A note on the D-optimality and D-efficiency of nonorthogonal blocked main effects plans

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Summary

This paper considers main effects plans used to study m two-level factors using n runs which are partitioned into b blocks of equal size $k = n/b$. The assumptions are adopted that $n \equiv 2 \pmod 8$ and $k > 2$ is even. Certain designs not having all main effects orthogonal to blocks were shown by Jacroux (2011a) to be D-optimal when $(m-2)(k-2)+2 \leqslant n \leqslant (m-1)(k-2)+2$. Here, we extend that result. For $(m-3)(k-2)+2 \leqslant n < (m-2)(k-2)+2$, the D-optimality of those designs is proved. Moreover, their D-efficiency is shown to be close to one for $2(m+1) \leqslant n < (m-3)(k-2)+2$, indicating their good performance under the criterion of D-optimality.

Key words: blocked main effects plan; D-efficiency; D-optimality; Fischer's inequality; Hadamard's inequality; nonorthogonality.

1. Introduction

Due to the expensive and time-consuming nature of experiments planned with a complete factorial design, optimal fractional factorial plans are widely applied in diverse fields such as agriculture, industry, and medical research. For example, they are commonly used in industrial research (Bose and Bagchi, 2007; Davies and Hay, 1950; Jacroux, 2009), where an important application is the improvement of manufacturing processes (e.g. chemical and biological processes or formulation of pharmaceutical preparations) and of product quality. In chemical research, optimal fractional factorial plans help to determine the effect of some changes in reaction conditions (e.g. temperature or time of reaction) or methods of manufacture (e.g. fermentation processes). In such research it is usually sufficient to use two-level factorial designs, to examine one change in each of the factors under investigation, e.g. an increase or decrease in the concentration and amounts of

one or more of the various constituents of the medium. Much of the work on optimal fractional factorial plans is valid in the absence of blocks, although the importance of blocking is emphasized by many researchers (see, for example, Cheng et al., 2004, and the references therein). A practical example of using fractional factorial design with blocks has already been given in section 7 of Davies and Hay (1950), where the effect of various factors on the yield of penicillin is investigated. Recently, interesting results on optimal main effect plans with blocking have been obtained (see references given below). Some of them are extended in the following sections.

In this paper, we consider experimental situations in which m two-level factors are to be studied in n runs, which are partitioned into b blocks of size $k = n/b$, where k is even, and where a main effects only design is to be used. By Jacroux (2011a), we use d to denote a design and the model for analyzing the data under this design is of the form

$$Y = X_d\beta + B_d\alpha + \epsilon, \tag{1}$$

where Y is an $n \times 1$ vector of observations, $X_d = (X_{d_1}, \ldots, X_{d_m}) = (x_{dij})$ is an $n \times m$ design matrix, $\beta = (\beta_1, \ldots, \beta_m)'$ is the vector of main effects parameters, B_d is an $n \times b$ zero-one block design matrix with entries $b_{dij} = 1$ if and only if the ith run occurs in the jth block, $\alpha = (\alpha_1, \ldots, \alpha_b)'$ is the vector of block parameters and ϵ is a vector of random error components, which are assumed to be uncorrelated with zero mean and constant variance σ^2. We interchangeably represent a design d by its design matrix X_d, whose ith row corresponds to run i and whose jth column corresponds to factor j, where $x_{dij} = 1, -1$ depending on whether factor j occurs at a high or low level during run i. We use $D(n, m, b)$ to denote the class of two-level main effects designs available where m two-level factors occur in n runs arranged in b blocks of size $k = n/b$, and $\bar{D}(n, m, b)$ to denote the subclass of designs within $D(n, m, b)$ having each factor occur at its high and low levels equally often within each block. We also use $D(n, m)$ to denote the entire class of two-level main effects plans having m factors occurring in n runs.

Under the model (1), the least squares estimate for β is any solution to the reduced normal equations for main effects given by $M_d\hat{\beta} = Q$, where $M_d = X_d'X_d - (1/k)X_d'B_dB_d'X_d$, $Q = X_d'(I_n - (1/k)B_dB_d')Y$ and I_n is the identity matrix of size n. The matrix M_d is called the information matrix of design d.

Among all designs d in the class $D(n, m, b)$, we often wish to choose

the best one with respect to some criterion. Many criteria are considered in the literature, we shell be interested in one of the most popular, namely the D-optimality criterion. We say a design d is D-optimal in $D(n, m, b)$ if $\det(M_d)$ is maximal. The other optimality criteria are also expressed in terms of the information matrix. Some results concerning such issues are found, among others, Bose and Bagchi (2007), Jacroux (2009, 2011a,b, 2013), Jacroux and Kealy-Dichone (2014, 2015) and Mukerjee et al. (2002). It is worth mentioning, that there are also many other considerations for optimal designs described in the literature (see, for example, Cheng and Tsai, 2009; Cheng et al., 2004; Das and Dey, 2004).

In this paper, we expand the results of the three papers by Jacroux (2011a,b, 2013), which concern the case when $n \equiv 2 \pmod 8$ and k is even (more precisely $k \equiv 2 \pmod 4$). Jacroux (2013) proved that a design $d_* \in \bar{D}(n, m, n/2)$ having

$$M_{d_*} = (n-2)I_m + 2J_{mm}, \tag{2}$$

where J_{mm} is the $m \times m$ matrix of ones, is optimal in $D(n, m, n/2)$ under the D-optimality criterion as well as most other widely used optimality criteria. When $n \geqslant (m-1)(k-2) + 2$ and $k > 2$, Jacroux (2011a) showed that a design $d_* \in \bar{D}(n, m, b)$ with M_{d_*} of the form (2) is D-optimal in $D(n, m, b)$. However, Jacroux (2011b) proved that a D-optimal design does not always belong to $\bar{D}(n, m, b)$, when $n \leqslant (m-1)(k-2) + 2$ and $k > 2$. In that paper, the following construction is considered.

1. Let $d_1 \in D((n-2)/2, m)$ have X_{d_1} which consists of m columns from an $(n-2)/2 \times (n-2)/2$ Hadamard matrix.

2. Let $d_2 \in D(n-2, m, (n-2)/2)$ have ($\otimes$ denotes the Kronecker product)

$$X_{d_2} = X_{d_1} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{3}$$

   and where blocks of size two are obtained by taking successive pairs of "foldover" runs in X_{d_2}.

3. Form $d_3 \in D(n, m, n/2)$ by adding a single block to d_2 consisting of one run of all 1's followed by another run consisting of m_1 1's followed by $n - m_1$ -1's where $m_1 > 0$.

4. Form $d_4 \in D(n, m, b)$ by combining $k/2$ successive runs of blocks of size two in X_{d_3} to form blocks of size k in d_4.

Jacroux (2011b) showed that a design d_4 obtained via (3) is D-better than the best design in $\bar{D}(n, m, b)$ provided that $n < (m-1)(k-2)+2$, whereas d_4 is D-equivalent to the best design in $\bar{D}(n, m, b)$ when $n = (m-1)(k-2)+2$. He also noted that for $n \leqslant (m-2)(k-2)+2$, the best design obtainable via (3) has m_1 which is closest to $\hat{m}_1 = (m(k-2)-n+2)/2(k-2)$ where as if $1 \leqslant (m(k-2)-n+2)/(k-2) < 2$, the best design will have $m_1 = 1$. From now on, we assume that d_4 is the best design under the D-optimality criterion obtained via (3), i.e. it has m_1 which is closest to $\hat{m}_1$.

In Jacroux (2011a), the D-optimality of a design d_4 constructed as in (3) is proved, when $(m-2)(k-2)+2 \leqslant n \leqslant (m-1)(k-2)+2$. Jacroux (2011b) also mentioned that designs d_4 obtained via (3) seem to be D-optimal when $n < (m-2)(k-2)+2$. In section 2, we prove that d_4 is D-optimal when $(m-3)(k-2)+2 \leqslant n < (m-2)(k-2)+2$, extending the result of Jacroux (2011a). For $n < (m-3)(k-2)+2$, it seems to be more difficult to prove the D-optimality of d_4, but in section 3 we show that the D-efficiency of designs d_4 is close to one, indicating their very good behavior under the D-optimality criterion and their practical usefulness.

2.   D-optimal designs when
$$(m-3)(k-2)+2 \leqslant n < (m-2)(k-2)+2$$

In this section, we prove the D-optimality of designs d_4 obtained via (3) for $(m-3)(k-2)+2 \leqslant n < (m-2)(k-2)+2$. In this way, we extend the results of Jacroux (2011a) and partially confirm the conjecture of Jacroux (2011b), as mentioned in the last paragraph of section 1.

Assume that $n \equiv 2 \pmod{8}$, $k = n/b > 2$, k is even and $(m-3)(k-2)+2 \leqslant n < (m-2)(k-2)+2$. Then, for $(m-3)(k-2)+2 < n < (m-2)(k-2)+2$, $\hat{m}_1 \in (1, 3/2)$, so $m_1 = 1$, but for $n = (m-3)(k-2)+2$, we have $\hat{m}_1 = 3/2$, and hence m_1 equals 1 or 2. By the proof of Theorem 3.1 in Jacroux (2011b), we see that the eigenvalues of the matrix M_{d_4} are equal to $z_{d_4,1} = \cdots = z_{d_4,m-2} = n - 2$, $z_{d_4,m-1} = n + 2(m_1 - 1) - 4m_1/k$, $z_{d_4,m} = n + 2(m - m_1 - 1)$. Thus for $m_1 = 1$, we have

$$\det(M_{d_4}) = (n-2)^{m-2}(n - \frac{4}{k})(n + 2(m-2)). \tag{4}$$

Since, for $n = (m-3)(k-2)+2$, we can take $m_1 = 2$, in this case we also

have

$$\det(M_{d_4}) = (n-2)^{m-2}(n+2-\frac{8}{k})(n+2(m-3)). \qquad (5)$$

In the following theorem, the D-optimality of the design d_4 in the class $D(n, m, b)$ is proven.

Theorem 2.1. *Let $n \equiv 2 \ (mod \ 8)$, $k = n/b > 2$, let k be even and let $d_4 \in D(n, m, b)$ be constructed as in (3). If $(m-3)(k-2) + 2 \leqslant n < (m-2)(k-2) + 2$, then d_4 is D-optimal in the class $D(n, m, b)$.*

The proof of Theorem 2.1 is quite long and so we present it in the Appendix.

Remark 2.1. *When $n \equiv 2 \ (mod \ 8)$, $k = n/b > 2$ and k is even, Theorem 2.1 and Theorem 4.1 of Jacroux (2011a) show that the designs d_4 obtained as in (3) are D-optimal in $D(n, m, b)$ for $(m-3)(k-2) + 2 \leqslant n \leqslant (m-1)(k-2) + 2$.*

Perhaps the technique presented in the proof of Theorem 2.1 can be used to show the D-optimality of the designs d_4 for $2(m+1) \leqslant n < (m-3)(k-2)+2$, but this would certainly be quite difficult. However, in the next section, we show the very satisfactory behavior of these designs in terms of D-efficiency.

3.   Highly D-efficient designs for $2(m+1) \leqslant n < (m-3)(k-2) + 2$

In this section, we investigate the efficiency of designs d_4 constructed as in (3) under the D-optimality criterion, i.e. D-efficiency as defined below. In the cases where a D-optimal design is not known (see Remark 2.1), we indicate that the D-efficiency of d_4 is very high and close to one.

Following the definition of Bulutoglu and Ryan (2009), the D-efficiency of a design d in the class $D(n, m, b)$ is

$$\text{D-eff}(d) = \left(\frac{\det(M_d)}{\max_{d_* \in D(n,m,b)} \det(M_{d_*})} \right)^{\frac{1}{m}}. \qquad (6)$$

Unfortunately, $\max_{d_* \in D(n,m,b)} \det(M_{d_*})$ is not known. Thus, we can not calculate the D-efficiency of designs. However, when we know an upper

bound UB for $\max_{d_* \in D(n,m,b)} \det(M_{d_*})$, we can approach D-eff$(d)$ by a lower bound of the form $[\det(M_d)/UB]^{1/m}$. Here we will proceed in this manner. Namely, in the following lemma we prove an upper bound for $\max_{d_* \in D(n,m,b)} \det(M_{d_*})$, which we will use to approximate the D-efficiency of a design $d \in D(n,m,b)$ as described above.

Lemma 3.1. *Assume that $n \equiv 2 \ (mod \ 8)$, $k = n/b > 2$ and k is even. If $2(m+1) \leqslant n < (m-1)(k-2)+2$ and $d \in D(n,m,b)$, then*

$$\det(M_d) \leqslant (n-2)^{m-l-1}(n+2 \left\lfloor \frac{n-2}{k-2} \right\rfloor)^l \cdot (n-2+2(m-l \left\lfloor \frac{n-2}{k-2} \right\rfloor - l)), \quad (7)$$

where $l \in \mathbb{N}$ is such that $l(\lfloor (n-2)/(k-2) \rfloor + 1) \leqslant m$ and $(l+1)(\lfloor (n-2)/(k-2) \rfloor + 1) > m$, and $\lfloor x \rfloor$ is the integral part of x.

Proof. Since $m > (n-2)/(k-2)+1 \geqslant \lfloor (n-2)/(k-2) \rfloor + 1$, the number l is correctly defined. Partition X_d so that $X_d = (X_{d_1}, \ldots, X_{d_{(l+1)}})$, where X_{d_i} is $n \times (\lfloor (n-2)/(k-2) \rfloor + 1)$ for $i = 1, \ldots, l$, and $X_{d_{(l+1)}}$ is $n \times (m - l(\lfloor (n-2)/(k-2) \rfloor + 1))$. Fischer's inequality (see, for example, Radhakrishna Rao and Bhaskara Rao, 1998, p. 453) implies

$$\det(M_d) \leqslant \det(M_{d_1}) \ldots \det(M_{d_{(l+1)}}), \quad (8)$$

where M_{d_i} is the information matrix of the design d_i with the design matrix X_{d_i}, $i = 1, \ldots, l+1$. Since $d_i \in D(n, \lfloor (n-2)/(k-2) \rfloor + 1, b)$ for $i = 1, \ldots, l$, and $d_{(l+1)} \in D(n, m - l(\lfloor (n-2)/(k-2) \rfloor + 1), b)$, Theorem 3.1 in Jacroux (2011a) shows that

$$\det(M_{d_i}) \leqslant (n-2)^{\lfloor \frac{n-2}{k-2} \rfloor} \left(n+2 \left\lfloor \frac{n-2}{k-2} \right\rfloor \right), \ i = 1, \ldots, l, \quad (9)$$

$$\det(M_{d_{(l+1)}}) \leqslant (n-2)^{m-l(\lfloor \frac{n-2}{k-2} \rfloor + 1)-1} \cdot (n-2+2(m-l \left\lfloor \frac{n-2}{k-2} \right\rfloor - l)). \quad (10)$$

Therefore, inequalities (8), (9) and (10) imply (7). $\qquad\square$

By (6) and Lemma 3.1, we conclude immediately the following corollary, which presents the lower bound for the D-efficiency of a design d in the class $D(n,m,b)$.

Corollary 3.1. *Under the assumptions of Lemma 3.1, if $d \in D(n,m,b)$,*

$$\text{D-eff}(d) \geqslant \left(\frac{\det(M_d)}{(n-2)^{m-l-1} \left[n+2 \left\lfloor \frac{n-2}{k-2} \right\rfloor \right]^l \left[n-2+2 \left(m - l \left\lfloor \frac{n-2}{k-2} \right\rfloor - l \right) \right]} \right)^{\frac{1}{m}}.$$

Using Corollary 3.1, we can examine the D-efficiency of the designs d_4 for $2(m+1) \leqslant n < (m-3)(k-2)+2$. The eigenvalues of the matrix M_{d_4} are $n-2$, $n+2(m_1-1)-4m_1/k$, $n+2(m-m_1-1)$ with multiplicities $m-2$, 1 and 1, respectively (see the proof of Theorem 3.1 in Jacroux, 2011b). Hence, by Corollary 3.1, it follows that

$$\text{D-eff}(d_4) \geqslant \left(\frac{(n-2)^{l-1} \left[n+2(m_1-1)-\frac{4m_1}{k} \right] (n+2(m-m_1-1))}{\left[n+2 \left\lfloor \frac{n-2}{k-2} \right\rfloor \right]^l \left[n-2+2 \left(m-l \left\lfloor \frac{n-2}{k-2} \right\rfloor -l \right) \right]} \right)^{\frac{1}{m}}, \quad (11)$$

where l is as in Lemma 3.1. We have calculated the values of the right hand side of (11) for many values of n, m, k, and we conclude that the lower bound for the D-efficiency of the designs d_4 is close to one. As an example we present values of this lower bound for some n, m and k in Table 1. We also observed that the lower bound for the D-efficiency of d_4 decreases when m increases for fixed n and k, which was to be expected. In Table 1 we present only its values for $m = n/2 - 1$, the largest number of factors for which we can construct the designs d_4. So the smallest values of D-efficiency of designs d_4 are given among all possible values for different m. Fortunately, for given k, this lower bound increases when n increases, which is also to be expected.

We see that the designs d_4 have D-efficiency close to one. This indicates that these designs perform very well under the D-optimality criterion and seem to be close to D-optimal. Since the D-efficiency of designs d_4 is so close to one, it seems that there do not exist designs better than them with respect to the D-optimality criterion, i.e. they are D-optimal. We do not know how to prove this, but we have confirmed it numerically. More precisely, we conducted a numerical search based on the tabu-search algorithm (Harman et al., 2016; Jung and Yum, 1996) to find the D-optimal designs in $D(n, m, b)$ for certain n, m and k. We used a modification of the R code of a tabu-search-based approach for chemical balance weighing designs by Katulska and Smaga (2016) (Domijan, 2012; R Core Team, 2015). It is significant that we did not find D-better designs than d_4. Summarizing, even if the designs d_4 obtained via (3) are not D-optimal, which seems to be impossible, they are the best known designs under the criterion of D-optimality, having D-efficiency very close to one. Therefore, they can be safely used in practice.

Although we have considered particular designs and a particular optimality criterion, the idea of approaching the efficiency of a design under

Table 1. Lower bound for the D-efficiency of designs d_4.

$k = 6$			$k = 10$			$k = 14$		
n	m	D-eff$(d_4) \geqslant$	n	m	D-eff$(d_4) \geqslant$	n	m	D-eff$(d_4) \geqslant$
18	8	0.9887	50	24	0.9942	42	20	0.9926
42	20	0.9952	90	44	0.9967	98	48	0.9967
66	32	0.9969	130	64	0.9977	154	76	0.9978
90	44	0.9977	170	84	0.9982	210	104	0.9984
114	56	0.9982	210	104	0.9986	266	132	0.9987

a chosen criterion of optimality, as used in this paper is widely applicable. It can be modified for other experimental designs and other optimality criteria, since it is usually quite easy to obtain a lower or upper (depending on the criterion) bound for the value of a criterion (see, for example, Katulska and Smaga, 2016). Studying efficiency in this way, may help to indicate very good or even optimal designs under a given optimality criterion.

Acknowledgement

Appendix

Proof of Theorem 2.1. Theorem 3.1 in Jacroux (2011b) implies that d_4 is D-better than any design $d \in \bar{D}(n, m, b)$. So let $d \in D(n, m, b)$, but $d \notin \bar{D}(n, m, b)$. Then, d has at least one factor that is non-orthogonal to blocks. So partition the factors in d so that factors $1, \ldots, p$ are not orthogonal to blocks whereas factors $p+1, \ldots, m$ are orthogonal to blocks. We correspondingly partition X_d so that $X_d = (X_{d_1}, X_{d_2})$, where X_{d_1} is $n \times p$ and X_{d_2} is $n \times (m - p)$. First, let $p = 1$. Since a factor in X_{d_1} is non-orthogonal to at least one block, the number $X'_{d_1} B_d B'_d X_{d_1}$ is at least 4 (k is even) and hence the first diagonal element of M_d cannot exceed $n - 4/k$. From Fischer's inequality (see, for example, Radhakrishna Rao and Bhaskara Rao, 1998, p. 453), it follows that

$$\det(M_d) \leqslant \left(X'_{d_1} X_{d_1} - \frac{1}{k} X'_{d_1} B_d B'_d X_{d_1} \right) \cdot \det \left(X'_{d_2} X_{d_2} - \frac{1}{k} X'_{d_2} B_d B'_d X_{d_2} \right). \quad (12)$$

Corollary 3.2 in Jacroux (2013) shows that

$$\det\left(X'_{d_2}X_{d_2} - \frac{1}{k}X'_{d_2}B_dB'_dX_{d_2}\right) \leqslant \det((n-2)I_{m-1} + 2J_{(m-1)(m-1)}) =$$
$$= (n-2)^{m-2}(n+2(m-2)). \tag{13}$$

Since $X'_{d_1}X_{d_1} - (1/k)X'_{d_1}B_dB'_dX_{d_1} \leqslant n - 4/k$ and by (4), (12) and (13), we have

$$\det(M_d) \leqslant (n-2)^{m-2}\left(n - \frac{4}{k}\right)(n+2(m-2)) = \det(M_{d_4}).$$

We now assume that $p \geqslant 2$ and partition X_{d_1} so that $X_{d_1} = (X_{d_11}, \ldots, X_{d_1p})$. Fischer's inequality implies

$$\det(M_d) \leqslant \det((X_{d_11}, X_{d_12})'\left(I_n - \frac{1}{k}B_dB'_d\right)(X_{d_11}, X_{d_12}))\cdot$$
$$\cdot \det((X_{d_13}, \ldots, X_{d_1p}, X_{d_2})'\left(I_n - \frac{1}{k}B_dB'_d\right)(X_{d_13}, \ldots, X_{d_1p}, X_{d_2})). \tag{14}$$

Since $n \geqslant ((m-2)-1)(k-2)+2$, by Theorem 3.1 in Jacroux (2011a), we conclude that

$$\det((X_{d_13}, \ldots, X_{d_1p}, X_{d_2})'\left(I_n - \frac{1}{k}B_dB'_d\right)(X_{d_13}, \ldots, X_{d_1p}, X_{d_2}))$$

is less than or equal to $(n-2)^{m-3}(n+2(m-3))$. We first consider the case $n = (m-3)(k-2)+2$. From (5) and (14), it follows that to show that $\det(M_d) \leqslant \det(M_{d_4})$, it is sufficient to prove that the difference $(n-2)(n+2-8/k) - \det((X_{d_11}, X_{d_12})'(I_n - (1/k)B_dB'_d)(X_{d_11}, X_{d_12}))$ is greater than or equal to zero. Denote by Σ_{ij} the sum of elements in X_{d_1i}, which corresponds to the j-th block, $i = 1, 2, j = 1, \ldots, b$. Let

$$L = (X_{d_11}, X_{d_12})'\left(I_n - \frac{1}{k}B_dB'_d\right)(X_{d_11}, X_{d_12}).$$

Then,

$$L = \begin{pmatrix} n - \frac{1}{k}\sum_{j=1}^b \Sigma_{1j}^2 & X'_{d_11}X_{d_12} - \frac{1}{k}\sum_{j=1}^b \Sigma_{1j}\Sigma_{2j} \\ X'_{d_12}X_{d_11} - \frac{1}{k}\sum_{j=1}^b \Sigma_{1j}\Sigma_{2j} & n - \frac{1}{k}\sum_{j=1}^b \Sigma_{2j}^2 \end{pmatrix}. \tag{15}$$

Since k is even, Σ_{ij} can be equal to $0, \pm 2, \pm 4, \ldots, \pm k$. However, there also exist j and j_* such that $\Sigma_{1j} \neq 0$ and $\Sigma_{2j_*} \neq 0$, because factors in $X_{d_1 1}$ and $X_{d_1 2}$ are non-orthogonal to at least one block. We have to consider four cases.

Case 1. Let

- $\Sigma_{1i}^2 \geqslant 4$, $\Sigma_{1j}^2 \geqslant 4$ for some $i, j, i \neq j$ and $\Sigma_{1r}^2 \geqslant 0$ for all $r \neq i$, $r \neq j$, and $\Sigma_{2s}^2 \geqslant 4$ for some s and $\Sigma_{2t}^2 \geqslant 0$ for all $t \neq s$,

or

- $\Sigma_{1i}^2 \geqslant 4$ for some i and $\Sigma_{1j}^2 \geqslant 0$ for all $j \neq i$, and $\Sigma_{2r}^2 \geqslant 4$, $\Sigma_{2s}^2 \geqslant 4$ for some $r, s, r \neq s$ and $\Sigma_{2t}^2 \geqslant 0$ for all $t \neq r$, $t \neq s$.

Then, in both cases

$$(n - \frac{1}{k} \sum_{j=1}^{b} \Sigma_{1j}^2)(n - \frac{1}{k} \sum_{j=1}^{b} \Sigma_{2j}^2) \leqslant (n - \frac{8}{k})(n - \frac{4}{k}). \tag{16}$$

By (15), (16) and Hadamard's inequality (see, for example, Marshall et al., 2011, p. 306), we obtain $\det(L) \leqslant (n - 8/k)(n - 4/k)$. Since $2 < k < n$, we have

$$(n - 2)(n + 2 - \frac{8}{k}) - \det(L) \geqslant (n - 2)(n + 2 - \frac{8}{k}) +$$
$$- (n - \frac{8}{k})(n - \frac{4}{k}) = \frac{4(k(n - k) + 4(k - 2))}{k^2} > 0.$$

Case 2. Let

- $\Sigma_{1i}^2 \geqslant 4$ for some i and $\Sigma_{1j}^2 \geqslant 0$ for all $j \neq i$, and $\Sigma_{2r}^2 \geqslant 16$ for some r and $\Sigma_{2s}^2 \geqslant 0$ for all $s \neq r$,

or

- $\Sigma_{1i}^2 \geqslant 16$ for some i and $\Sigma_{1j}^2 \geqslant 0$ for all $j \neq i$, and $\Sigma_{2r}^2 \geqslant 4$ for some r and $\Sigma_{2s}^2 \geqslant 0$ for all $s \neq r$.

In both of these cases, we have

$$(n - \frac{1}{k} \sum_{j=1}^{b} \Sigma_{1j}^2)(n - \frac{1}{k} \sum_{j=1}^{b} \Sigma_{2j}^2) \leqslant (n - \frac{16}{k})(n - \frac{4}{k}).$$

But, $(n - 16/k)(n - 4/k) \leqslant (n - 8/k)(n - 4/k)$, so the same arguments as in Case 1 show that $(n - 2)(n + 2 - 8/k) > \det(L)$.

Case 3. Let $\Sigma_{1i}^2 = 4$, $\Sigma_{2j}^2 = 4$ for some $i, j, i \neq j$, and $\Sigma_{1r} = 0$ for all $r \neq i$, and $\Sigma_{2s} = 0$ for all $s \neq j$. Since b is odd and $k \equiv 2 \pmod 4$, the number of ones in X_{d_11} and in X_{d_12} is even. Thus, Lemma 2.2 in Jacroux et al. (1983) implies $|X'_{d_11} X_{d_12}| \geqslant 2$. Therefore, by (15), we obtain

$$\det(L) = \det \begin{pmatrix} n - \frac{4}{k} & X'_{d_11} X_{d_12} \\ X'_{d_12} X_{d_11} & n - \frac{4}{k} \end{pmatrix} \leqslant \left(n - \frac{4}{k} \right)^2 - 4.$$

Hence

$$(n - 2)\left(n + 2 - \frac{8}{k} \right) - \det(L) \geqslant (n - 2)\left(n + 2 - \frac{8}{k} \right) - \left(n - \frac{4}{k} \right)^2 + 4 =$$

$$= \frac{16(k - 1)}{k^2} > 0.$$

Case 4. Let $\Sigma_{1i}^2 = \Sigma_{2i}^2 = 4$ for some i, and $\Sigma_{1j} = \Sigma_{2j} = 0$ for all $j \neq i$. Hence, by (15), we have

$$\det(L) = (n - \frac{4}{k})^2 - (X'_{d_11} X_{d_12} \pm \frac{4}{k})^2. \tag{17}$$

As in Case 3, we conclude that $|X'_{d_11} X_{d_12}| \geqslant 2$. Since $k \geqslant 6$,

$$(X'_{d_11} X_{d_12} \pm \frac{4}{k})^2 \geqslant (2 - \frac{4}{k})^2,$$

which together with (17) gives

$$\det(L) \leqslant (n - \frac{4}{k})^2 - (2 - \frac{4}{k})^2 = (n - 2)(n + 2 - \frac{8}{k}).$$

Thus, we have proved that $\det(M_{d_4}) \geqslant \det(M_d)$ for arbitrary $d \in D(n, m, b)$ when $n = (m - 3)(k - 2) + 2$. Observe that

$$(n - \frac{4}{k})(n + 2(m - 2)) - (n + 2 - \frac{8}{k})(n + 2(m - 3))$$

$$= 4k^{-1}(n - ((m - 3)(k - 2) + 2)).$$

So from (4), for $(m-3)(k-2)+2 < n < (m-2)(k-2)+2$, it follows that

$$\det(M_{d_4}) > (n-2)^{m-2}(n+2-\frac{8}{k})(n+2(m-3)) \geqslant \det(M_d),$$

by the above considerations. This implies that the design d_4 is D-optimal in the class $D(n, m, b)$.

$\square$

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