optimal design matrices.

The case d=8. The following is an example of a D-optimal $A \in M_{5,8}(0,1)$,

$$B_8 = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 \end{bmatrix}.$$

In order to show that B_8 is D-optimal we let $A \in M_{5,8}(0,1)$. By Table 3, $\det AA^T < 384$ unless $\delta(A) \leq 5$. If $n_1+n_5 \geq 1$, then $\det AA^T \leq G(5,7)+G(4,7) = 192+84 = 276 < 384 = \det B_8B_8^T$. So we may assume that $n_1+n_5=0$ and $0 \leq n_2+n_4 \leq 5$. If $n_2+n_4=0$, then $\det AA^T \leq F(5,8) = 324 < 384 = \det B_8B_8^T$. So $1 \leq n_2+n_4 \leq 5$. Thus $n_3 \geq 3$. All possibilities were checked using a computer, which produced the above example as one of many D-optimal design matrices. See Section 5 for the details.

5. The action of $S_{j+1} \times S_d$ on $M_{j,d}(0,1)$. Any permutation of the columns of a matrix A leaves the determinant of AA^T invariant. Column permutations induce a right action of S_d on $M_{j,d}(0,1)$ via

$$\begin{aligned} M_{j,d}(0,1) \times S_d &\longrightarrow M_{j,d}(0,1) \\ (A,\sigma) &\longmapsto AP_\sigma, \end{aligned}$$

where P_σ is the permutation matrix of σ.

There is a left action of S_{j+1} on $M_{j,d}(0,1)$ which is best explained by enlarging $M_{j,d}(0,1)$ to the set $C_{j,d}(-1,0,1)$ the set of all $j \times d$ matrices such that each column contains either -1 and 0, or 0 and 1. Since multiplication of columns of B by -1 does not change the value of $\det BB^T$ the maximum $\det XX^T$ over $C_{j,d}(-1,0,1)$ is the same as $G(j,d)$. We can recover $M_{j,d}(0,1)$ by introducing an equivalence relation on $C_{j,d}(-1,0,1)$ which identifies two elements $B_1, B_2 \in C_{j,d}(-1,0,1)$ if $B_1 = B_2 Q$ where Q is a diagonal matrix with diagonal entries ± 1. Every equivalence class contains exactly one element in $M_{j,d}(0,1)$ and the value of $\det BB^T$ is constant on equivalence classes.

It is clear that any permutation of the rows of B also leaves the determinant of BB^T invariant. This gives rise to a left action of S_j on $C_{j,d}(-1,0,1)$. Let S_j be given by the generators $(1,2),(2,3),\cdots,(j-1,j)$ and let the corresponding elements acting on $C_{j,d}(-1,0,1)$ be denoted by $x_1,...,x_{j-1}$.

More importantly, there is another row operation on $C_{j,d}(0,1)$ which leaves the determinant of BB^T invariant for all $B \in C_{j,d}(-1,0,1)$. The operation is given by multiplying row j of B by -1 and adding it to every other row of B. Let this operation be denoted by x_j. In [HKL], Proof of Lemma 7.3, this operation was described as a reflection of the simplex spanned by the rows of A through a hyperplane.

It is easy to see that

$$\begin{aligned} x_i^2 &= \textit{identity map} \text{ for all } 1 \le i \le j \\ (x_i x_{i+1})^3 &= \textit{identity map} \text{ for all } 1 \le i \le j-1 \\ x_i x_k &= x_k x_i \text{ if } 1 \le i, k \le j, |i-k| > 1. \end{aligned}$$

For $1 \le i, k < j$ these relations follow directly from the fact $x_1,...,x_{j-1}$ generate S_j while the relations $x_j^2 = (x_{j-1}x_j)^3 = $ identity map can easily be verified by inspection. It is well-known that the above relation define S_{j+1} (see [Jo]).

The left action of S_{j+1} on $C_{j,d}(-1,0,1)$ is in fact an action on the equivalence classes of $C_{j,d}(-1,0,1)$ and hence induces an action on $M_{j,d}(0,1)$.

Especially in Section 4 we have made use of this group action to simplify computational problems. The group theory program GAP was used to compute orbits of this group action on certain sets of vectors as was mentioned in Section 4.

We give examples of how this group action allows us to make certain assumptions on design matrices by choosing suitable ones in each equivalence class. Keep in mind that if A and B are equivalent under the group action, then $\det AA^T = \det BB^T$.

If $d = 1$ there are 3 orbits of the group action on the nonzero, (0,1) column vectors: the orbit of all vectors having exactly 3 ones, the orbit of vectors having exactly 2 or 4 ones, and the orbit of vectors having exactly 1 or 5 ones.

Just before the analysis of the case $d = 5$ in Section 4, we commented that if $n_1 + n_5 > 0$, for some design matrix A, then there is another design matrix, A_1 whose first column is $(1,0,0,0,0)^T$ and $\det AA^T = \det A_1 A_1^T$. The reason for this is that $(1,0,0,0,0)^T$ and $(1,1,1,1,1)^T$ are in the same orbit. Thus any design matrix with a column equal to $(1,1,1,1,1)^T$ is equivalent, via the group action, to a design matrix A_1 as above.

Similarly, if $n_2+n_4 \geq 1$ we may assume that $n_2 \geq 1$ and that the first column of A is $(1,1,0,0,0)^T$. We used this argument throughout Section 4.

Another example of how the group action can be used to reduce the amount of calculation occurs in the analysis of the case $d=8$. The argument shows that if A is D-optimal, then $n_1+n_5=0$ and $n_3 \geq 3$. One of the several subcases that need to considered is the one where $n_3=4$, $n_2+n_4=4$, and the 4 columns of A having exactly 3 ones are distinct. On the sets of 4 distinct vectors with exactly three ones, the group action generates 3 orbits represented by

$$\begin{array}{l}\{(1,1,1,0,0),(1,1,0,1,0),(1,1,0,0,1),(0,1,1,1,0)\}\\ \{(1,1,1,0,0),(1,1,0,1,0),(1,1,0,0,1),(0,0,1,1,1)\}\\ \{(1,1,1,0,0),(1,1,0,1,0),(0,1,1,0,1),(0,1,0,1,1)\}.\end{array}$$

Thus any such D-optimal design matrix A is equivalent (via the group action on $M_{5,8}(0,1)$) to a D-optimal matrix A' whose first 4 columns are equal to one of the 3 sets above. Thus all D-optimal matrices can be discovered by checking only the A' whose first four columns are as above.

Finally, we used the group action in Section 4 to argue that if $n_2+n_4=2$ and $n_3=d-2$, we may assume that $n_2=2$ and $n_4=0$. If $n_2=1=n_4$, then after suitable row interchanges we may assume that one column of A is $(0,1,1,1,1)^T$ while the other is either $(1,1,0,0,0)^T$ or $(0,1,1,0,0)^T$. Using the operation x_5 above, these two pairs of column vectors become either $(1,0,0,0,1)^T,(1,1,0,0,0)^T$ or $(1,0,0,0,1)^T,(0,1,1,0,0)^T$, i.e. n_2 is now 2. If $n_2=0$ and $n_4=2$, then after suitable row interchanges we may assume that either the column $(0,1,1,1,1)^T$ is repeated twice or there are two columns $(0,1,1,1,1)^T,(1,0,1,1,1)^T$. In both cases the operation x_5 transforms both pairs to a pair of columns with exactly 2 ones, i.e. $n_2=2$. Since the set of vectors with exactly 3 ones is invariant under the group action we still have $n_3=d-2$ in all cases.

6. Cohn's inequality. We present a new version and a new proof of Cohn's inequality (see [Co1]). Our view point is that Cohn's inequality is a variation of the arithmetic-geometric mean inequality

$$\prod_{i=1}^{n} x_i \leq \left(\frac{1}{n}\sum_{i=1}^{n} x_i\right)^n,$$

which can also be stated as: The product $\prod_{i=1}^n x_i$ subject to the condition $\sum_{i=1}^n x_i = s$, $x_i \geq 0$ is maximized when $x_1=\cdots=x_n=\frac{s}{n}$. Cohn's inequality deals with maximizing $\prod_{i=1}^n x_i$ subject to two conditions, one of them linear and the other one quadratic.

THEOREM 6.1. *Let $w_i \in \mathbb{R}$ for $i \in \{1,\ldots,n\}$, $n>1$, such that*

1. $w_i \geq 0$ *for* $i \in \{1,\ldots,n\}$.
2. $\sum_{i=1}^n w_i = n$
3. $\sum_{i=1}^n w_i^2 = n + c^2(1-\frac{1}{n})$.

Then,

$$\prod_{i=1}^{n} w_i \le \left(1 + c - \frac{c}{n}\right)\left(1 - \frac{c}{n}\right)^{n-1}. \tag{16}$$

The result in [Co1] is a logarithmic version of the above result. Throughout the paper we have made use of the fact that the bound in inequality (16) is a decreasing function of the quantity c.

Proof. We start out as in the proof of the lemma in [Co1] and use Lagrange multipliers to maximize the target function $p(w_1, ..., w_n) = p(w) = \prod_{i=1}^{n} w_i$. Set

$$\begin{aligned} f(w_1, ..., w_n) = f(w) &= \sum_{i=1}^{n} w_i - n \\ g(w_1, ..., w_n) = g(w) &= \sum_{i=1}^{n} w_i^2 - (n + c^2(1 - \frac{1}{n})). \end{aligned}$$

Then,

$$\begin{aligned} \nabla p(w) &= p(w)\,(\frac{1}{w_1}, ..., \frac{1}{w_n}) \\ \nabla f(w) &= (1, ..., 1) \\ \nabla g(w) &= 2w. \end{aligned}$$

Let $S = \{w | w_i \ge 0, f(w) = g(w) = 0\}$. Since $p(w)$ is continuous and S is compact, $p(w)$ has a maximum value M on S. If $p(w) = M$, then by the Lagrange Multiplier Theorem there exist $\lambda, \mu \in \mathbb{R}$ such that for all $i \in \{1, ..., n\}$ we have

$$\begin{aligned} \frac{M}{w_i} &= \lambda + 2\mu w_i \text{ or} \\ 0 &= 2\mu w_i^2 + \lambda w_i - M. \end{aligned}$$

Thus $\{w_1, ..., w_n\}$ contains at most two elements. If $c = 0$, then we have $w_1 = \cdots = w_n = 1$. If $c > 0$, then we may assume that $v_1 = w_1 = \cdots = w_k > w_{k+1} = \cdots = w_n = v_2$, $1 \le k < n$. The problem now is to maximize

$$\begin{aligned} &p(v_1, v_2, k) = v_1^k v_2^{n-k}, \\ &\text{subject to} \\ &\qquad 0 < v_2 < v_1, \\ &\qquad 1 \le k < n, \\ &f(v_1, v_2, k) = kv_1 + (n-k)v_2 - n = 0, \\ &g(v_1, v_2, k) = kv_1^2 + (n-k)v_2^2 - \left(n + c^2(1 - \frac{1}{n})\right) = 0. \end{aligned}$$

Solving the last two equations for v_1, v_2 yields

$$v_1 = 1 + \sqrt{s}\frac{\sqrt{n-k}}{\sqrt{n}\sqrt{k}} v_2 = 1 - \sqrt{s}\frac{\sqrt{k}}{\sqrt{n}\sqrt{n-k}},$$

where $s = c^2(1-\frac{1}{n})$. The problem now reduces to maximizing the function

$$p(k) = \left(1 + \frac{\sqrt{s}\sqrt{n-k}}{\sqrt{n}\sqrt{k}}\right)^k \left(1 - \frac{\sqrt{s}\sqrt{k}}{\sqrt{n}\sqrt{n-k}}\right)^{n-k}.$$

The function $p(k)$ is defined for $k \in (0,n)$ and we want to find its maximum in the interval $[1, n-1]$. Equivalently we can find the maximum of $\ln p(k)$ in the interval $[1, n-1]$. Differentiating $q(k) = \ln p(k)$ we get

$$q'(k) = \ln v_1 - \ln v_2 - \frac{v_1 - v_2}{2}\left(\frac{1}{v_1} + \frac{1}{v_2}\right).$$

Now $q'(k) < 0$ is a consequence of the fact that the function $\frac{1}{x}$ is convex. We have

$$\begin{aligned}\ln v_1 - \ln v_2 &= \int_{v_2}^{v_1} \frac{1}{x}\, dx \\ &< \frac{v_1 - v_2}{2}\left(\frac{1}{v_1} + \frac{1}{v_2}\right).\end{aligned}$$

Thus the maximum of $q(k)$ on $[1, n-1]$ occurs at $k = 1$ and the maximum is equal to

$$\begin{aligned} v_1 v_2^{n-1} &= \left(1 + \frac{\sqrt{s}\sqrt{n-1}}{\sqrt{n}}\right)\left(1 - \frac{\sqrt{s}}{\sqrt{n}\sqrt{n-1}}\right)^{n-1} \\ &= \left(1 + c(1-\frac{1}{n})\right)\left(1 - \frac{c}{n}\right)^{n-1}, \end{aligned}$$

which is what we had to show. □

REMARK 6.2. The last part of the proof is an argument used in in Lemma 2.1 of [NR] and the reduction to the case of only two values follows the argument in [Co1].

In [Neu], Theorem 1, Cohn's inequality was used to prove an inequality for determinants of positive-definite matrices. The next result improves the inequality of [Neu] slightly to better suit our purposes here. Let $||R||$ denote the Euclidean norm of the matrix $R = (r_{ij})$, i.e. $||R||^2 = \sum_{i,j} |r_{i,j}|^2$.

COROLLARY 6.3. *Let $R = (r_{ij}) \in M_n(\mathbb{C})$ be a positive-definite Hermitian matrix. Let c be the positive square root of*

$$\frac{n}{n-1}\left(-n + \left(\frac{n||R||}{\operatorname{trace} R}\right)^2\right).$$

Then,

$$\det R \le \left(\frac{\operatorname{trace} R}{n}\right)^n \left(1 + c - \frac{c}{n}\right)\left(1 - \frac{c}{n}\right)^{n-1}. \tag{17}$$

Proof. Let $\lambda_1, ..., \lambda_n$ be the eigenvalues of R. Then,

$$\begin{aligned}\sum_{i=1}^{n} \lambda_i &= \text{trace } R \text{ and}\\ \sum_{i=1}^{n} \lambda_i^2 &= \text{trace } R^2\\ &= \text{trace } RR^*\\ &= \sum_{1\le i,j\le n} r_{ij}\overline{r}_{ij}\\ &= \sum_{1\le i,j\le n} |r_{ij}|^2\\ &= ||R||^2.\end{aligned}$$

Set $w_i = n\lambda_i/\text{trace}\, R$. Then $\sum_{i=1}^{n} w_i = n$ and $\sum_{i=1}^{n} w_i^2 = n + c^2(1 - \frac{1}{n})$. We can now apply Cohn's inequality to $w_1, ..., w_n$. The result of the corollary follows by multiplying both sides by $(\text{trace}\, R/n)^n$. □

If all columns of $A \in M_{j,d}(0,1)$ have exactly k ones, then $\text{trace}\, AA^T = kd$, the number of ones in A. The previous corollary then takes on a special form which is the one we apply in Section 3.

COROLLARY 6.4. *Assume $A \in M_{j,d}(0,1)$ such that $J_jA = kJ_{j,d}$. Then*

$$\det AA^T \le \left(\frac{kd}{j}\right)^j \left(1 + c - \frac{c}{j}\right) \left(1 - \frac{c}{j}\right)^{j-1},$$

where c is defined as in Corollary 6.3 with $R = AA^T$.

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