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# D-OPTIMAL PARTIALLY REPLICATED TWO-LEVEL FACTORIAL DESIGNS

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*Abstract:* When designing a two-level factorial experiment, a cost-effective compromise for obtaining a replication-based estimate of the error variance is to conduct a partial replication on unreplicated designs. In this article, based on the D-optimality criterion, we focus on selecting a partial replication from the orthogonal designs derived from Hadamard matrices. It is shown that the augmented designs, composed of the chosen partial replication and the orthogonal designs, are highly efficient. We obtain (i) sufficient conditions for the augmented designs to be D-optimal over their corresponding classes; (ii) a construction method for the desired designs.

*Key words and phrases:* Hadamard matrix, orthogonal array, projection property, pure error.

## 1. Introduction

At the early stages of a factorial experiment, unreplicated two-level designs are commonly used to identify important or active effects. Under the situation that there is no prior information available on which effects might be active, minimum aberration designs may serve as reasonable choices for gaining more information about a large set of potential effects. However, the analysis methods for unreplicated data may perform unsatisfactorily in identifying truly active effects, particularly when the effect sparsity principle does not hold. This is due mainly to the lack of a replication-based estimate of the error variance. Thus, one might begin with an economical design, not necessarily a minimum aberration design, for estimating specified possibly active effects. Then, if some additional runs remain, can consider running repeated treatment combinations to obtain a realistic estimate of experimental error in order to test whether the specified possibly active effects are truly active. A simple approach to obtain pure replicates is to duplicate all the treatment combinations of the unreplicated design. However, the number of runs required can rapidly outgrow the resources of most experiments. Therefore, a practical compromise is to carry out a partial replication. Partially replicated designs usually work well regardless of the effect sparsity, see Liao and Chai (2009).

Dykstra (1959) proposed some high-resolution designs including repeated runs. Also, Pigeon and McAllister (1989) and Lupinacci and Pigeon (2008) discussed orthogonal main-effect plans with a partial replication. According to Mukerjee (1999), a two-level orthogonal array augmented with precisely one additional interior or exterior run is universally optimal among all possible two-level designs. A treatment combination is said to be an interior run if it is in the original design, otherwise an exterior run. Moreover, Hedayat and Zhu (2003) explored the augmentation of a set of interior or exterior runs to a saturated D-optimal two-level design. Chan, Ma, and Goh (2003) proposed a stochastic algorithm to generate D-optimal or highly D-efficient lean designs, which sometimes may include repeated runs. Butler and Ramos (2007) provided sufficient conditions for adding runs to, or deleting runs from a two-level orthogonal array so that the resulting design is optimal with respect to a general class of optimality criteria.

Liao and Chai (2004) first investigated the parallel-flats designs with a replicated flat. Most recently, Liao and Chai (2009) proposed a set of sufficient conditions and an algorithm for constructing D-optimal designs over the class of parallel-flats designs. However, there are still some limitations in their study. First, they considered only regular designs with a partial replication. Second, the number of repeated runs in their designs must be a power of 2. In this study, we extend the results beyond the above limitations and obtain a more general class of partially replicated designs, taking both regular and nonregular designs into account. More interestingly, we discuss selecting repeated runs of any number less than the run-size of an orthogonal design.

The rest of this article is organized as follows. We formulate the problem of interest in the next section. In Section 3, we present sufficient conditions for an augmented design to be D-optimal in various design settings. An approach to find the desired D-optimal designs is provided in Section 4. Concluding remarks are given in the final section.

## 2. The Problem of Interest

Let $\boldsymbol{X}_0$ be a Hadamard matrix of order $N$. Thus, $\boldsymbol{X}_0^T\boldsymbol{X}_0 = \boldsymbol{X}_0\boldsymbol{X}_0^T = N\boldsymbol{I}_N$, where $\boldsymbol{I}_N$ is the identity matrix of order $N$. Without loss of generality, $\boldsymbol{X}_0$ can be written as

$$\boldsymbol{X}_0 = \left[\boldsymbol{1}_N \; \boldsymbol{X}_0^*\right],$$

where $\boldsymbol{1}_N$ is the vector of length $N$ with all entries equal to 1 and $\boldsymbol{X}_0^*$ is the model matrix of an orthogonal array with strength two. An $N \times n$ array with entries equal to 1 or $-1$ is said to be an orthogonal array with strength $t$ if all possible $t$-tuples appear equally often as row vectors in any $N \times t$ submatrix, denoted by

$\mathrm{OA}(N, 2^n, t)$. In the context of two-level factorial design, $\boldsymbol{X}_0$ represents the model matrix of a saturated orthogonal design. Let $\boldsymbol{\beta}$ denote the specified possibly active effects to consist of the constant term $\mu$ and all the effects requested to be estimated in the model. The other effects not specified in $\boldsymbol{\beta}$ are assumed to be negligible. A design is said to be saturated, if the number of its distinct treatment combinations is equal to the number of terms in $\boldsymbol{\beta}$.

Let $v$ denote the number of terms in $\boldsymbol{\beta}$. It is assumed that $\boldsymbol{\beta}$ can be estimated using the design whose model matrix is obtained by eliminating the last $N-v$ columns of $\boldsymbol{X}_0$. This unreplicated orthogonal design is denoted by $d_N^v$. Moreover, let $d_{N+k}^v$ be a plan derived from $d_N^v$ by augmenting any $k$ distinct interior runs, that is, there are $k$ repeated runs in $d_{N+k}^v$. Let $\mathcal{D}(N, v, k)$ denote the collection of $d_{N+k}^v$ derived from all possible $d_N^v$. Also, let $\boldsymbol{X}_0$ be partitioned as

$$\boldsymbol{X}_0 = \begin{bmatrix} \boldsymbol{X}_{11} \ \boldsymbol{X}_{12} \\ \boldsymbol{X}_{21} \ \boldsymbol{X}_{22} \end{bmatrix},$$

where $\boldsymbol{X}_{11}$, $\boldsymbol{X}_{12}$, $\boldsymbol{X}_{21}$, and $\boldsymbol{X}_{22}$ are of orders $k \times v$, $k \times v_0$, $(N-k) \times v$, and $(N-k) \times v_0$, respectively. Note that $v_0 = N - v$. The experimental outcomes $\boldsymbol{Y}$, collected from a $d_{N+k}^v$, can be typically fitted by the linear model.

$$\boldsymbol{Y} = \boldsymbol{X\beta} + \boldsymbol{\epsilon},$$

where the model matrix

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{X}_{11} \\ \boldsymbol{X}_{21} \\ \boldsymbol{X}_{11} \end{bmatrix}.$$

The vector $\boldsymbol{\epsilon}$ consists of random variables assumed to be pairwise uncorrelated with common mean 0 and variance $\sigma^2$. $\boldsymbol{X}_{11}$ represents the partial replication of the design.

A design is said to be D-optimal for $\boldsymbol{\beta}$ over a specified class of designs, if its information matrix achieves the maximal determinant within the class. In this study, we consider the problem of finding the D-optimal design for $\boldsymbol{\beta}$ over $\mathcal{D}(N, v, k)$. Since $\boldsymbol{X}_0$ is a Hadamard matrix, one has $\boldsymbol{X}_{11}\boldsymbol{X}_{11}^T + \boldsymbol{X}_{12}\boldsymbol{X}_{12}^T = N\boldsymbol{I}_k$. Moreover, $|\boldsymbol{I}_n + \boldsymbol{G}^T\boldsymbol{G}| = |\boldsymbol{I}_m + \boldsymbol{G}\boldsymbol{G}^T|$ and $|\boldsymbol{I}_n - \boldsymbol{G}^T\boldsymbol{G}| = |\boldsymbol{I}_m - \boldsymbol{G}\boldsymbol{G}^T|$ for any $m \times n$ matrix $\boldsymbol{G}$. For a $d_{N+k}^v \in \mathcal{D}(N, v, k)$, based on these identities, the determinant of its information matrix can be expressed as

$$\begin{aligned} |\boldsymbol{M}| &= |N\boldsymbol{I}_v + \boldsymbol{X}_{11}^T\boldsymbol{X}_{11}| \\ &= N^v 2^k \left| \boldsymbol{I}_{v_0} - \frac{1}{2N}\boldsymbol{X}_{12}^T\boldsymbol{X}_{12} \right|. \end{aligned}$$

Therefore, maximizing $|\boldsymbol{M}|$ is equivalent to maximizing

$$\left|\boldsymbol{I}_{v_0} - \frac{1}{2N}\boldsymbol{A}\right|, \tag{2.1}$$

where $\boldsymbol{A} = \boldsymbol{X}_{12}^T\boldsymbol{X}_{12}$. Let $a_{ij}$ denote the $(ij)$th element of $\boldsymbol{A}$. Since $\boldsymbol{A}$ is a symmetric matrix of order $v_0$ and its diagonal elements are all equal to $k$, we can consider $\boldsymbol{A}$ on only its off-diagonal elements $a_{ij}$ for $i < j$. Consequently, our main concern is to determine an appropriate $\boldsymbol{X}_{12}$ with order $k \times v_0$ (the complementary part of $\boldsymbol{X}_{11}$) from $\boldsymbol{X}_0$, so that (2.1) is maximized over $\mathcal{D}(N, v, k)$; and the corresponding $\boldsymbol{X}_{11}$ indicates the optimal selection of $k$ repeated runs.

## 3. Sufficient Conditions for the D-optimal Designs

In this section, the optimal selection of a partial replication on saturated and nearly saturated designs with $0 \le v_0 \le 4$ are investigated. The result concerning the saturated case $v_0 = 0$ is proved by Hedayat and Zhu (2003). We rephrase their result as follows.

**Theorem 1.** *Any design $d_{N+k}^{N} \in \mathcal{D}(N, N, k)$ is D-optimal for $\boldsymbol{\beta}$ over all possible two-level designs plus any $k$ repeated runs plans.*

Now we turn to the nearly saturated case with $v_0 = 1$. It can be verified that the value of (2.1) is $1 - k/(2N)$ when $v_0 = 1$. Therefore, the determinants of the information matrices are all the same for any designs $d_{N+k}^{N-1} \in \mathcal{D}(N, N-1, k)$. The result is summarized as follows.

**Theorem 2.** *When $v_0 = 1$, any $d_{N+k}^{N-1}$ is D-optimal for $\boldsymbol{\beta}$ over $\mathcal{D}(N, N-1, k)$.*

On the other hand, when $2 \le v_0 \le 4$, the values of (2.1) can be different for selecting distinct sets of $k$ repeated runs. Theorems 3, 4 and 5 summarize the results for these cases.

**Theorem 3.** *When $v_0 = 2$, the sufficient conditions for a $d_{N+k}^{N-2}$ to be D-optimal for $\boldsymbol{\beta}$ over $\mathcal{D}(N, N-2, k)$ are as follows.*

(1) *If $k$ is even, then $a_{12} = 0$.*

(2) *If $k$ is odd, then $a_{12} = \pm 1$.*

It is straightforward to find that $a_{12} \in \{0, \pm 2, \ldots, \pm k\}$ when $k$ is even, and $a_{12} \in \{\pm 1, \pm 3, \ldots, \pm k\}$ when $k$ is odd. The results of Theorem 3 are immediately obtained by calculating (2.1). For ease of presentation, the proofs of Theorems 4 and 5 are relegated to the Appendix.

**Theorem 4.** *When $v_0 = 3$, the sufficient conditions for a $d_{N+k}^{N-3}$ to be D-optimal for $\boldsymbol{\beta}$ over $\mathcal{D}(N, N-3, k)$ are as follows.*

(1) *If* $k \equiv 0$ (*mod* 4), *then* $a_{ij} = 0$ *for all* $i < j$.

(2) *If* $k \equiv 1$ (*mod* 4), *then* (i) $a_{ij} = 1$ *for all* $i < j$; *or* (ii) *one of the* $a_{ij}$*'s is* 1, *and the other two* $-1$.

(3) *If* $k \equiv 2$ (*mod* 4), *then one of the* $a_{ij}$*'s is* 2 *or* $-2$, *and the other two* 0.

(4) *If* $k \equiv 3$ (*mod* 4), *then* (i) $a_{ij} = -1$ *for all* $i < j$; *or* (ii) *one of the* $a_{ij}$*'s is* $-1$, *and the other two* 1.

**Theorem 5.** *When* $v_0 = 4$, *the sufficient conditions for a* $d_{N+k}^{N-4}$ *to be D-optimal for* $\boldsymbol{\beta}$ *over* $\mathcal{D}(N, N-4, k)$ *are as follows.*

(1) *If* $k \equiv 0$ (*mod* 4), *then* $a_{ij} = 0$ *for all* $i < j$.

(2) *If* $k \equiv 1$ (*mod* 4), *then* (i) $a_{ij} = 1$ *for all* $i < j$; *or* (ii) *for a fixed integer* $1 \le r \le 4$, *three of the* $a_{ij}$*'s are* 1 *for* $i \ne r$ *or* $j \ne r$, *and the remaining three are* $-1$; *or* (iii) *for two fixed integers* $1 \le r < r' \le 4$, *one of the* $a_{ij}$*'s is* 1 *for* $i \ne r, r'$ *and* $j \ne r, r'$, *and the remaining five are* $-1$.

(3) *If* $k \equiv 2$ (*mod* 4), *then two of the* $a_{ij}$*'s, say* $a_{rs}$ *and* $a_{r's'}$ *where* $r$, $s$, $r'$ *and* $s'$ *are all distinct, are* 2 *or* $-2$, *and the remaining four are* 0.

(4) *If* $k \equiv 3$ (*mod* 4), *then* (i) $a_{ij} = -1$ *for all* $i < j$; *or* (ii) *for a fixed integer* $1 \le r \le 4$, *three of the* $a_{ij}$*'s are* $-1$, $i \ne r$ *or* $j \ne r$, *and the remaining three are* 1; *or* (iii) *for two fixed integers* $1 \le r < r' \le 4$, *one of the* $a_{ij}$*'s is* $-1$, $i \ne r, r'$ *and* $j \ne r, r'$, *and the remaining five are* 1.

Let $\bar{d}_N^v$ be an orthogonal design (a regular design, Plackett and Burman (1946) design, one from a Hadamard matrix, or other) for $\boldsymbol{\beta}$. Also, let $\bar{d}_{N+k}^v$ be a plan derived from $\bar{d}_N^v$ by augmenting any $k$ distinct interior runs, and let $\bar{\mathcal{D}}(N, v, k)$ denote the collection of $\bar{d}_{N+k}^v$ derived from all possible $\bar{d}_N^v$. Then all the D-optimal $d_{N+k}^v$ may not be optimal over $\bar{\mathcal{D}}(N, v, k)$, since not every model matrix of an orthogonal design can be embedded into a Hadamard matrix. However, Vijayan (1976) showed that any $N \times (N - v_0)$ Hadamard submatrix can be embedded into a Hadamard matrix of order $N$ for $1 \le v_0 \le 4$. Also, all the D-optimal partially replicated designs discussed in Theorems 2 to 5 have the same D-efficiency if their orthogonal designs are derived from Hadamard matrices of equal order. Therefore, we have the stronger conclusion that the D-optimal $d_{N+k}^{N-v_0}$ of Theorems 2 to 5 are actually optimal over $\bar{\mathcal{D}}(N, N - v_0, k)$ for $1 \le v_0 \le 4$.

The run-sizes of orthogonal designs for two-level factorials, except the trivial ones ($N = 1, 2$), must be a multiple of 4. If a minimal run-size orthogonal design ($v \le N \le v + 3$) for $\boldsymbol{\beta}$ is available, then we must have $0 \le v_0 \le 3$. Thus, from Theorems 1 to 4, the D-optimal $d_{N+k}^v$ are always attainable if there exists a minimal run-size orthogonal design for $\boldsymbol{\beta}$. For example, if $\boldsymbol{\beta}$ consists of only the constant term $\mu$ and main effects, then a Plackett-Burman design can serve as the desired orthogonal design. Liao, Iyer, and Vecchia (1996) provided a heuristic algorithm for searching a minimal run-size orthogonal design for any specified $\boldsymbol{\beta}$.

## 4. Construction of the Partially Replicated Designs

From Theorems 1 and 2, any two designs both in $\mathcal{D}(N,N,k)$ or in $\mathcal{D}(N,N-1,k)$ are of equal performance, we thus proceed with the cases $v_0 = 2$, 3 and 4. We propose a systematic approach to arranging the rows of a given Hadamard matrix $\boldsymbol{X}_0$ so that the sufficient conditions of Theorems 3, 4 and 5 are fulfilled. Let $\boldsymbol{P}$ be a permutation matrix such that $\boldsymbol{P}\boldsymbol{X}_0 = \tilde{\boldsymbol{X}}_0 = [\tilde{\boldsymbol{X}}_1 \;\; \tilde{\boldsymbol{X}}_2]$, where $\tilde{\boldsymbol{X}}_1$ consists of the first $v$ columns of $\tilde{\boldsymbol{X}}_0$ and $\tilde{\boldsymbol{X}}_2$ is an $\mathrm{OA}(N, 2^{v_0}, 2)$. Also, let $\tilde{\boldsymbol{X}}_{11}$ and $\tilde{\boldsymbol{X}}_{12}$ be composed of the first $k$ rows of $\tilde{\boldsymbol{X}}_1$ and $\tilde{\boldsymbol{X}}_2$, respectively. In the following, we show that there must exist at least one appropriate $\boldsymbol{P}$ such that the resulting $\tilde{\boldsymbol{X}}_{12}$ satisfies the sufficient conditions. This leads to the fact that the D-optimal partial replication can be easily obtained from $\tilde{\boldsymbol{X}}_{11}$.

(1) When $v_0 = 2$, $\tilde{\boldsymbol{X}}_2$ is an $\mathrm{OA}(N, 2^2, 2)$. This guarantees that $\tilde{\boldsymbol{X}}_2$ can be expressed as
$$\tilde{\boldsymbol{X}}_2 = \boldsymbol{l}_{N/2} \otimes \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$
where $\otimes$ denotes Kronecker product and $\boldsymbol{l}_{N/2}$ is a $(1,-1)$-vector of length $N/2$. Note that a $(1,-1)$-vector means that each of its entries is 1 or $-1$. In this case, the $\boldsymbol{l}_{N/2}$ contains equal occurrences of 1 and $-1$. It is straightforward to verify that the resulting $\tilde{\boldsymbol{X}}_{12}$ satisfies the sufficient conditions of Theorem 3 for any $1 \le k \le N$.

(2) When $v_0 = 3$, $\tilde{\boldsymbol{X}}_2$ is an $\mathrm{OA}(N, 2^3, 2)$. According to Lin and Draper (1992) and Cheng (1995), the projection of an orthogonal array with strength two onto any three factors is one of three types: one or more copies of the complete $2^3$ factorial; one or more copies of a half-replicate of the $2^3$ factorial with the product of level combinations all equal to 1 or $-1$; a combination of both types. Therefore, for any Hadamard matrix $\boldsymbol{X}_0$, there must exist an appropriate $\boldsymbol{P}$ such that $\tilde{\boldsymbol{X}}_2$ is
$$\tilde{\boldsymbol{X}}_2 = \boldsymbol{l}_{N/4} \otimes \begin{bmatrix} 1 & 1 & 1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \end{bmatrix}, \tag{4.1}$$
where $\boldsymbol{l}_{N/4}$ is a $(1,-1)$-vector of length $N/4$. Similarly, it is straightforward to check that such a $\tilde{\boldsymbol{X}}_{12}$ satisfies the sufficient conditions of Theorem 4 for any $1 \le k \le N$.

(3) When $v_0 = 4$, $\tilde{\boldsymbol{X}}_2$ is an OA$(N, 2^4, 2)$. Based on Corollary 3.1 of Cheng (1995), there exist nonnegative integers $\alpha$ and $\beta$ such that a $(1, -1)$-vector $\boldsymbol{x} = (x_1, x_2, x_3, x_4)$ and its mirror image $\bar{\boldsymbol{x}} = (-x_1, -x_2, -x_3, -x_4)$ appear as row vectors of $\tilde{\boldsymbol{X}}_2$ $\alpha$ times in total for any $\boldsymbol{x}$ with $x_1x_2x_3x_4 = 1$, and $\beta$ times in total for any $\boldsymbol{x}$ with $x_1x_2x_3x_4 = -1$. This ensures that $\tilde{\boldsymbol{X}}_2$ can be expressed as

$$\tilde{\boldsymbol{X}}_2 = \begin{bmatrix} \boldsymbol{H}_1 \\ \boldsymbol{H}_2 \\ \vdots \\ \boldsymbol{H}_{N/4} \end{bmatrix}, \tag{4.2}$$

where $\boldsymbol{H}_1, \cdots, \boldsymbol{H}_{N/4}$ are $4 \times 4$ Hadamard matrices of the forms

$$\boldsymbol{H}_i = \boldsymbol{D}_i \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & -1 \end{bmatrix} \text{ or } \boldsymbol{H}_i = \boldsymbol{D}_i \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}.$$

Here $\boldsymbol{D}_i$ is a diagonal matrix of order 4 with diagonal entries 1 or $-1$. It is straightforward to verify that the sufficient conditions of Theorem 5 are fulfilled for any $1 \le k \le N$ based on the resulting $\tilde{\boldsymbol{X}}_{12}$.

The following two examples, including both nonregular and regular designs, are given to illustrate the construction approach.

**Example 1.** The Plackett-Burman design with $N = 12$ is used to study the constant term $\mu$ and main effects for 8 factors. So, there are $v = 9$ terms in $\boldsymbol{\beta}$. After performing an appropriate permutation on the rows of $\boldsymbol{X}_0$, we have

$$\tilde{\boldsymbol{X}}_0 = [\tilde{\boldsymbol{X}}_1 \;\; \tilde{\boldsymbol{X}}_2] = \left[\begin{array}{ccccccccc|ccc}
1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\
1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\
1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\
1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\
1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 \\
1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 \\
1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 \\
1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1
\end{array}\right],$$

where the columns of $\tilde{\boldsymbol{X}}_1$ correspond to the terms in $\boldsymbol{\beta}$, and $\tilde{\boldsymbol{X}}_2$ can be written as

$$\tilde{\boldsymbol{X}}_2 = \begin{bmatrix} 1 \\ -1 \\ -1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 1 & 1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \end{bmatrix}.$$

Clearly, this $\tilde{\boldsymbol{X}}_2$ is of the form (4.1). Hence, the first $k$ row vectors of $\tilde{\boldsymbol{X}}_1$ correspond exactly to the desired $k$ repeated runs for any $1 \le k \le 12$. For example, suppose that there are $k = 3$ additional runs available for estimating the pure error variance. This results in

$$\tilde{\boldsymbol{X}}_{11} = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 \end{bmatrix},$$

namely, the treatment combinations $(-1, 1, 1, -1, 1, -1, -1, -1)$, $(1, 1, -1, 1, 1, -1, 1, -1)$ and $(-1, -1, 1, 1, 1, -1, 1, 1)$ are the optimal selection. Moreover if $k = 5$, then the two runs $(-1, 1, 1, 1, -1, 1, 1, -1)$ and $(1, 1, 1, -1, 1, 1, -1, 1)$ together with the above three runs, form the D-optimal augmentation.

**Example 2.** Suppose $\boldsymbol{\beta} = \{\mu, F_1, F_2, F_3, F_4, F_5, F_6, F_1F_2, F_1F_3, F_1F_4, F_1F_5, F_1F_6\}$ are the effects of interest in an experiment including 6 two-level factors. Here $F_i$ denotes the main effect of factor $i$ and $F_iF_j$ denotes the two-factor interaction of factors $i$ and $j$. The regular $2^{6-2}$ design determined by the generators $F_5 = F_1F_3F_4$ and $F_6 = F_1F_2F_3$ is adopted to estimate these $v = 12$ possibly active effects. The Hadamard matrix $\boldsymbol{X}_0$ of this regular design can be constructed by the standard method, e.g., see Wu and Hamada (2009). First, write down $\mathbf{1}_{16}$ as column 1 and the basic design consisting of the $2^4$ full factorial associated with $F_1$, $F_2$, $F_3$, and $F_4$ as columns 2-5. Then, generate the remaining 11 columns by performing a Hadamard product (componentwise product) among any $k$ columns of the basic design, $k = 2, 3, 4$. Rearrange the resulting columns through the relations $F_5 = F_1F_3F_4$ and $F_6 = F_1F_2F_3$, so that $F_1F_5 = F_3F_4$ and $F_1F_6 = F_2F_3$, to yield the desired $\boldsymbol{X}_0 = [\boldsymbol{X}_1 \;\; \boldsymbol{X}_2]$. Here $\boldsymbol{X}_1$ corresponds to $\boldsymbol{\beta}$, and $\boldsymbol{X}_2$ consists of the four columns associated with $F_2F_4$, $F_1F_2F_4$, $F_2F_3F_4$, and $F_1F_2F_3F_4$. The projection of $\boldsymbol{X}_2$ onto all of its columns gives two copies of a regular $2^{4-1}$ design, because $(F_2F_4)(F_1F_2F_4)(F_2F_3F_4)(F_1F_2F_3F_4) = I$. Therefore, there exists a permutation matrix $\boldsymbol{P}$ such that $\boldsymbol{P}\boldsymbol{X}_0 = [\tilde{\boldsymbol{X}}_1 \;\; \tilde{\boldsymbol{X}}_2]$, and $\tilde{\boldsymbol{X}}_2$ is given by

$$\tilde{\boldsymbol{X}}_2 = \begin{bmatrix} \boldsymbol{H}_1 \\ \boldsymbol{H}_2 \\ \boldsymbol{H}_3 \\ \boldsymbol{H}_4 \end{bmatrix},$$

where

$$\boldsymbol{H}_1 = \boldsymbol{H_2} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & -1 \end{bmatrix} \text{ and } \boldsymbol{H_3} = \boldsymbol{H_4} = \begin{bmatrix} -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Clearly, $\tilde{\boldsymbol{X}}_2$ is of the form as (4.2). Thus, we can obtain the desired $k$ twice-replicated runs for any $1 \leq k \leq 16$ exactly from the first $k$ rows of $\tilde{\boldsymbol{X}}_1$.

## 5. Discussion

A partially replicated design can save runs compared to the fully replicated design. It also provides more power in identifying truly active effects than the unreplicated design, even without the effect sparsity assumption. In our study, we have proposed a systematic method for obtaining the best partial replication on an orthogonal design according to the D-optimality criterion. We have focused on saturated and nearly saturated designs with $0 \leq v_0 \leq 4$. The D-optimality for other cases with $v_0 \geq 5$ could be derived by complex algebraic calculations. However, construction of such designs would need further investigation, because the projection properties of an orthogonal array with strength two onto 5 or more factors are not available in the literature.

Other than the case of saturated design presented in Theorem 1, the D-optimality of the nearly saturated designs is proved to hold only within the class of their original designs from all possible orthogonal designs. It is known that an orthogonal design is D-optimal over the class of all possible two-level designs. Thus, it is reasonable to conjecture that the proposed D-optimal partially replicated designs could be also D-optimal over the whole class of two-level designs plus $k$ repeated runs plans. To support this conjecture, we produced all possible nonsingular designs with $N = 8$ and $v = 6$ using an exhaustive search. That is, we generated all possible $8 \times 6$ $(1, -1)$-matrices whose entries of the first column were all fixed to be 1. We then kept all the nonsingular designs that had full-column rank. For each nonsingular design, we generated all of its possible augmented designs with any $k$ repeated runs, $1 \leq k \leq 7$. As expected, the D-optimal designs over these all possible competing designs are exactly the proposed D-optimal partially replicated designs. As mentioned earlier, the proof for the case $k = 1$ can be found in Mukerjee (1999). It could be an interesting challenge to analytically verify this conjecture for $k \geq 2$.

In practice, there could be some nonzero effects not specified in $\boldsymbol{\beta}$. These nonzero effects, likely small individually, may cumulatively affect the power for identifying the truly active effects from $\boldsymbol{\beta}$. Therefore, one might apply some reasonable measures, such as generalized resolution and generalized minimum aberration by Deng and Tang (1999), minimum $G_2$-aberration by Tang and Deng (1999) and minimum moment aberration by Xu (2003), to quantify the reduced information of partially replicated designs in unraveling the confounding between the specified possibly active effects of $\boldsymbol{\beta}$ and the nonzero effects not specified in $\boldsymbol{\beta}$. Furthermore, one might modify the criterion for constructing optimal partially replicated designs by simultaneously maximizing the efficiency in estimation of $\boldsymbol{\beta}$, and minimizing the alias or bias for the possible existence of the nonzero effects not specified in $\boldsymbol{\beta}$. These are interesting issues for future research.

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## Appendix

The following lemmas are needed in the proofs of Theorems 4 and 5.

**Lemma A.1.** *Suppose that $k \equiv 1$ (mod 4). Let $\lambda_{12}$, $\lambda_{13}$, and $\lambda_{23}$ be the pairwise inner product between three $(1,-1)$-vectors of length $k$. Let*

$$f(\lambda_{12},\lambda_{13},\lambda_{23}) = \eta(\lambda_{12}^2+\lambda_{13}^2+\lambda_{23}^2)+2\lambda_{12}\lambda_{13}\lambda_{23}, \tag{A.1}$$

*for some $\eta > 1$. Then $f(\lambda_{12},\lambda_{13},\lambda_{23})$ is minimized if $\lambda_{12}\lambda_{13}\lambda_{23}=1$.*

**Proof.** For $k \equiv 1$ (*mod* 4), $\lambda_{12},\lambda_{13},\lambda_{23} \in \{\pm 1, \pm 3, \ldots, \pm k\}$. From the inequality of arithmetic and geometric means, we have $\lambda_{12}^2+\lambda_{13}^2+\lambda_{23}^2 \geq 3(\lambda_{12}\lambda_{13}\lambda_{23})^{2/3}$. Then,

$$\begin{aligned} f(\lambda_{12},\lambda_{13},\lambda_{23}) &= \eta(\lambda_{12}^2+\lambda_{13}^2+\lambda_{23}^2)+2\lambda_{12}\lambda_{13}\lambda_{23} \\ &\geq 3\eta(\lambda_{12}\lambda_{13}\lambda_{23})^{2/3}+2\lambda_{12}\lambda_{13}\lambda_{23}. \end{aligned}$$

Let $w = \lambda_{12}\lambda_{13}\lambda_{23}$ and $g(w) = 3\eta w^{2/3}+2w$. It is easy to see that $g(w)$ is an increasing function when $w > 1$, and a decreasing function when $w < -1$. Thus, the minimum of $g(w)$ occurs at $w = \pm 1$. However, $w$ cannot be $-1$, so $f(\lambda_{12},\lambda_{13},\lambda_{23})$ is minimized when $\lambda_{12}\lambda_{13}\lambda_{23}=1$.

**Lemma A.2.** *Suppose that $k \equiv 2$ (mod 4). Let $\boldsymbol{u}_1$, $\boldsymbol{u}_2$, $\boldsymbol{u}_3$ and $\boldsymbol{u}_4$ be $(1,-1)$-vectors of length $k$. Also, let $\lambda_{ij} = \boldsymbol{u}_i^T\boldsymbol{u}_j$ for $i<j$. Then, we have*

(1) *the minimum of $\lambda_{12}^2+\lambda_{13}^2+\lambda_{23}^2$ is 4 provided one of these three $\lambda_{ij}$'s is 2 or $-2$, and the other two are 0;*

(2) *the minimum of* $\sum_{i<j}^{4} \lambda_{ij}^2$ *is* 8 *provided two of these six* $\lambda_{ij}$*'s are* 2 *or* $-2$*, and the other four are* 0.

**Proof.** For $k \equiv 2$ $(mod\ 4)$, $\lambda_{12}$, $\lambda_{13}$, $\lambda_{23} \in \{0, \pm 2, \pm 4, \ldots, \pm k\}$. We claim that it is not possible to have $\lambda_{12} = \lambda_{13} = \lambda_{23} = 0$. Let $\boldsymbol{u}_1 = [u_1, \ldots, u_k]^T$. To force $\lambda_{12} = \lambda_{13} = 0$, without loss of generality, let

$$\begin{aligned}\boldsymbol{u}_2 &= \left[-u_1, \cdots, -u_{\frac{k}{2}}, u_{\frac{k}{2}+1}, \cdots, u_k\right]^T, \\ \boldsymbol{u}_3 &= \left[-u_1, \cdots, -u_m, u_{m+1}, \cdots, u_{\frac{k}{2}}, -u_{\frac{k}{2}+1}, \cdots, -u_{k-m}, u_{k-m+1}, \cdots, u_k\right]^T.\end{aligned}$$

Here $\boldsymbol{u}_2$ is obtained by reversing the signs of the first $k/2$ entries of $\boldsymbol{u}_1$; $\boldsymbol{u}_3$ is obtained by reversing the signs of the first $m$ entries of $\boldsymbol{u}_1$ and the first $k/2 - m$ entries among the last $k/2$ ones of $\boldsymbol{u}_1$, where $1 \leq m \leq k/2$. However,

$$\begin{aligned}\boldsymbol{u}_2^T \boldsymbol{u}_3 &= m - \left(\frac{k}{2} - m\right) - \left(\frac{k}{2} - m\right) + m \\ &= 4m - k.\end{aligned}$$

Thus, $\lambda_{23}$ is nonzero and the minimum of $\lambda_{23}^2$ is 4 because $k \equiv 2$ $(mod\ 4)$. Consequently, the minimum of $\lambda_{12}^2 + \lambda_{13}^2 + \lambda_{23}^2$ is 4 provided one of these three $\lambda_{ij}$'s is 2 or $-2$, and the other two are 0. This completes the proof of (1). The proof of (2) is similar.

**Proof of Theorem 4.** For $v_0 = 3$, (2.1) is given by

$$\left|\boldsymbol{I}_3 - \frac{1}{2N}\boldsymbol{A}\right| = \left(1 - \frac{k}{2N}\right)^3 - \frac{1}{(2N)^3}\left[(2N-k)(a_{12}^2 + a_{13}^2 + a_{23}^2) + 2a_{12}a_{13}a_{23}\right].$$

Thus, the maximization of (2.1) is to find $a_{12}$, $a_{13}$ and $a_{23}$ such that

$$(2N-k)(a_{12}^2 + a_{13}^2 + a_{23}^2) + 2a_{12}a_{13}a_{23} \tag{A.2}$$

is minimized.

(1) When $k \equiv 0$ $(mod\ 4)$, $\boldsymbol{I}_3 - (1/2N)\boldsymbol{A}$ is a diagonal matrix provided $a_{12} = a_{13} = a_{23} = 0$. Thus, (2.1) attains the maximum.

(2) When $k \equiv 1$ $(mod\ 4)$, from Lemma 1, (A.2) is minimized if $a_{12}a_{13}a_{23} = 1$. Equivalently, conditions (i) and (ii) hold.

(3) When $k \equiv 2$ $(mod\ 4)$, let $\Omega$ be the collection of all possible 3-tuples $(a_{12}, a_{13}, a_{23})$. Also, let $\Omega_0$ be the subset of $\Omega$ satisfying $a_{12}a_{13}a_{23} = 0$ and $\Omega_1 = \Omega \backslash \Omega_0$,

the complement of $\Omega_0$. We claim that the minimum of (A.2) occurs over $\Omega_0$. From Lemma 2, (A.2) attains the minimum over $\Omega_0$ when one of the $a_{ij}$'s is 2 or $-2$, and the other two are 0. On the other hand, the $a_{ij}$'s are all in the set $\{\pm 2, \pm 4, \ldots, \pm k\}$ over $\Omega_1$. By similar arguments to those of Lemma 1, (A.2) is minimized over $\Omega_1$ if $a_{12}a_{13}a_{23} = 8$, resulting in $a_{12} = a_{13} = a_{23} = 2$, or one of the $a_{ij}$'s is 2 and the other two are $-2$. The minimums of (A.2) over $\Omega_0$ and $\Omega_1$ are $4(2N - k)$ and $12(2N - k) + 16$, respectively. Obviously, the former is smaller, and this proves the condition.

(4) When $k \equiv 3$ ($mod$ 4), by arguments as in proving (2), (A.2) is minimized if $a_{12}a_{13}a_{23} = -1$. Thus, conditions (i) and (ii) hold.

**Proof of Theorem 5.** Let $\boldsymbol{A}^* = -[1/(2N)]\boldsymbol{X}_{12}^T\boldsymbol{X}_{12} = -[1/(2N)]\boldsymbol{A}$ and apply the diagonal expansion in calculating the determinant, see Searle (1982). For $v_0 = 4$, (2.1) can be expressed as

$$\begin{aligned}\left|\boldsymbol{I}_4 - \frac{1}{2N}\boldsymbol{X}_{12}^T\boldsymbol{X}_{12}\right| &= |\boldsymbol{I}_4 + \boldsymbol{A}^*| \\ &= 1 + tr_1(\boldsymbol{A}^*) + tr_2(\boldsymbol{A}^*) + tr_3(\boldsymbol{A}^*) + tr_4(\boldsymbol{A}^*) \\ &= 1 + \left(-\frac{2k}{N}\right) + tr_2(\boldsymbol{A}^*) + tr_3(\boldsymbol{A}^*) + |\boldsymbol{A}^*|,\end{aligned}$$

where $tr_i(\boldsymbol{A}^*)$ denotes the sum of the principal minors of order $i$ of $\boldsymbol{A}^*$. Moreover,

$$\begin{aligned}tr_2(\boldsymbol{A}^*) + tr_3(\boldsymbol{A}^*) = &\frac{3k^2}{2N^2} - \frac{k^3}{2N^3} \\ &- \frac{1}{8N^3}\Bigg\{2(N-k)\sum_{i<j}^{4} a_{ij}^2 + 2(a_{12}a_{13}a_{23} + a_{12}a_{14}a_{24} \\ &+ a_{13}a_{14}a_{34} + a_{23}a_{24}a_{34})\Bigg\},\end{aligned}$$

$$\begin{aligned}|\boldsymbol{A}^*| = \frac{k^4}{16N^4} - \frac{1}{16N^4}\Bigg\{&k^2\sum_{i<j}^{4} a_{ij}^2 + 2(a_{13}a_{14}a_{23}a_{24} + a_{12}a_{14}a_{23}a_{34} + a_{12}a_{13}a_{24}a_{34}) \\ &- (a_{12}^2a_{34}^2 + a_{13}^2a_{24}^2 + a_{14}^2a_{23}^2) \\ &- 2k(a_{12}a_{13}a_{23} + a_{12}a_{14}a_{24} + a_{13}a_{14}a_{34} + a_{23}a_{24}a_{34})\Bigg\}.\end{aligned}$$

Thus, the maximization of (2.1) is equivalent to finding a set of $a_{ij}$'s such that $tr_2(\boldsymbol{A}^*)+tr_3(\boldsymbol{A}^*)$ and $|\boldsymbol{A}^*|$ are both maximized. That is, the following expressions are both minimized:

$$2(N-k)\sum_{i<j}^{4} a_{ij}^2 + 2(a_{12}a_{13}a_{23} + a_{12}a_{14}a_{24} + a_{13}a_{14}a_{34} + a_{23}a_{24}a_{34}); \tag{A.3}$$

$$k^2\sum_{i<j}^{4} a_{ij}^2 + 2(a_{13}a_{14}a_{23}a_{24} + a_{12}a_{14}a_{23}a_{34} + a_{12}a_{13}a_{24}a_{34}) - (a_{12}^2a_{34}^2 + a_{13}^2a_{24}^2 + a_{14}^2a_{23}^2)$$
$$-2k(a_{12}a_{13}a_{23} + a_{12}a_{14}a_{24} + a_{13}a_{14}a_{34} + a_{23}a_{24}a_{34}). \tag{A.4}$$

(1) When $k \equiv 0$ $(mod\ 4)$, $\boldsymbol{I}_4 - (1/2N)\boldsymbol{X}_{12}^T\boldsymbol{X}_{12}$ is a diagonal matrix provided $a_{ij} = 0$ for all $i < j$. Thus, (2.1) achieves the maximum.

(2) When $k \equiv 1$ $(mod\ 4)$, (A.3) can be expressed as the sum of $f(a_{12}, a_{13}, a_{23})$, $f(a_{12}, a_{14}, a_{24})$, $f(a_{13}, a_{14}, a_{34})$, and $f(a_{23}, a_{24}, a_{34})$ of the form as (A.1). From Lemma 1, (A.3) is minimized if $a_{12}a_{13}a_{23} = a_{12}a_{14}a_{24} = a_{13}a_{14}a_{34} = a_{23}a_{24}a_{34} = 1$, equivalently $a_{ij} = 1$ for all $i < j$. From Theorem 2.1 of Cheng (1980), $|\boldsymbol{A}^*|$ is maximized if $a_{ij} = 1$ for all $i < j$. Consequently, condition (i) is proved. Now

$$|\boldsymbol{I}_4 + \boldsymbol{A}^*| = |\boldsymbol{D}(\boldsymbol{I}_4 + \boldsymbol{A}^*)\boldsymbol{D}| = \left|\boldsymbol{I}_4 - \frac{1}{2N}\boldsymbol{DAD}\right|, \tag{A.5}$$

where $\boldsymbol{D}$ is a diagonal matrix whose diagonal elements are 1 or $-1$. Thus, it is easy to verify that (2.1) has the same value under conditions (i), (ii), and (iii).

(3) When $k \equiv 2$ $(mod\ 4)$, let $\Omega$ be the collection of all possible 6-tuples ($a_{12}$, $a_{13}$, $a_{14}$, $a_{23}$,$a_{24}$,$a_{34}$). Also, let $\Omega_0$ be the subset of $\Omega$ satisfying $a_{12}a_{13}a_{14}a_{23}a_{24}a_{34} = 0$ and $\Omega_1 = \Omega \setminus \Omega_0$, the complement of $\Omega_0$. We claim that the maximum of (2.1) occurs over $\Omega_0$. By Lemma 2, it is straightforward to observe that both (A.3) and (A.4) attain their minimums over $\Omega_0$ if both $a_{rs}$ and $a_{r's'}$ are 2 or $-2$, where $r$, $s$, $r'$ and $r'$ are all distinct, and the remaining four are 0. On the other hand, the $a_{ij}$'s are in the set $\{\pm 2, \pm 4, \ldots, \pm k\}$ over $\Omega_1$. By arguments as in proving (2), both (A.3) and (A.4) achieve their minimums over $\Omega_1$ when $a_{ij} = 2$ for all $i < j$. The maximums of (2.1) over $\Omega_0$ and $\Omega_1$ are $(1-(k/2N)+1/N)^2(1-(k/2N)-1/N)^2$ and $(1-(k/2N)+1/N)^2[(1-(k/2N)-1/N)^2-(2/N)^2]$, respectively. The former is greater, and this completes the proof of (3).

(4) When $k \equiv 3$ $(mod\ 4)$, $\boldsymbol{I}_4 - (1/2N)\boldsymbol{A} = (1-[(k+1)/2N])\,\boldsymbol{I}_4 + (1/2N)\,\boldsymbol{J}_4$, provided $a_{ij} = -1$ for all $i < j$. Again, condition (i) follows directly from Theorem 2.1 of Cheng (1980). According to (A.5), conditions (ii) and (iii) can be derived immediately from condition (i).

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