Construction of Minimal-Point Mixed-Level Screening Designs Using Conference Matrices

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Screening designs are frequently used to identify active effects from a large number of factors. Small size designs are preferred when the experiments are costly. Two-level or three-level minimal-point screening designs have been well studied in the literature. However, minimal-point mixed-level designs have not been thoroughly explored. In this paper, a new class of minimal-point mixed-level designs is constructed using conference matrices. The constructed designs can be used to estimate the main effects and quadratic effects with a good performance of *D*-efficiency and variance of estimates.

Key Words: *D*-Efficiency; Main Effect; Maximal Determinant Matrix; Orthogonal Array; Quadratic Effect.

1. Introduction

Screening designs are often used to identify the most important factors during the early stages of an experimentation process that typically involves a large number of factors. When the experimentation is expensive, time-consuming or difficult, small size designs are preferred. A minimal-point design is a saturated design in which the number of runs is the same as the number of the parameters to be estimated. It makes use of the minimal effort to estimate all the parameters. For experiments with two-level factors, it is a desirable choice to use D-optimal designs as the screening designs. For experiments with three-level factors, a new type of definitive screening designs was developed by Jones and Nachtsheim (2011). These designs have desirable properties for screening factors. Xiao et al. (2012) proposed a systematic method to construct such definitive screening designs via conference matrices. However, minimal-point designs with mixed two-level and three-level factors are lacking. In this paper, the construction of mixed-level screening designs with minimal points is provided and the properties of the designs are discussed.

Consider the following linear model with $m + p$ factors:

$$y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i=1}^{p} \alpha_i z_i + \epsilon, \quad (1)$$

where x_i is a three-level factor ($i = 1, \dots, m$), z_i is a two-level factor ($i = 1, \dots, p$), and ϵ is the error term with zero mean and a finite variance σ^2. This

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model has a constant term, $m+p$ first-order terms, m quadratic terms, and thus has a total of $2m+p+1$ parameters. A new type of design with desirable properties based on conference matrices will be proposed for such a model.

This paper is organized as follows. The construction of the minimal-point mixed-level designs and examples are proposed in Section 2. Section 3 discusses the design properties, while applications are illustrated in Section 4. Conclusions are given in Section 5.

2. Design Construction and Examples

In this section, the construction of mixed-level designs with m three-level factors and p two-level factors is presented. First, we introduce the definitions of conference matrix and maximal determinant matrix. The existence of these designs will be discussed in Section 5.

Definition 1 (Goethals and Seidel (1967))

An m-order square matrix $\mathbf{C} = (c_{ij})$ is called a *conference matrix* (also called a **C**-matrix) if it satisfies $\mathbf{C}^{\mathrm{T}}\mathbf{C} = (m-1)\mathbf{I}_m$, with $c_{ii} = 0$ $(i = 1, 2, \ldots, m)$, $c_{ij} \in \{1, -1\}$ $(i \neq j,\ i, j = 1, 2, \ldots m)$, where $\mathbf{I}_m$ is the m-order identity matrix.

Definition 2

An $n \times n$ matrix is called an n-order *maximal determinant matrix* if it has the largest possible determinant among the $n \times n$ matrices whose entries are ± 1.

D-optimal designs are good choices for two-level screening designs, and $\mathbf{P} = (\mathbf{C}^{\mathrm{T}}, \mathbf{0}_m,\ -\mathbf{C}^{\mathrm{T}})^{\mathrm{T}}$ is a desirable structure for three-level screening designs, where $\mathbf{0}_m$ is an $m \times 1$ column vector with all elements zero and $\mathbf{C}$ is an m-order conference matrix (see Jones and Nachtsheim (2011)). This fold-over structure can guarantee that the estimates of all the main effects are uncorrelated with the estimates of quadratic effects and two-factor interactions. We thus propose the following design $\mathbf{D}$ for the mixed-level screening problem in model (1):

$$\mathbf{D} = \begin{pmatrix} \mathbf{P} & \mathbf{B} \\ \mathbf{A} & \mathbf{M} \end{pmatrix},$$

where $\mathbf{P}$ is $(\mathbf{C}^{\mathrm{T}}, \mathbf{0}_m, -\mathbf{C}^{\mathrm{T}})^{\mathrm{T}}$, $\mathbf{M}$ is a two-level maximal determinant matrix, $\mathbf{A}$ is a $p \times m$ matrix with entries 0 and ± 1, and $\mathbf{B}$ is a $(2m+1) \times p$ matrix with entries ± 1. Note that matrices $\mathbf{A}$ and $\mathbf{B}$ can be obtained by computer search once the design optimality is specified. In this paper, we focus on constructing $\mathbf{A}$ and $\mathbf{B}$ systematically. Here we propose the forms of $\mathbf{A}$ and $\mathbf{B}$ that result in good performance in terms of design efficiencies.

Considering the fold-over structure $(\mathbf{C}^{\mathrm{T}}, -\mathbf{C}^{\mathrm{T}})^{\mathrm{T}}$ in $\mathbf{P}$, it is wise to take matrix $\mathbf{B}$ with the form $(\mathbf{H}^{\mathrm{T}}, \mathbf{g}, \mathbf{H}^{\mathrm{T}})^{\mathrm{T}}$, where $\mathbf{g}$ is a $p \times 1$ column vector, $\mathbf{H}$ is an $m \times p$ matrix with entries ± 1. Such a structure guarantees $\mathbf{P}^{\mathrm{T}}\mathbf{B} = \mathbf{0}_{m\times p}$, where $\mathbf{0}_{m\times p}$ is an $m \times p$ matrix with entries zero. Namely,

$$\mathbf{D} = \begin{pmatrix} \mathbf{P} & \mathbf{B} \\ \mathbf{A} & \mathbf{M} \end{pmatrix} = \begin{pmatrix} \mathbf{C} & \mathbf{H} \\ \mathbf{0}_m^{\mathrm{T}} & \mathbf{g}^{\mathrm{T}} \\ -\mathbf{C} & \mathbf{H} \\ \mathbf{A} & \mathbf{M} \end{pmatrix}.$$

According to the different sizes of m and p, the designs are constructed in four cases as shown in Table 1. Basically, matrices $\mathbf{A}$ and $\mathbf{H}$ are chosen to have low correlation between any two columns. Because $\mathbf{C}$ is an orthogonal matrix and the correlation between any two distinct columns of matrix $\mathbf{M}$ is low, a natural choice for matrices $\mathbf{A}$ and $\mathbf{H}$ is a portion of matrices $\mathbf{C}$ and $\mathbf{M}$, respectively. Here we make use of the first few rows of $\mathbf{C}$ and $\mathbf{M}$ (other rows can be used as well, although our experiences indicate that the choice of these rows is not critical at all). Take $m = 4$ as an example, various designs for various p are given below.

Case 1

For $m = p$, take $\mathbf{B} = (-\mathbf{M}^{\mathrm{T}}, \mathbf{1}_p, -\mathbf{M}^{\mathrm{T}})^{\mathrm{T}}$, $\mathbf{A} = \mathbf{C}$, where $\mathbf{1}_p$ is a $p \times 1$ column vector with all elements unity; then the design for $m = p = 4$ is

$$\mathbf{D} = \left(\begin{array}{c|c} \mathbf{C} & -\mathbf{M} \\ \mathbf{0}_m^{\mathrm{T}} & \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{C} & -\mathbf{M} \\ \hline \mathbf{C} & \mathbf{M} \end{array}\right) = \left(\begin{array}{cccc|cccc} 0 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ -1 & 0 & -1 & 1 & -1 & 1 & -1 & 1 \\ -1 & 1 & 0 & -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 0 & -1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 0 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 0 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 0 & -1 & 1 & 1 & -1 \\ \hline 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 0 & -1 & 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 0 & 1 & -1 & -1 & 1 \end{array}\right).$$

TABLE 1. Proposed Design Structure

Condition	Choice of matrix **A**	Choice of matrix **B**	Resulting design **D**	Remark
$m = p$	$\mathbf{A} = \mathbf{C}$	$\mathbf{B} = \begin{pmatrix} -\mathbf{M} \\ \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{M} \end{pmatrix}$	$\mathbf{D} = \begin{pmatrix} \mathbf{C} & -\mathbf{M} \\ \mathbf{0}_m^{\mathrm{T}} & \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{C} & -\mathbf{M} \\ \mathbf{C} & \mathbf{M} \end{pmatrix}$	a
$m > p$	$\mathbf{A} = \mathbf{C}_1$	$\mathbf{B} = \begin{pmatrix} \mathbf{E} \\ \mathbf{1}_p^{\mathrm{T}} \\ \mathbf{E} \end{pmatrix}$	$\mathbf{D} = \begin{pmatrix} \mathbf{C} & \mathbf{E} \\ \mathbf{0}_m^{\mathrm{T}} & \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{C} & \mathbf{E} \\ \mathbf{C}_1 & \mathbf{M} \end{pmatrix}$	b
$m = p - 1$	$\mathbf{A} = \begin{pmatrix} \mathbf{C} \\ \mathbf{0}_m^{\mathrm{T}} \end{pmatrix}$	$\mathbf{B} = \begin{pmatrix} -\mathbf{M}_2 \\ -\mathbf{r} \\ -\mathbf{M}_2 \end{pmatrix}$	$\mathbf{D} = \begin{pmatrix} \mathbf{C} & -\mathbf{M}_2 \\ \mathbf{0}_m^{\mathrm{T}} & -\mathbf{r} \\ -\mathbf{C} & -\mathbf{M}_2 \\ \mathbf{A} & \mathbf{M} \end{pmatrix}$	c
$m < p - 1$	$\mathbf{A} = \begin{pmatrix} \mathbf{C} \\ \mathbf{C}_2 \end{pmatrix}$	$\mathbf{B} = \begin{pmatrix} -\mathbf{M}_2 \\ \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{M}_2 \end{pmatrix}$	$\mathbf{D} = \begin{pmatrix} \mathbf{C} & -\mathbf{M}_2 \\ \mathbf{0}_m^{\mathrm{T}} & \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{C} & -\mathbf{M}_2 \\ \mathbf{A} & \mathbf{M} \end{pmatrix}$	d

a. $\mathbf{D} = \begin{pmatrix} \mathbf{P} & \mathbf{B} \\ \mathbf{A} & \mathbf{M} \end{pmatrix}$ with $\mathbf{P} = (\mathbf{C}^{\mathrm{T}}, \mathbf{0}_m, -\mathbf{C}^{\mathrm{T}})^{\mathrm{T}}$, where $\mathbf{C}$ is a conference matrix and $\mathbf{M}$ is a $p \times p$ maximal determinant matrix.

b. $\mathbf{C}_1$ is composed of the first p rows of $\mathbf{C}$; $\mathbf{E} = (\mathbf{N}^{\mathrm{T}}, \mathbf{M}_1^{\mathrm{T}})^{\mathrm{T}}$, where $\mathbf{N} = \mathbf{l}_{\lfloor m/p \rfloor} \otimes \mathbf{M}$, $\mathbf{l}_k$ is a $k \times 1$ matrix of which the $(2i-1)$th element is -1, for $i = 1, \ldots, \lceil k/2 \rceil$ and the other elements are 1; $\otimes$ denotes Kronecker product, $\lfloor a \rfloor$ stands for the largest integer not greater than a, and $\lceil b \rceil$ is the smallest integer not less than b; and $\mathbf{M}_1$ is a matrix of which the rows are the first $m - \lfloor m/p \rfloor \times p$ rows of $\mathbf{M}$.

c. $\mathbf{M}_2$ is composed of the first m rows of $\mathbf{M}$ and $\mathbf{r}$ is the last row of M.

d. $\mathbf{C}_2$ is composed of the first $p - m$ rows of $\mathbf{C}$.

Case 2

For $m > p$, take $\mathbf{B} = (\mathbf{E}_{m\times p}^{\mathrm{T}}, \mathbf{1}_p, \mathbf{E}_{m\times p}^{\mathrm{T}})^{\mathrm{T}}$, $\mathbf{E} = (\mathbf{N}^{\mathrm{T}}, \mathbf{M}_1^{\mathrm{T}})^{\mathrm{T}}$, and $\mathbf{A} = \mathbf{C}_1$, where $\mathbf{N} = \mathbf{l}_{\lfloor m/p \rfloor} \otimes \mathbf{M}$, $\mathbf{l}_k$ is a $k \times 1$ matrix whose $(2i-1)$th element is -1, for $i = 1, \ldots, \lceil k/2 \rceil$ and the other elements are 1, $\otimes$ denotes Kronecker product, $\lfloor a \rfloor$ stands for the largest integer not greater than a and $\lceil b \rceil$ is the smallest integer not less than b; $\mathbf{M}_1$ is a matrix for which the rows are the first $m - \lfloor m/p \rfloor \times p$ rows of $\mathbf{M}$; and $\mathbf{C}_1$ is composed of the first p rows of $\mathbf{C}$. Then the design for $p = 3$ is

$$\mathbf{D} = \left(\begin{array}{c|c} \mathbf{C} & \mathbf{E} \\ \mathbf{0}_m^{\mathrm{T}} & \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{C} & \mathbf{E} \\ \hline \mathbf{C}_1 & \mathbf{M} \end{array}\right)$$

$$= \left(\begin{array}{cccc|ccc} 0 & 1 & 1 & 1 & 1 & -1 & -1 \\ -1 & 0 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & -1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & -1 & -1 & -1 & 1 & -1 & -1 \\ 1 & 0 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 0 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 0 & -1 & 1 & 1 \\ \hline 0 & 1 & 1 & 1 & -1 & 1 & 1 \\ -1 & 0 & -1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 0 & -1 & 1 & 1 & -1 \end{array}\right).$$

Case 3

For $m = p - 1$, take $\mathbf{B} = (-\mathbf{M}_2^{\mathrm{T}}, -\mathbf{r}^{\mathrm{T}}, -\mathbf{M}_2^{\mathrm{T}})^{\mathrm{T}}$ and $\mathbf{A} = (\mathbf{C}^{\mathrm{T}}, \mathbf{0}_m)^{\mathrm{T}}$, where $\mathbf{M}_2$ is composed of the first m rows of $\mathbf{M}$ and $\mathbf{r}$ is the last row of $\mathbf{M}$. Then the design for $p = 5$ is

$$\mathbf{D} = \left(\begin{array}{c|c} \mathbf{C} & -\mathbf{M}_2 \\ \mathbf{0}_m^{\mathrm{T}} & -\mathbf{r} \\ -\mathbf{C} & -\mathbf{M}_2 \\ \hline \mathbf{A} & \mathbf{M} \end{array}\right) = \left(\begin{array}{rrrr|rrrrr} 0 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ -1 & 0 & -1 & 1 & -1 & 1 & -1 & -1 & -1 \\ -1 & 1 & 0 & -1 & -1 & -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 0 & -1 & -1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 1 \\ 0 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 0 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 0 & 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 0 & -1 & -1 & -1 & 1 & -1 \\ \hline 0 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 0 & -1 & 1 & 1 & -1 & 1 & 1 & 1 \\ -1 & 1 & 0 & -1 & 1 & 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 0 & 1 & 1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & -1 \end{array}\right).$$

Case 4

For $m < p - 1$, take $\mathbf{A} = (\mathbf{C}^{\mathrm{T}}, \mathbf{C}_2^{\mathrm{T}})^{\mathrm{T}}$ and $\mathbf{B} = (-\mathbf{M}_2^{\mathrm{T}}, \mathbf{1}_p, -\mathbf{M}_2^{\mathrm{T}})^{\mathrm{T}}$, where $\mathbf{C}_2$ is composed of the first $p - m$ rows of $\mathbf{C}$. Then the design for $p = 6$ is

$$\mathbf{D} = \left(\begin{array}{c|c} \mathbf{C} & -\mathbf{M}_2 \\ \mathbf{0}_m^{\mathrm{T}} & \mathbf{1}_p^{\mathrm{T}} \\ -\mathbf{C} & -\mathbf{M}_2 \\ \hline \mathbf{A} & \mathbf{M} \end{array}\right) = \left(\begin{array}{rrrr|rrrrrr} 0 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 0 & -1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 \\ -1 & 1 & 0 & -1 & -1 & -1 & 1 & -1 & -1 & -1 \\ -1 & -1 & 1 & 0 & 1 & 1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 0 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 0 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & 0 & 1 & 1 & 1 & 1 & -1 & -1 \\ \hline 0 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 0 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 0 & -1 & 1 & 1 & -1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 0 & -1 & -1 & -1 & -1 & 1 & 1 \\ 0 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 \\ -1 & 0 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 \end{array}\right).$$

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3. Design Properties

Here we discuss the properties of the proposed designs. We first adopt the D-efficiency criterion to evaluate the performance of the designs,

$$D_{\mathrm{eff}}(\mathbf{D}) = \frac{\|\mathbf{X}^{\mathrm{T}}(\mathbf{D})\mathbf{X}(\mathbf{D})\|^{1/k}}{n},$$

where $\mathbf{X}(\mathbf{D})$ is the model matrix of design $\mathbf{D}$, n is the run size of $\mathbf{D}$, and k is the number of parameters to be estimated in the model. For the first-order model, the model matrix is $\mathbf{X}_1 = (\mathbf{1}_n, \mathbf{x}_1, \ldots, \mathbf{x}_m, \mathbf{z}_1, \ldots, \mathbf{z}_p)$ and for the pure-quadratic model, the model matrix is $\mathbf{X}_2 = (\mathbf{1}_n, \mathbf{x}_1, \ldots, \mathbf{x}_m, \mathbf{x}_1^2, \ldots, \mathbf{x}_m^2, \mathbf{z}_1, \ldots, \mathbf{z}_p)$. The D-efficiencies for the proposed designs for $m = 4, 6, \ldots, 12$ (with $p = 0, 1, \ldots, m + 4$) are given in Appendix A. The special cases of $m = p$ are displayed in Table 2 for illustration. The orthogonal arrays (OAs) in Table 2 are taken from Hedayat et al. (1999). Mixed-level OAs are good choices for the mixed-level screening problem of model (1), but the run sizes of the OAs are not minimal. As a comparison, we evaluate the D-efficiencies if the smallest OAs are used with specific numbers of m and p. We define the D-efficiency ratio as

$$D\text{-efficiency ratio} = \frac{D_{\mathrm{eff}}(\mathbf{D}_{\mathrm{P}})}{D_{\mathrm{eff}}(\mathrm{OA})},$$

where $\mathbf{D}_{\mathrm{P}}$ is the proposed design.

TABLE 2. D-Efficiencies for the Cases of $m = p$

m	p	$n = 2m + p + 1$	OA size	1st-order D-efficiency ratio (%)	Pure-quadratic D-efficiency ratio (%)
4	4	13	36	93.3 (0.7794/0.8351)	82.6 (0.4592/0.5557)
6	6	19	36	94.3 (0.7820/0.8293)	77.6 (0.4244/0.5472)
8	8	25	36	102.7 (0.8491/0.8263)	75.8 (0.4115/0.5428)
10	10	31	72	101.5 (0.8367/0.8244)	70.5 (0.3806/0.5401)
12	12	37	72	107.3 (0.8828/0.8231)	68.6 (0.3684/0.5383)

From Table 2, it is obvious that the first-order D-efficiencies of the proposed designs are comparable with the ones of OAs. In some cases, the proposed designs are superior to OAs in terms of the first-order D-efficiency. The pure-quadratic D-efficiency ratios are between 68.6% and 82.6%, while the sizes of the proposed designs are much smaller than the ones of OAs. For other m and p, the D-efficiencies of the proposed designs have a similar performance (see Appendix A).

The D-efficiencies of the designs are also plotted in Figure 1: Fig. 1(a) displays the first-order D-efficiencies (y-axis) versus the values of p (x-axis) for various values of m, while Fig. 1(b) displays the pure-quadratic D-efficiencies. In Fig. 1(a), for any fixed p, as m increases, the D-efficiency for the first-order model increases. For given m, the D-efficiencies when "$m < p$" are in general smaller than the values when "$m \geq p$". In Fig. 1(b), in most cases, for any fixed p, as m increases, the D-efficiency for the pure-quadratic model decreases. For given m, when p increases, the value increases in most cases.

Next, we calculate the variances of the two-level main effects and three-level main and quadratic effects for model (1): $\mathrm{Var}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}_2^{\mathrm{T}}\mathbf{X}_2)^{-1}\sigma^2$, where $\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_m, \hat{\beta}_{11}, \ldots, \hat{\beta}_{mm}, \hat{\alpha}_1, \ldots, \hat{\alpha}_p)^{\mathrm{T}}$, and $\sigma^2 = \mathrm{Var}(\epsilon)$. For the proposed designs, $\mathrm{Var}(\hat{\beta}_i)$ is a constant and this is stated as Theorem 1 below (the proof of which is given in Appendix B). It is obvious that there is a negative relationship between m and the variance value.

Theorem 1

For the proposed designs with model (1), $\mathrm{Var}(\hat{\beta}_i)$ has a constant value of $\sigma^2/[2(m-1)]$, for all $i = 1, \ldots, m$, where m is the number of the three-level factors.

The variances of the designs are plotted in Figure 2: Fig. 2(a) displays the average variances of two-level main effects (y-axis) versus the values of p (x-axis) for various values of m. Fig. 2(b) displays the variances of three-level main effects. In Fig. 2(a), given p and m, the average variance of two-level main effects equals $\sum_{i=1}^{p} \mathrm{Var}(\hat{\alpha}_i)/p$. For $p \leq 5$, the average variances are nearly the same for different m. The average variance decreases dramatically as p increases, especially for small p. For the same m, the average variance decreases when p increases from 1 to $m+1$ and the average variance increases slightly as p increases from $m+2$ to $m+4$. For $p > 3$, the average variances of two-level main effects are smaller than $0.2\sigma^2$ for all m, and for $p > 4$, the values are smaller than $0.1\sigma^2$ for all m but $m = 4$. These values are reasonably low. In Fig. 2(b), $\mathrm{Var}(\hat{\beta}_i)$ is a constant of $\sigma^2/[2(m-1)]$; thus, as m increases, $\mathrm{Var}(\hat{\beta}_i)$ decreases dramatically. For all m but $m = 4$, the variances of three-level main effects are not larger than $0.1\sigma^2$. Fig. 2(c) displays the average variances of three-level quadratic effects. Given p and m, the average variance of three-level quadratic effects equals $\sum_{i=1}^{p} \mathrm{Var}(\hat{\beta}_{ii})/p$. For given m, the average variance decreases dramatically for $p \leq m+1$. In most cases, the average variance is no more than $0.7\sigma^2$. The values are smaller than $0.5\sigma^2$ for $p \geq m$ except for the case of $m = 4$.

Now we calculate the correlation coefficients for the proposed designs. The performance of the correlation structure is described by $\rho_{\min}$, $\rho_{\max}$, and ρ_{ave}. The correlation coefficient of vectors $\mathbf{u} = (u_1, \ldots, u_n)^{\mathrm{T}}$ and $\mathbf{v} = (v_1, \ldots, v_n)^{\mathrm{T}}$ is

$$\rho = \frac{\sum_{i=1}^{n}(u_i - \bar{\mathbf{u}})(v_i - \bar{\mathbf{v}})}{\sqrt{\sum(u_i - \bar{\mathbf{u}})\sum(v_i - \bar{\mathbf{v}})}},$$

where $\bar{\mathbf{u}} = n^{-1}\sum u_i$ and $\bar{\mathbf{v}} = n^{-1}\sum v_i$. For the $(2m+p+1) \times (2m+p)$ model matrix $(x_1, \ldots, x_m, x_1^2, \ldots, x_m^2, z_1, \ldots, z_p)$, the correlation matrix is

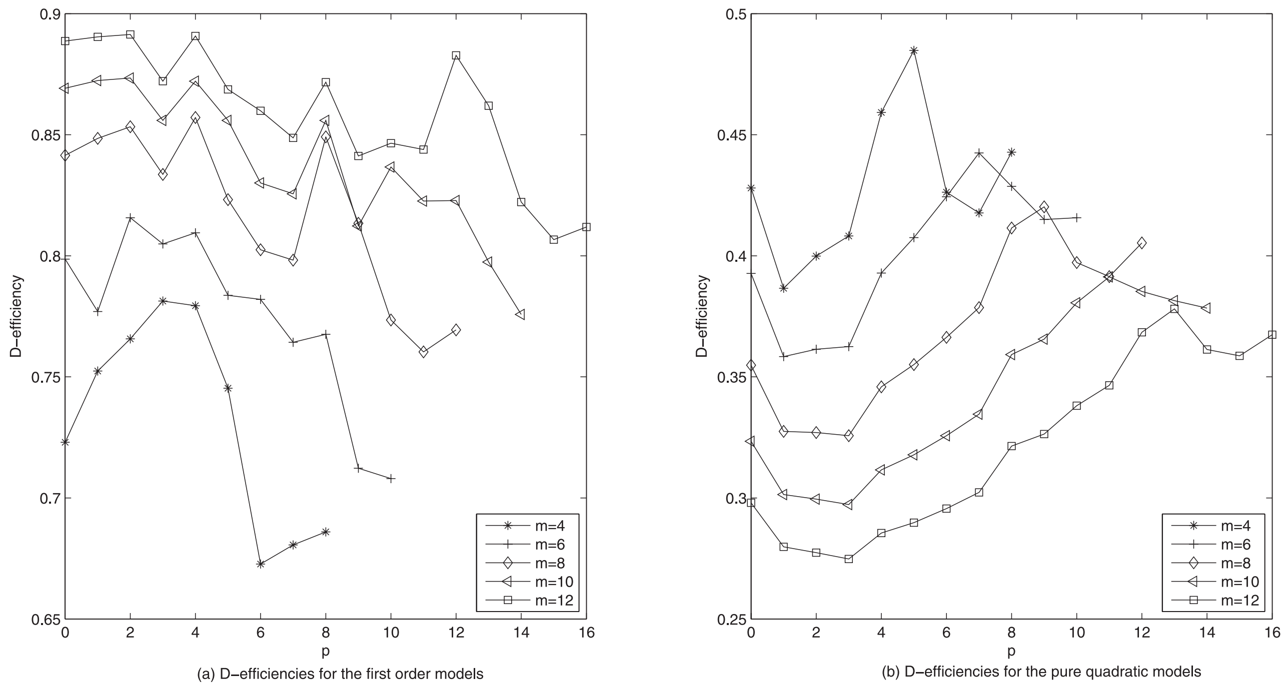

FIGURE 1. *D*-Efficiencies of the Proposed Designs.

$$\begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1(2m+p)} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{2(2m+p)} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{(2m+p)1} & \rho_{(2m+p)2} & \cdots & \rho_{(2m+p)(2m+p)} \end{pmatrix},$$

where ρ_{ij} is the correlation coefficient between the ith and jth columns of the model matrix. $\rho_{\min} = \min_{i\neq j} |\rho_{ij}|$, $\rho_{\max} = \max_{i\neq j} |\rho_{ij}|$, and $\rho_{\text{ave}} = \sum_{i\neq j} |\rho_{ij}|/((2m+p)^2 - 2m - p)$. The values of $\rho_{\min}$, $\rho_{\max}$ and ρ_{ave} are listed in Appendix C. It is obvious to see that most values of ρ_{ave} are smaller than 0.1, and all the values of $\rho_{\min}$ are 0. Thus, only a few of the correlation coefficients are a little large, and most of them are rather small.

Recently, Jones and Nachtsheim (2013) proposed a new class of definitive screening designs with added two-level categorical factors (called DSD-augment designs and ORTH-augment designs). It is interesting to compare the design efficiencies (mainly based on *D*-efficiency here) between the proposed designs (with minimal point) and their designs (not of minimal point). The comparisons on *D*-efficiencies are given in Appendix D, because the *D*-efficiencies for the ORTH-augment designs are similar to that for the DSD-augment designs, only the *D*-efficiencies for the DSD-augment designs are listed there. The general observation from the comparisons is that the proposed designs are comparable with the DSD-augment designs in terms of the *D*-efficiency of the first-order and the pure-quadratic models. The proposed designs outperform the DSD-augment designs in some cases (in terms of the first-order *D*-efficiency).

4. Simulation Study

Two examples are given here to illustrate the analysis procedure. R software is used to generate the responses and analyze the data. An experiment with 6 two-level factors and 6 three-level factors is considered in the examples. The design is displayed in Table 3. It is a minimal-point design for the pure-quadratic model. As will be shown in Example 1, the analysis of the proposed design is straightforward if only the main effects of all factors and quadratic effects of three-level factors are active. A multiple regression model including main effects and pure-quadratic effects can be employed. However, when both two-factor interactions and pure-quadratic effects are active, the analysis becomes more challenging—some effects may be correlated. For example, Figure 3 displays the absolute values of the column correlations for the design shown in Table 3. Most of the second-order effects have nonzero correlations with each other for this design. This is inevitable, because the proposed design is a minimal-point design. Any

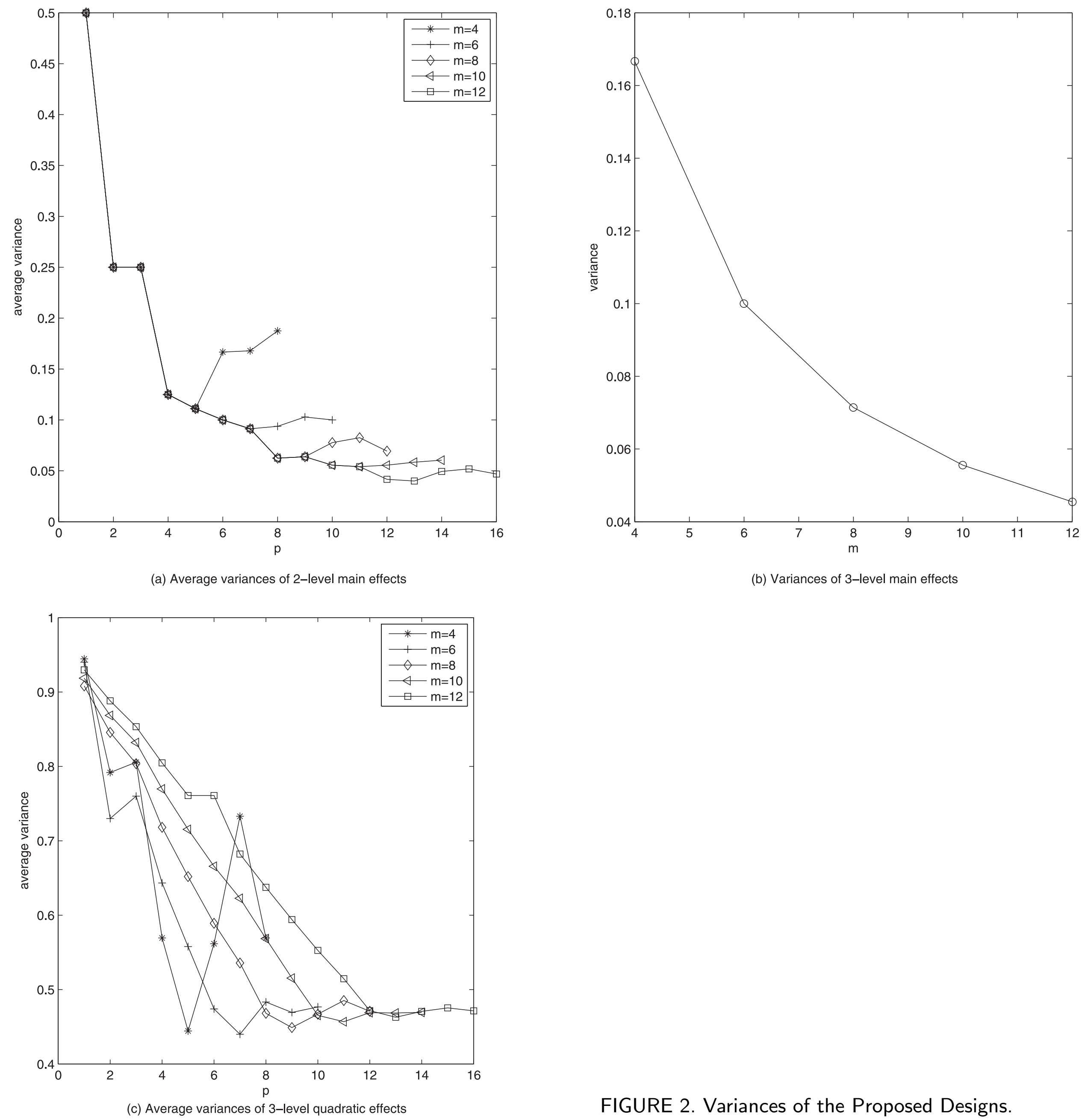

FIGURE 2. Variances of the Proposed Designs.

interaction effect has to be correlated with some main effects or pure-quadratic effects.

Example 1

In this example, only main effects and pure-quadratic effects are active. The underlying model is

$$y = \beta_0 + \sum_{i=1}^{6} \beta_i x_i + \sum_{i=1}^{6} \beta_{ii} x_i^2 + \sum_{i=1}^{6} \alpha_i z_i + \epsilon.$$

The random error is distributed as $N(0, 1)$. The design matrix is chosen as the design in Table 3. Two different models are considered.

I. Four active effects for which the coefficient vector is $\boldsymbol{\beta} = (\beta_0, \beta_k, \beta_{kk}, \alpha_q)^{\mathrm{T}} = (3, 5, -8,\ 10)^{\mathrm{T}}$, where k and q are randomly chosen from $\{1, \ldots, 6\}$;

II. Six active effects for which the coefficient vector is $\boldsymbol{\beta} = (\beta_0, \beta_{k_1}, \beta_{k_2}, \beta_{k_3}, \beta_{ll}, \alpha_q)^{\mathrm{T}} =$

TABLE 3. The Proposed Design and the Simulative Data

Run	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$	$\mathbf{x}_5$	$\mathbf{x}_6$	$\mathbf{z}_1$	$\mathbf{z}_2$	$\mathbf{z}_3$	$\mathbf{z}_4$	$\mathbf{z}_5$	$\mathbf{z}_6$	$\mathbf{y}$
1	0	1	1	1	1	1	1	−1	−1	−1	−1	−1	−9.93
2	1	0	1	1	−1	−1	−1	1	−1	−1	−1	−1	3.74
3	1	1	0	−1	−1	1	−1	−1	1	−1	−1	−1	−10.09
4	1	1	−1	0	1	−1	1	1	1	1	−1	−1	−2.78
5	1	−1	−1	1	0	1	1	1	1	−1	1	−1	−8.54
6	1	−1	1	−1	1	0	1	1	1	−1	−1	1	−5.49
7	0	0	0	0	0	0	1	1	1	1	1	1	19.58
8	0	−1	−1	−1	−1	−1	1	−1	−1	−1	−1	−1	−38.70
9	−1	0	−1	−1	1	1	−1	1	−1	−1	−1	−1	−8.09
10	−1	−1	0	1	1	−1	−1	−1	1	−1	−1	−1	−27.30
11	−1	−1	1	0	−1	1	1	1	1	1	−1	−1	−6.06
12	−1	1	1	−1	0	−1	1	1	1	−1	1	−1	20.40
13	−1	1	−1	1	−1	0	1	1	1	−1	−1	1	−2.63
14	0	1	1	1	1	1	−1	1	1	1	1	1	21.01
15	1	0	1	1	−1	−1	1	−1	1	1	1	1	12.26
16	1	1	0	−1	−1	1	1	1	−1	1	1	1	19.10
17	1	1	−1	0	1	−1	−1	−1	−1	−1	1	1	7.24
18	1	−1	−1	1	0	1	−1	−1	−1	1	−1	1	−35.18
19	1	−1	1	−1	1	0	−1	−1	−1	1	1	−1	2.42

$(-7, 18, -10, 12, 15, 4)^{\mathrm{T}}$, where k_1, k_2, k_3, and q are randomly chosen from $\{1, \ldots, 6\}$ and l is randomly chosen from $\{k_1, k_2, k_3\}$.

The coefficient of any inactive effect is zero. For each model, we perform 1000 simulations independently using the stepwise approach. The candidate terms for the stepwise procedure are $\{\beta_0, \beta_1, \ldots, \beta_6, \beta_{11}, \ldots, \beta_{66}, \alpha_1, \ldots, \alpha_6\}$.

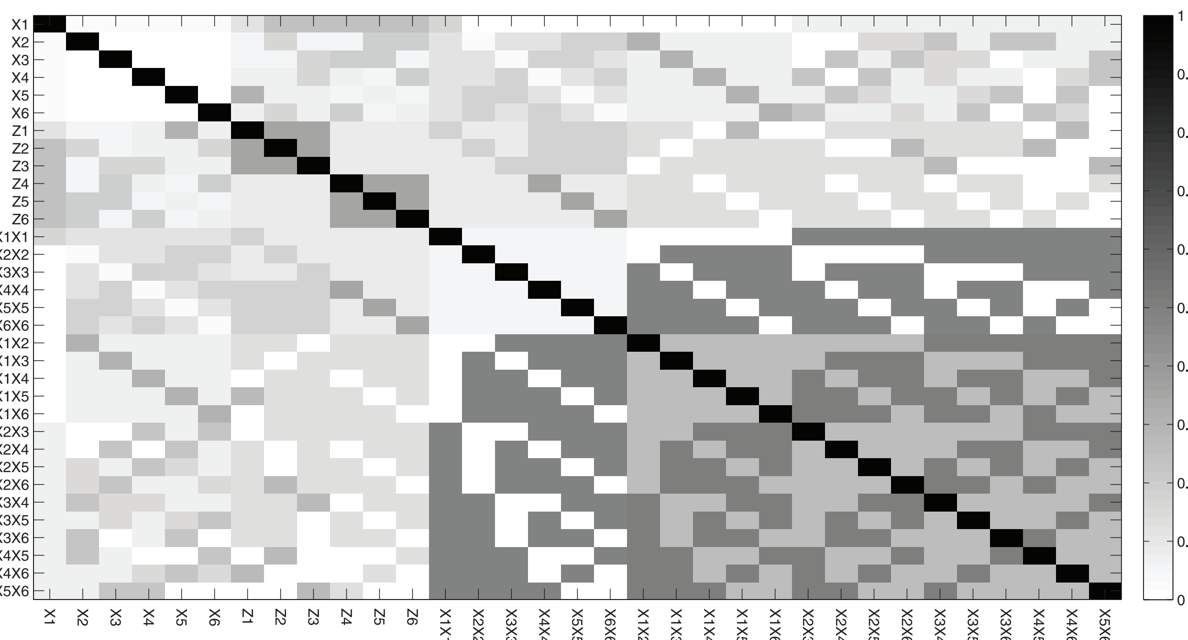

FIGURE 3. Absolute Correlation Map.

TABLE 4. Simulation Results of Example 1

Model	TMIR	SEIR	AEIR	IEIR	MFac
I	96.6%	100%	100%	0.39%	3.03
II	95.2%	100%	100%	0.78%	5.04

The simulation results are displayed in Table 4, where TMIR is the rate of the selected model that is the same as the true model, SEIR is the rate of the selected model that includes the true model, AEIR is the rate at which active effects are correctly identified, IEIR is the rate at which inactive effects are identified and MFac is the average of the number of the selected effects (the intercept is not included here). The TMIR is no less than 95%, SEIR and AEIR are all 100%. This indicates that all the active effects are selected into the model for all the simulations. The IEIR is no more than 0.8%. The design performs very well.

Example 2

In this example, besides main effects and pure-quadratic effects, one interaction effect is also assumed to be active. It is shown that our design/analysis works well with active interactions. Specifically, the response column y in Table 3 is generated by the model

$$y = 3 + 8x_2 + 6x_3 + 5z_2 + 10z_5 - 7x_2^2 - 4x_2x_3 + \epsilon,$$

where ϵ is distributed as $N(0, 1)$.

We perform Dantzig selector (Candes and Tao (2007)) to select effects considering all the main and pure-quadratic effects and interactions of two three-level factors and one three-level factor with one two-level factor. The result is shown in Table 5.

Then a multiple regression is adopted to estimate the coefficients for the selected variables. The result is listed in Table 6. It is obvious that x_2, x_3, z_2, z_5, x_2x_3, and x_2^2 are active. The analysis perfectly identifies the same active effects as the true model.

In general, we recommend first using a variable-selection strategy, such as the Dantzig selector for the analysis of these designs; then using multiple regression or a model-selection tool for the estimation. The Dantzig selector is used here, upon the suggestion of the editor; other methods, such as Lasso (Tibshirani (1996)), could be used as well. For Example 2 here, the results via Lasso are similar to the results presented in Table 6.

TABLE 5. Sequence of Dantzig Selector Moves

Variable	z_5	x_2	x_3	z_2	x_2x_2	x_4x_4	x_6x_6	x_2x_3
Step	1	2	3	4	5	6	7	8

TABLE 6. Estimates of the Coefficients

	Estimate	Std. error	t value	Pr(> $\|t\|$)	
(Intercept)	4.35	0.60	7.27	2.68e-05	***
x_2	8.02	0.16	49.07	2.98e-13	***
x_3	5.99	0.16	37.12	4.80e-12	***
z_2	5.40	0.15	36.90	5.08e-12	***
z_5	9.80	0.15	64.83	1.86e-14	***
x_2x_2	−6.87	0.34	−20.17	1.98e-09	***
x_4x_4	−1.58	0.42	−3.77	0.00364	**
x_6x_6	−0.11	0.42	−0.26	0.79797	
x_2x_3	−3.54	0.24	−14.55	4.69e-08	***

Note: Significance levels are coded as 0 (***) 0.001 (**) 0.01 (*) 0.05 (.) 0.1.

5. Conclusions

A new class of minimal-point designs for mixed two-level and three-level factors is presented. The proposed designs can be used to estimate the main effects of all factors and quadratic effects of three-level factors. These designs have minimal experimental points with good performance of D-efficiency and variance.

The maximal determinant matrices have been well developed. They can be found on the website http://www.indiana.edu/∼maxdet/. The method proposed in this paper only works when the number of three-level factors m is even (such that a conference matrix exists). When m is odd, we suggest using the $(m+1)$-order conference matrix without the last column. However, the number of runs will not be minimal in this case. For saturated cases, the designs in Jones and Nachtsheim (2011) are recommended to replace the conference matrices in the proposed designs. The conference matrix is a special class of weighing matrix (Raghavarao (1959)). A weighing matrix may be used to replace the conference matrix in the presented design and generate a design with desirable properties. This deserves further study.

Appendix A

D-Efficiencies of the Proposed Designs for $m = 4, 6, 8, 10, 12$ and $p = 0, 1, \ldots, m + 4$

m	p	$n = 2m + p + 1$	OA size	1st-order D-efficiency ratio (%)	Pure-quadratic D-efficiency ratio (%)
4	0	9	9	100.0 (0.7320/0.7320)	100.0 (0.4280/0.4280)
4	1	10	18	98.6 (0.7524/0.7631)	83.0 (0.3866/0.4659)
4	2	11	36	96.5 (0.7657/0.7932)	80.1 (0.3999/0.4994)
4	3	12	36	92.9 (0.7585/0.8165)	77.2 (0.4082/0.5291)
4	4	13	36	93.3 (0.7794/0.8351)	82.6 (0.4592/0.5557)
4	5	14	36	87.6 (0.7453/0.8503)	83.7 (0.4848/0.5795)
4	6	15	36	80.0 (0.6727/0.8629)	70.9 (0.4263/0.6010)
4	7	16	36	77.2 (0.6806/0.8736)	67.3 (0.4177/0.6204)
4	8	17	36	77.7 (0.6860/0.8827)	69.4 (0.4428/0.6381)
6	0	13	18	113.1 (0.7986/0.7064)	94.8 (0.3927/0.4142)
6	1	14	18	105.3 (0.7770/0.7378)	81.3 (0.3584/0.4411)
6	2	15	36	106.9 (0.8157/0.7631)	77.6 (0.3614/0.4659)
6	3	16	36	102.7 (0.8049/0.7841)	74.2 (0.3625/0.4887)
6	4	17	36	101.0 (0.8095/0.8016)	77.1 (0.3929/0.5097)
6	5	18	36	97.2 (0.7940/0.8165)	77.1 (0.4075/0.5291)
6	6	19	36	94.3 (0.7820/0.8293)	77.6 (0.4244/0.5472)
6	7	20	36	90.9 (0.7643/0.8405)	78.5 (0.4425/0.5639)
6	8	21	36	90.3 (0.7676/0.8503)	74.0 (0.4287/0.5795)
6	9	22	36	82.9 (0.7123/0.8589)	69.9 (0.4150/0.5941)
6	10	23	36	81.7 (0.7080/0.8667)	68.4 (0.4157/0.6077)
8	0	17	27	120.6 (0.8415/0.6974)	87.2 (0.3548/0.4071)
8	1	18	36	117.4 (0.8485/0.7230)	76.5 (0.3275/0.4280)
8	2	19	36	114.6 (0.8533/0.7446)	73.1 (0.3270/0.4475)
8	3	20	36	109.2 (0.8336/0.7631)	70.0 (0.3257/0.4659)
8	4	21	36	110.0 (0.8571/0.7792)	71.6 (0.3459/0.4831)
8	5	22	36	103.8 (0.8232/0.7932)	71.2 (0.3551/0.4994)
8	6	23	36	99.6 (0.8025/0.8055)	71.2 (0.3663/0.5147)
8	7	24	36	98.6 (0.8048/0.8165)	71.6 (0.3786/0.5291)
8	8	25	36	102.7 (0.8491/0.8263)	75.8 (0.4115/0.5428)
8	9	26	72	97.4 (0.8134/0.8351)	75.6 (0.4202/0.5557)
8	10	27	72	91.7 (0.7735/0.8431)	70.0 (0.3972/0.5679)
8	11	28	72	89.4 (0.7603/0.8503)	67.5 (0.3914/0.5795)
8	12	29	72	89.8 (0.7694/0.8569)	68.6 (0.4053/0.5905)
10	0	21	27	125.6 (0.8692/0.6917)	80.3 (0.3234/0.4028)
10	1	22	36	122.3 (0.8724/0.7133)	71.9 (0.3014/0.4193)
10	2	23	36	119.3 (0.8734/0.7321)	68.7 (0.2995/0.4359)
10	3	24	72	114.4 (0.8559/0.7485)	65.9 (0.2973/0.4513)
10	4	25	72	114.3 (0.8721/0.7631)	66.9 (0.3116/0.4659)
10	5	26	72	110.3 (0.8559/0.7761)	66.2 (0.3178/0.4798)
10	6	27	72	105.4 (0.8301/0.7878)	66.1 (0.3257/0.4930)
10	7	28	72	103.4 (0.8256/0.7983)	66.2 (0.3346/0.5056)
10	8	29	72	106.0 (0.8559/0.8078)	69.4 (0.3592/0.5176)

Appendix A *(continued)*

m	p	$n = 2m + p + 1$	OA size	1st-order D-efficiency ratio (%)	Pure-quadratic D-efficiency ratio (%)
10	9	30	72	101.5 (0.8284/0.8165)	69.1 (0.3656/0.5291)
10	10	31	72	101.5 (0.8367/0.8244)	70.5 (0.3806/0.5401)
10	11	32	72	98.9 (0.8226/0.8317)	71.7 (0.3913/0.5506)
10	12	33	72	98.1 (0.8228/0.8384)	68.7 (0.3853/0.5607)
10	13	34	72	94.4 (0.7974/0.8446)	66.9 (0.3815/0.5703)
10	14	35	72	91.2 (0.7758/0.8503)	65.3 (0.3784/0.5795)
12	0	25	27	129.2 (0.8887/0.6878)	74.5 (0.2980/0.3999)
12	1	26	54	125.8 (0.8904/0.7064)	72.0 (0.2798/0.4142)
12	2	27	72	123.3 (0.8914/0.7230)	64.8 (0.2774/0.4280)
12	3	28	72	118.2 (0.8721/0.7378)	62.3 (0.2748/0.4411)
12	4	29	72	118.6 (0.8908/0.7511)	62.9 (0.2855/0.4538)
12	5	30	72	113.8 (0.8687/0.7631)	62.2 (0.2898/0.4659)
12	6	31	72	111.1 (0.8599/0.7741)	62.0 (0.2956/0.4775)
12	7	32	72	108.2 (0.8487/0.7841)	61.9 (0.3023/0.4887)
12	8	33	72	109.9 (0.8717/0.7932)	64.4 (0.3214/0.4994)
12	9	34	72	104.9 (0.8412/0.8016)	64.1 (0.3264/0.5097)
12	10	35	72	104.6 (0.8465/0.8093)	65.1 (0.3381/0.5196)
12	11	36	72	103.7 (0.8468/0.8156)	65.5 (0.3465/0.5291)
12	12	37	72	107.3 (0.8828/0.8231)	68.6 (0.3684/0.5383)
12	13	38	72	103.9 (0.8620/0.8293)	69.1 (0.3781/0.5472)
12	14	39	72	98.5 (0.8222/0.8351)	65.1 (0.3613/0.5557)
12	15	40	72	96.0 (0.8067/0.8405)	63.6 (0.3587/0.5639)
12	16	41	72	96.1 (0.8119/0.8455)	64.2 (0.3674/0.5718)

Note: For $p = 0$, these are the designs from Xiao et al. (2012).

Appendix B
Proof of Theorem 1

The model matrix $\mathbf{X}_2$ has the following form:

$$\mathbf{X}_2 = \begin{pmatrix} \mathbf{1}_m & \mathbf{C} & \mathbf{C}\circ\mathbf{C} & \mathbf{H} \\ 1 & \mathbf{0}_m^{\mathrm{T}} & \mathbf{0}_m^{\mathrm{T}} & \mathbf{g}^{\mathrm{T}} \\ \mathbf{1}_m & -\mathbf{C} & \mathbf{C}\circ\mathbf{C} & \mathbf{H} \\ \mathbf{1}_p & \mathbf{A} & \mathbf{A}\circ\mathbf{A} & \mathbf{M} \end{pmatrix},$$

where $\circ$ denotes the element-wise product. From the structure of $\mathbf{X}_2$, assuming

$$\mathbf{X}_2^{-1} = \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \mathbf{Y}_3 & \mathbf{Y}_4 \\ \mathbf{Y}_5 & \mathbf{Y}_6 & \mathbf{Y}_7 & \mathbf{Y}_8 \\ \mathbf{Y}_9 & \mathbf{Y}_{10} & \mathbf{Y}_{11} & \mathbf{Y}_{12} \\ \mathbf{Y}_{13} & \mathbf{Y}_{14} & \mathbf{Y}_{15} & \mathbf{Y}_{16} \end{pmatrix},$$

where the sizes of the submatrices of $\mathbf{Y}_1$, $\mathbf{Y}_2$, $\mathbf{Y}_3$, and $\mathbf{Y}_4$ are $1\times m$, 1×1, $1\times m$, and $1\times p$, respectively; the sizes of $\mathbf{Y}_5$, $\mathbf{Y}_6$, $\mathbf{Y}_7$, and $\mathbf{Y}_8$ are $m\times m$, $m\times 1$, $m\times m$, and $m\times p$, respectively; the sizes of $\mathbf{Y}_9$, $\mathbf{Y}_{10}$, $\mathbf{Y}_{11}$, and $\mathbf{Y}_{12}$ are $m\times m$, $m\times 1$, $m\times m$, and $m\times p$, respectively; and the sizes of $\mathbf{Y}_{13}$, $\mathbf{Y}_{14}$, $\mathbf{Y}_{15}$, and $\mathbf{Y}_{16}$ are $p\times m$, $p\times 1$, $p\times m$, and $p\times p$, respectively. Due to the multiplication of submatrices, we can have

$$\begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \mathbf{Y}_3 & \mathbf{Y}_4 \\ \mathbf{Y}_9 & \mathbf{Y}_{10} & \mathbf{Y}_{11} & \mathbf{Y}_{12} \\ \mathbf{Y}_{13} & \mathbf{Y}_{14} & \mathbf{Y}_{15} & \mathbf{Y}_{16} \end{pmatrix}\mathbf{X}_2 = \begin{pmatrix} 1 & \mathbf{0}_m^{\mathrm{T}} & \mathbf{0}_m^{\mathrm{T}} & \mathbf{0}_p^{\mathrm{T}} \\ \mathbf{0}_m & \mathbf{0}_{m\times m} & \mathbf{1}_m & \mathbf{0}_{m\times p} \\ \mathbf{0}_p & \mathbf{0}_{p\times m} & \mathbf{0}_{p\times m} & \mathbf{1}_p \end{pmatrix},$$

where $\mathbf{0}_{m\times p}$ is a matrix with all elements zero; then because

$$\left(\frac{1}{2(m-1)}\mathbf{C}^{\mathrm{T}}, \mathbf{0}_m, -\frac{1}{2(m-1)}\mathbf{C}^{\mathrm{T}}, \mathbf{0}_{m\times p}\right)\mathbf{X}_2 = (\mathbf{0}_m, \mathbf{I}_m, \mathbf{0}_{m\times m}, \mathbf{0}_{m\times p}),$$

it can thus be deduced that

$$(\mathbf{Y}_5, \mathbf{Y}_6, \mathbf{Y}_7, \mathbf{Y}_8) = \left(\frac{1}{2(m-1)}\mathbf{C}^{\mathrm{T}}, \mathbf{0}_m, -\frac{1}{2(m-1)}\mathbf{C}^{\mathrm{T}}, \mathbf{0}_{m\times p}\right).$$

Let t_i denote the ith diagonal element of $(\mathbf{X}_2^{\mathrm{T}}\mathbf{X}_2)^{-1}$, $i = 1, \ldots, 2m+p+1$, then $\mathrm{Var}(\hat{\beta}_i) = t_{i+1}\sigma^2$, $i = 1, \ldots, m$. Denote

$$(\mathbf{X}_2^{\mathrm{T}}\mathbf{X}_2)^{-1} = \begin{pmatrix} \mathbf{Q}_{11} & \mathbf{Q}_{12} & \mathbf{Q}_{13} & \mathbf{Q}_{14} \\ \mathbf{Q}_{21} & \mathbf{Q}_{22} & \mathbf{Q}_{23} & \mathbf{Q}_{24} \\ \mathbf{Q}_{31} & \mathbf{Q}_{32} & \mathbf{Q}_{33} & \mathbf{Q}_{34} \\ \mathbf{Q}_{41} & \mathbf{Q}_{42} & \mathbf{Q}_{43} & \mathbf{Q}_{44} \end{pmatrix},$$

where the sizes of $\mathbf{Q}_{11}$, $\mathbf{Q}_{12}$, $\mathbf{Q}_{13}$, and $\mathbf{Q}_{14}$ are 1×1, $1\times m$, $1\times m$, and $1\times p$, respectively; the sizes of $\mathbf{Q}_{21}$, $\mathbf{Q}_{22}$, $\mathbf{Q}_{23}$, and $\mathbf{Q}_{24}$ are $m\times 1$, $m\times m$, $m\times m$, and $m\times p$, respectively; the sizes of $\mathbf{Q}_{31}$, $\mathbf{Q}_{32}$, $\mathbf{Q}_{33}$, and $\mathbf{Q}_{34}$ are $m\times 1$, $m\times m$, $m\times m$, and $m\times p$, respectively; and the sizes of $\mathbf{Q}_{41}$, $\mathbf{Q}_{42}$, $\mathbf{Q}_{43}$, and $\mathbf{Q}_{44}$ are $p\times 1$, $p\times m$, $p\times m$ and $p\times p$, respectively; then the diagonal elements of $\mathbf{Q}_{22}$ are t_{i+1}, $i = 1, \ldots, m$. From the form of $\mathbf{X}_2^{-1}$, we can get

$$\begin{pmatrix} \mathbf{Q}_{11} & \mathbf{Q}_{12} & \mathbf{Q}_{13} & \mathbf{Q}_{14} \\ \mathbf{Q}_{21} & \mathbf{Q}_{22} & \mathbf{Q}_{23} & \mathbf{Q}_{24} \\ \mathbf{Q}_{31} & \mathbf{Q}_{32} & \mathbf{Q}_{33} & \mathbf{Q}_{34} \\ \mathbf{Q}_{41} & \mathbf{Q}_{42} & \mathbf{Q}_{43} & \mathbf{Q}_{44} \end{pmatrix} = \begin{pmatrix} \mathbf{Y}_1 & \mathbf{Y}_2 & \mathbf{Y}_3 & \mathbf{Y}_4 \\ \mathbf{Y}_5 & \mathbf{Y}_6 & \mathbf{Y}_7 & \mathbf{Y}_8 \\ \mathbf{Y}_9 & \mathbf{Y}_{10} & \mathbf{Y}_{11} & \mathbf{Y}_{12} \\ \mathbf{Y}_{13} & \mathbf{Y}_{14} & \mathbf{Y}_{15} & \mathbf{Y}_{16} \end{pmatrix} \times \begin{pmatrix} \mathbf{Y}_1^{\mathrm{T}} & \mathbf{Y}_5^{\mathrm{T}} & \mathbf{Y}_9^{\mathrm{T}} & \mathbf{Y}_{13}^{\mathrm{T}} \\ \mathbf{Y}_2^{\mathrm{T}} & \mathbf{Y}_6^{\mathrm{T}} & \mathbf{Y}_{10}^{\mathrm{T}} & \mathbf{Y}_{14}^{\mathrm{T}} \\ \mathbf{Y}_3^{\mathrm{T}} & \mathbf{Y}_7^{\mathrm{T}} & \mathbf{Y}_{11}^{\mathrm{T}} & \mathbf{Y}_{15}^{\mathrm{T}} \\ \mathbf{Y}_4^{\mathrm{T}} & \mathbf{Y}_8^{\mathrm{T}} & \mathbf{Y}_{12}^{\mathrm{T}} & \mathbf{Y}_{16}^{\mathrm{T}} \end{pmatrix}.$$

Due to the multiplication of submatrices, it is obvious that

$$\mathbf{Q}_{22} = (\mathbf{Y}_5, \mathbf{Y}_6, \mathbf{Y}_7, \mathbf{Y}_8)(\mathbf{Y}_5, \mathbf{Y}_6, \mathbf{Y}_7, \mathbf{Y}_8)^{\mathrm{T}} = \left(\frac{1}{2(m-1)}\mathbf{C}^{\mathrm{T}}, \mathbf{0}_m, -\frac{1}{2(m-1)}\mathbf{C}^{\mathrm{T}}, \mathbf{0}_{m\times p}\right) \times \begin{pmatrix} \frac{1}{2(m-1)}\mathbf{C} \\ \mathbf{0}_m^{\mathrm{T}} \\ -\frac{1}{2(m-1)}\mathbf{C} \\ \mathbf{0}_{p\times m} \end{pmatrix} = \frac{1}{2(m-1)^2}\mathbf{C}^{\mathrm{T}}\mathbf{C} = \frac{1}{2(m-1)}\mathbf{I}_m.$$

So $t_{i+1} = 1/[2(m-1)]$, $i = 1, \ldots, m$; furthermore, $\mathrm{Var}(\hat{\beta}_i) = \sigma^2/[2(m-1)]$. □

Appendix C

The Correlation Coefficients of the Proposed Designs

m	p	$\rho_{\min}$	$\rho_{\max}$	ρ_{ave}	m	p	$\rho_{\min}$	$\rho_{\max}$	ρ_{ave}
4	1	0	0.65	0.10	10	1	0	0.36	0.08
4	2	0	0.55	0.13	10	2	0	0.37	0.08
4	3	0	0.48	0.13	10	3	0	0.41	0.09
4	4	0	0.36	0.12	10	4	0	0.41	0.09
4	5	0	0.37	0.12	10	5	0	0.31	0.10
4	6	0	0.72	0.16	10	6	0	0.53	0.10
4	7	0	0.75	0.16	10	7	0	0.56	0.10
4	8	0	0.61	0.11	10	8	0	0.37	0.09
6	1	0	0.32	0.08	10	9	0	0.43	0.09
6	2	0	0.47	0.10	10	10	0	0.33	0.09
6	3	0	0.42	0.11	10	11	0	0.31	0.09
6	4	0	0.43	0.10	10	12	0	0.24	0.09
6	5	0	0.44	0.10	10	13	0	0.32	0.09
6	6	0	0.35	0.11	10	14	0	0.31	0.09
6	7	0	0.50	0.11	12	1	0	0.36	0.07
6	8	0	0.40	0.11	12	2	0	0.37	0.08
6	9	0	0.45	0.12	12	3	0	0.32	0.09
6	10	0	0.45	0.13	12	4	0	0.37	0.09
8	1	0	0.44	0.08	12	5	0	0.33	0.09

Appendix C *(continued)*

m	p	$\rho_{\min}$	$\rho_{\max}$	ρ_{ave}	m	p	$\rho_{\min}$	$\rho_{\max}$	ρ_{ave}
8	2	0	0.45	0.09	12	6	0	0.35	0.09
8	3	0	0.46	0.10	12	7	0	0.50	0.09
8	4	0	0.39	0.10	12	8	0	0.31	0.09
8	5	0	0.43	0.11	12	9	0	0.39	0.10
8	6	0	0.47	0.10	12	10	0	0.35	0.09
8	7	0	0.50	0.10	12	11	0	0.33	0.08
8	8	0	0.46	0.08	12	12	0	0.26	0.07
8	9	0	0.58	0.09	12	13	0	0.31	0.08
8	10	0	0.41	0.10	12	14	0	0.28	0.09
8	11	0	0.43	0.10	12	15	0	0.40	0.09
8	12	0	0.35	0.10	12	16	0	0.46	0.08

Appendix D

Comparisons of *D*-Efficiencies Between the Proposed Designs and the DSD-Augment Designs

m	p	$n = 2m + p + 1$	DSD-augment size	1st-order *D*-efficiency ratio (%)	Pure-quadratic *D*-efficiency ratio (%)
4	1	10	14	96.1 (0.7524/0.7831)	88.2 (0.3866/0.4381)
4	2	11	14	97.4 (0.7657/0.7864)	86.4 (0.3999/0.4631)
4	3	12	18	90.4 (0.7585/0.8392)	86.6 (0.4082/0.4715)
4	4	13	18	92.7 (0.7794/0.8410)	93.0 (0.4592/0.4936)
6	1	14	18	95.0 (0.7770/0.8179)	92.8 (0.3584/0.3861)
6	2	15	18	98.8 (0.8157/0.8257)	88.6 (0.3614/0.4082)
6	3	16	22	93.7 (0.8049/0.8594)	88.8 (0.3625/0.4083)
6	4	17	22	94.4 (0.8095/0.8574)	92.2 (0.3929/0.4260)
8	1	18	22	100.5 (0.8485/0.8445)	94.5 (0.3275/0.3467)
8	2	19	22	100.4 (0.8533/0.8503)	89.6 (0.3270/0.3648)
8	3	20	26	94.7 (0.8336/0.8804)	89.3 (0.3257/0.3648)
8	4	21	26	96.9 (0.8571/0.8842)	90.7 (0.3459/0.3814)
10	1	22	26	100.9 (0.8724/0.8648)	95.3 (0.3014/0.3163)
10	2	23	26	100.5 (0.8734/0.8692)	90.4 (0.2995/0.3314)
10	3	24	30	96.5 (0.8559/0.8868)	90.2 (0.2973/0.3295)
10	4	25	30	98.6 (0.8721/0.8841)	91.1 (0.3116/0.3422)
12	1	26	30	101.1 (0.8904/0.8806)	95.8 (0.2798/0.2921)
12	2	27	30	101.1 (0.8914/0.8816)	91.1 (0.2774/0.3045)
12	3	28	34	96.7 (0.8721/0.9016)	90.4 (0.2748/0.3040)
12	4	29	34	98.5 (0.8908/0.9041)	90.3 (0.2855/0.3162)

Acknowledgments

We are most grateful to the Editor and two referees, whose sharply focused comments were extremely helpful. This work was supported by the National Natural Science Foundation of China (grant nos. 11271205 and 11101024), the Specialized Research Fund for the Doctoral Program of Higher Education of China (grant no. 20130031110002), and the "131" Talents Program of Tianjin.

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