Statistics and Probability Letters 208 (2024) 110079

Contents lists available at ScienceDirect

Statistics and Probability Letters

journal homepage: www.elsevier.com/locate/stapro

# Mixed-level screening designs based on skew-symmetric conference matrices

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ARTICLE INFO

*MSC:*
primary 62K15
secondary 62K05

*Keywords:*
Correlation
Definitive screening design
Fold-over
J-characteristic
Pure-quadratic effect

ABSTRACT

Screening is an important step of experimental design. It aims to identify a few active factors, among a large number of potential factors. In this paper, we propose two classes of mixed-level screening designs with desirable design properties; such as, low correlations between any two design columns, high design efficiencies (e.g., D- or A-efficiencies), and orthogonality between main effects and two-factor interactions. Conference matrices with skew-symmetric structure play an important role in the proposed construction. Two new construction methods for conference matrices with skew-symmetric structure, recursive and algebraic constructions, are provided. It is shown that the proposed mixed-level screening designs have all desirable design properties and do not require any computer search.

## 1. Introduction

Screening design aims to identify active factors from a large number of potential factors and is popularly used in industrial research; such as, bio-medical engineering, drug discovery (Dean and Lewis, 2006). Some machine learning algorithms also involve the issue of identifying active factors by fractional factorial designs (Rodrigues et al., 2021). For cost-saving, the run size of screening design is typically small. Conventionally, two-level fractional factorial designs with resolutions III (or IV) have been widely used for screening. However, designs of resolution III have their main effects and some two-factor interactions fully confounded, while designs of resolution IV (or higher) are rather expensive in terms of run size. Moreover, two-level design is not able to capture any curvature or any active pure-quadratic effects that may exist in the underlying true model.

Jones and Nachtsheim (2011) proposed a new class of three-level screening design, called definitive screening design, which provides the estimates of main effects that are unbiased by all second-order effects, and takes only twice as many runs of factors plus one. Numerical constructions on definitive screening designs have been studied in Jones and Nachtsheim (2011), Nguyen and Stylianou (2013) and Schoen et al. (2022). Xiao et al. (2012) provided a systematic construction of definitive screening designs using conference matrices. Moreover, Phoa and Lin (2015) proposed a theoretically driven approach to construct definitive screening designs. Blocking of definitive screening designs has also received widespread attention; see Jones and Nachtsheim (2016), Lin (2015) and Wang et al. (2016). Conference matrices play a prominent role in the construction of definitive screening designs. It is noteworthy that conference matrices can be substituted with alternative matrices, such as weight matrices; see Alhelali et al. (2020) and Georgiou et al. (2014). Moreover, definitive screening designs have other theoretical studies; see Liu et al. (2023), Schoen et al. (2019), and Wang et al. (2022).

The definitive screening designs by Jones and Nachtsheim (2011), however, can only accommodate three-level factors, although two-level categorical factors are rather common for screening problems. Jones and Nachtsheim (2013) presented a new type of design

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https://doi.org/10.1016/j.spl.2024.110079
Received 27 August 2023; Received in revised form 5 February 2024; Accepted 6 February 2024
Available online 10 February 2024
0167-7152/

including both two- and three-level factors, referred to mixed-level screening designs. The mixed-level screening designs proposed in Jones and Nachtsheim (2013) are generated by a searching algorithm to convert some three-level columns of a conference matrix to two-level columns under the D-optimal criterion. This algorithm requires the evaluation of the determinants of $2^{2m_2}$ information matrices (where $m_2$ is the number of two-level factors). Hence, this procedure will lead to a large amount of evaluation and typically obtain an inefficient design. Furthermore, the absolute correlation between any pair of two-level design columns of Jones and Nachtsheim (2013)'s designs may fail to reach the lower bound (see Proposition 1 below), and the correlation between two pure-quadratic effect columns is $1/2 - 1/(m-1)$, where $m$ is the run size of the conference matrix (this value tends to $1/2$ as run size tends to large).

To overcome the limitations of existing designs, two classes of mixed-level screening designs are proposed here (without using any computer search), called Type I and Type II designs. Compared with the designs found by Jones and Nachtsheim (2013), the proposed designs have the same first-order design efficiencies (see Table A.1) and other desired theoretical properties. The proposed designs match with the optimal designs found by Jones and Nachtsheim (2013), when $m$ is small. Moreover, the correlation between two pure-quadratic effects of Type II is in the order $O(1/m)$ (tends to 0 as run size tends to infinity). For large $m_2$, the searching algorithm of Jones and Nachtsheim (2013) may not be feasible, because it needs to calculate determinants of all $2^{2m_2}$ information matrices.

This paper is organized as follows. Section 2 reviews some preliminaries, including the construction method of Jones and Nachtsheim (2013). Section 3 provides a new class of conference matrices. Two types of mixed-level screening designs with high D- and A-efficiencies are generated by these conference matrices. Theoretical properties of the proposed designs are then discussed. Section 4 provides further results on the construction of skew-symmetric conference matrices and some discussions. All supplementary materials (including required tables and proofs) are provided in Appendix.

## 2. Preliminaries

Assume that the response follows the second-order model,

$$y = \beta_0 + \sum_{i=1}^{m_2+m_3} \beta_i x_i + \sum_{i=1}^{m_2+m_3-1} \sum_{j=i+1}^{m_2+m_3} \beta_{ij} x_i x_j + \sum_{i=1}^{m_3} \beta_{ii} x_i^2 + \epsilon, \tag{1}$$

where $y$ is the response variable; $x_1, x_2, \ldots, x_{m_3}$ are three-level factors; $x_{m_3+1}, x_{m_3+2}, \ldots, x_{m_3+m_2}$ are two-level factors; and $x_i x_j$ and $x_i^2$ are the interactions of factors and the pure-quadratic effects of three-level factors, respectively. $\beta_i$, $\beta_{ij}$ and $\beta_{ii}$ denote the unknown constant coefficients, and $\epsilon$ is the random error with zero mean and a finite variance $\sigma^2$. Our primary concern is screening, so we assume that the experimenter initially fits the (reduced) first-order model to the response, which can be written as

$$y = \beta_0 + \sum_{i=1}^{m_2+m_3} \beta_i x_i + \epsilon. \tag{2}$$

As previously mentioned, to ensure the orthogonality between main effects and two-factor interactions, fractional factorial designs with resolutions of at least IV are required. This involves a substantial large number of experimental runs. Hence, we utilize conference matrices and fold-over structures to construct screening designs, aiming to save resources and costs. We call a matrix $C = (c_{ij})_{m\times m}$ a conference matrix if it satisfies $C'C = (m-1)I_m$, with $c_{ii} = 0$ $(i = 1, 2, \ldots, m)$, and $c_{ij} \in \{-1, 1\}$ $(i \neq j,\ i, j = 1, 2, \ldots, m)$, where $I_m$ is an identity matrix of order $m$ (Xiao et al., 2012). Further, we call $C$ skew-symmetric if $C' = -C$. The construction of mixed-level screening design by Jones and Nachtsheim (2013) with $n = 2m+2$ runs involving $m_2$ two-level factors and $m_3$ three-level factors is summarized as follows.

**Construction 1** (*Jones and Nachtsheim's Construction Method, 2013*).
*Step 1. Let $m$ denote the size of the smallest conference matrix $C$ satisfying $m \geq m_2 + m_3$. Take the first $m_3 + m_2$ columns of $C$, and change the 0's in the last $m_2$ columns to 1's or $-1$'s. We denote the resulting matrix as $C^*$;*
*Step 2. Create*

$$D_{\mathrm{JN}} = \begin{pmatrix} C^* \\ -C^* \\ b' \\ -b' \end{pmatrix}, \tag{3}$$

*where $b = (b_1, \ldots, b_{m_3}, b_{m_3+1}, \ldots, b_{m_3+m_2})'$ with $b_i = 0$ for $i = 1, 2, \ldots, m_3$ and $b_i = 1$ or $-1$ for $i = m_3+1, m_3+2, \ldots, m_3+m_2$. Here, $D_{\mathrm{JN}}$ is a screening design with $m_3$ three-level factors (first $m_3$ columns) and $m_2$ two-level factors (last $m_2$ columns);*
*Step 3. There are $2^{m_2}$ choices of $C^*$ and $2^{m_2}$ choices of $b$; thus, there are $2^{2m_2}$ choices for $D_{JN}$. Take the optimal $D_{JN}$ under the D-optimal or A-optimal criteria.*

Conference matrices used in $D_{\mathrm{JN}}$ are given in Xiao et al. (2012) and Schoen et al. (2019). The optimal designs generated by Construction 1 can be obtained by a searching algorithm. However, such a searching is time consuming for large $m_2$. Here, the performances of a design are reported (mainly via D- and A-efficiencies). Specifically, $\mathrm{D}_{\mathrm{eff}} = |X'X|^{1/p}/n$ (Draper and Lin, 1990), and $\mathrm{A}_{\mathrm{eff}} = (p/n)\big/\mathrm{tr}(X'X)^{-1}$, where $X$ is the model matrix, $p$ is the number of parameters in the model, and $n$ is the run size of design. Note that if a matrix $X$ has only 0's and $\pm1$'s, we have $tr(X'X)^{-1} \geq p/n$.

Two constructions of mixed-level screening designs, via skew-symmetric conference matrices, are proposed. These two construction methods do not require computer search, and the resulting designs achieve the lower bound given in Propositions 1 and 2 below. Furthermore, these mixed-level screening designs have high D- and A-efficiencies.

**Proposition 1.** *For a $D_{JN}$ generated by Construction 1, the absolute correlation between two two-level design columns is greater than or equal to $1/(m+1)$.*

We use $J_2$ defined in Eq. (4) below, proposed by Deng and Tang (1999), to measure the correlations among the design columns of $D_{\mathrm{JN}} = (d_{ij})_{(2m+2)\times(m_3+m_2)}$, and a smaller $J_2$ value is preferred.

$$J_2(D_{\mathrm{JN}}) = \sum_{1\le j_1<j_2\le m_3+m_2} \left| \sum_{i=1}^{2m+2} d_{ij_1} d_{ij_2} \right| . \tag{4}$$

**Proposition 2.** *For a $D_{JN}$ generated by Construction 1, we have $J_2(D_{JN}) \ge 2m_2m_3 + m_2(m_2-1)$.*

## 3. Main results

### 3.1. Type I mixed-level screening designs

We first present the construction of skew-symmetric conference matrices. These matrices are the main components of mixed-level screening designs. The recursive construction steps of these conference matrices are as follows.

**Construction 2** (*Construction of Skew-Symmetric Conference Matrices*).

1. *For $k=1$, let*

$$O_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}; C_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix};$$

2. *For $k>1$, define $O_k$ and $C_k$ as*

$$O_k = \begin{pmatrix} O_{k-1} & O_{k-1} \\ O_{k-1} & -O_{k-1} \end{pmatrix}; C_k = \begin{pmatrix} C_{k-1} & O_{k-1} \\ -O_{k-1} & C_{k-1} \end{pmatrix}.$$

**Theorem 1.** *The $C_k$ obtained from Construction 2 is a $2^k \times 2^k$ skew-symmetric conference matrix.*

We next provide a construction method for mixed-level screening designs based on the newly proposed conference matrices in Theorem 1. The resulting designs are referred to as Type I mixed-level screening designs. The specific construction processes are as follows.

**Construction 3** (*Construction of Type I Mixed-Level Screening Designs*).

*Step 1. Let $m$ denote the size of the smallest skew-symmetric conference matrix $C$ satisfying $m \ge m_2+m_3$. Take the first $m_3+m_2$ columns of $C$, denoting $\widetilde{C}$, and change the 0's in the last $m_2$ columns of $\widetilde{C}$ to 1's. We denote the resulting matrix as $C^*$;*

*Step 2. Create*

$$D_{Type\ I} = \begin{pmatrix} C^* \\ -C^* \\ b' \\ -b' \end{pmatrix}, \tag{5}$$

*where* $b = (\underbrace{0,\dots,0}_{m_3},\underbrace{1,\dots,1}_{m_2})'$.

The above steps provide a convenient construction for mixed-level screening designs with $2m+2$ runs involving $m_2$ two-level factors and $m_3$ three-level factors, which do not need an algorithmic search. Next, the theoretical properties of the proposed designs are obtained below.

**Proposition 3.** *$D_{Type\ I}$ achieves the lower bounds displayed in Propositions 1 and 2.*

**Proposition 4.** *The correlation of $D_{Type\ I}$ between two three-level design columns is 0, and the correlation between a three-level design column and a two-level design column is $\pm 1/(m^2-1)^{1/2}$.*

Proposition 3 indicates that the absolute correlation between two two-level design columns and the $J_2$-characteristic for $D_{\text{Type I}}$ are less than or equal to that of $D_{\text{JN}}$. Additionally, Propositions 3 and 4 demonstrate that the correlations between two design columns in $D_{\text{Type I}}$ are either 0 or decrease to 0 as $m$ goes to infinity. These results guarantee that $D_{\text{Type I}}$ have high D-efficiencies and A-efficiencies.

**Theorem 2.** *For a $D_{Type\ I}$ generated by Construction 3, the first-order D-efficiency and the first-order A-efficiency have the following lower bounds, respectively,*

$$D_{\text{eff}}(\text{Type I}) \geq 1 - \frac{2}{m}; \tag{6}$$

$$A_{\text{eff}}(\text{Type I}) \geq 1 - \frac{6}{m+1}. \tag{7}$$

From (6) and (7), the lower bounds of the D- and A-efficiencies of $D_{\text{Type I}}$ tend to 1 as $m$ increases. Hence, $D_{\text{Type I}}$ achieves high estimation efficiencies with large $m$. Table A.1 (in Appendix) exhibits the first-order efficiencies for $D_{\text{Type I}}$ and $D_{\text{JN}}$ for different values $m_2$ and $m_3$ and some other columns to be explained later. The cases with $m_2 > 10$ are not provided, because these designs are computationally expensive for $D_{\text{JN}}$. From Table A.1, it can be seen that the efficiencies of $D_{\text{Type I}}$ and $D_{\text{JN}}$ are basically identical.

In summary, the construction of $D_{\text{Type I}}$ is straightforward (without any computer search). The correlation between two two-level design columns and the $J_2$ value for $D_{\text{Type I}}$ reach the lower bound. In addition, $D_{\text{Type I}}$ have excellent first-order D- and A-efficiencies.

### 3.2. Type II mixed-level screening designs

When exploring the response surface model, (1) is under consideration. The pure-quadratic effects determine the curve of the response surface in model (1). However, the correlations between two pure-quadratic effect columns are $1/2 - 1/(m-1)$ for both $D_{\text{Type I}}$ and $D_{\text{JN}}$ (for large $m$, this is about $1/2$). To reduce the correlation between two pure-quadratic effect columns, we introduce another type of mixed-level screening design, called Type II mixed-level screening designs, which have the following form

$$D_{\text{Type II}} = \begin{pmatrix} C^* \\ -C^* \end{pmatrix}, \tag{8}$$

where $C^*$ is defined in Construction 3. As a result of the fold-over structure, main effects are uncorrelated with both the two-factor interactions and the pure-quadratic effects. The following proposition provides the correlation between two pure-quadratic effect columns of $D_{\text{Type II}}$.

**Proposition 5.** *For a $D_{Type\ II}$ with $n = 2m$ runs involving $m_2$ two-level factors and $m_3$ three-level factors, the correlation between two pure-quadratic effect columns is $-1/(m-1)$.*

Proposition 5 shows that the correlation between two pure-quadratic effect columns approaches 0 as $m$ tends to infinity for $D_{\text{Type II}}$. This also implies that $D_{\text{Type II}}$ is able to estimate the pure-quadratic effects more accurately than $D_{\text{Type I}}$ and $D_{\text{JN}}$. The correlations for other cases are shown in Proposition 6 below.

**Proposition 6.** *For a $D_{Type\ II}$ with $n = 2m$ runs involving $m_2$ two-level factors and $m_3$ three-level factors,*

*(i) the correlation between two two-level design columns is 0;*
*(ii) the correlation between two three-level design columns is 0;*
*(iii) the correlation between a three-level design column and a two-level design column is $\pm 1/(m^2 - m)^{1/2}$.*

Proposition 6 implies that the correlations between any two design columns in $D_{\text{Type II}}$ are either 0 or decrease to 0 as $m$ tends to infinity.

**Proposition 7.** *Let $D^*_{JN}$ be the design by deleting the last two rows of $D_{JN}$ in Construction 1; then, $J_2(D^*_{JN}) \geq 2m_3m_2 = J_2(D_{Type\ II})$.*

Propositions 5–7 guarantee that $D_{\text{Type II}}$ have high D- and A-efficiencies, as presented in Theorem 3.

**Theorem 3.** *For a $D_{Type\ II}$ with $n = 2m$ runs involving $m_2$ two-level factors and $m_3$ three-level factors, the first-order D-efficiency and the first-order A-efficiency have the following lower bounds, respectively,*

$$D_{\text{eff}}(\text{Type II}) \geq 1 - \frac{1}{m-1}; \tag{9}$$

$$A_{\text{eff}}(\text{Type II}) \geq 1 - \frac{3}{m}. \tag{10}$$

Theorem 3 provides the lower bounds of the D- and A-efficiencies of $D_{\text{Type II}}$, which tends to 1 as $m$ increases. Table A.1 in Appendix further illustrates that $D_{\text{Type II}}$ have the highest first-order D-efficiencies and A-efficiencies compared to those of $D_{\text{Type I}}$ and $D_{\text{JN}}$.

## 4. Further results and discussion

Skew-symmetric conference matrices play a crucial role for two types of mixed-level screening designs. However, Construction 2 provides the skew-symmetric conference matrices of order $m = 2^k$ only. For $m \equiv 0 \pmod 4$ and $s = m - 1$ is a prime power, another construction for skew-symmetric conference matrices with order $m$ is proposed below.

Let $s$ be a prime power and $s \equiv 3 \pmod 4$, and let $\alpha_0 = 0, \alpha_1, \ldots, \alpha_{s-1}$ denote the elements of $GF(s)$. Define map $\chi$ on $GF(s)$ by

$$\chi(\beta) = \begin{cases} 1, & \text{if } \beta = \alpha^2 \text{ for some } \alpha \in GF(s), \\ 0, & \text{if } \beta = 0, \\ -1, & \text{otherwise.} \end{cases}$$

The map $\chi$ has been used for constructing the Paley conference matrix by Wang et al. (2022).

**Theorem 4.** *Suppose $m \equiv 0 \pmod 4$ and $s = m - 1$ is a prime power. Let $Q = (q_{ij})_{s \times s}$ with $q_{ij} = \chi(\alpha_i - \alpha_j)$, for $i, j = 0, \ldots, s-1$. Then,*

$$C_m = \begin{pmatrix} 0 & -\mathbf{1}_s' \\ \mathbf{1}_s & Q \end{pmatrix}$$

*is a skew-symmetric conference matrix of order $m$, where $\mathbf{1}_s$ is a column vector of $s$ ones.*

The orders of skew-symmetric conference matrices of order $m \le 100$ constructed by Theorem 4 are $m = 4$, 8, 12, 20, 24, 28, 32, 44, 48, 60, 68, 72, 80, 84. The mixed-level screening designs generated by these conference matrices have the same desired properties as those constructed in Construction 2. The generated designs have high D- and A-efficiencies; see Table A.1 in Appendix for cases $m = 12$ and $m = 20$.

In summary, two types of mixed-level screening designs are proposed. The proposed designs aim to achieve desirable properties, such as low correlations between design columns, high design efficiencies (D- or A-efficiencies), and orthogonality between main effects and two-factor interactions (as stated in the review comments). The correlation between two pure-quadratic effect columns approaches 0 as $m$ tends to infinity for $D_{\text{Type II}}$. This implies that $D_{\text{Type II}}$ provides more accurate estimates of pure-quadratic effects compared to $D_{\text{Type I}}$ and $D_{\text{JN}}$. Hence, if the pure-quadratic effect columns are under consideration, $D_{\text{Type II}}$ is preferred. In contrast to $D_{\text{JN}}$, both $D_{\text{Type I}}$ and $D_{\text{Type II}}$ are constructed without any computer search. This highlight has been repeatedly mentioned in the review comments. However, the run size of $D_{\text{Type I}}$ and $D_{\text{Type II}}$ are limited. The issues of how to construct a mixed-level orthogonal screening design with flexible runs is a subject of future work.

## Data availability

No data was used for the research described in the article.

## Acknowledgments

This research is supported by the National Natural Science Foundation of China (Nos. 12371259 and 11971098), the Fundamental Research Funds for the Central Universities, China (No. 2412023YQ003), the National Key Research and Development Program of China (Nos. 2020YFA0714102 and 2022YFA1003701) and the National Science Foundation, United States (Grant DMS-18102925).

## Appendix A. Comparison of the first-order efficiencies among $D_{\text{Type I}}$, $D_{\text{Type II}}$ and $D_{\text{JN}}$

See Table A.1.

## Appendix B. Proofs

To prove the conclusions, we need the following lemmas.

**Lemma 1.** *Let $A$ and $B$ be an $n \times n$ real symmetric matrix, and let $A_m$ be any principal submatrix of order $m$ of $A$. Then,*

*(i)*

$$\lambda_{\min}(A) \le \lambda(A_m) \le \lambda_{\max}(A),$$

*where $\lambda_{\max}(A)$ and $\lambda_{\min}(A)$ are the largest and smallest eigenvalues of $A$, respectively.*

*(ii)*

$$\lambda_{\min}(B) \le \lambda_i(A+B) - \lambda_i(A) \le \lambda_{\max}(B), \ i = 1, 2, \ldots, n,$$

*where $\lambda_i(\cdot)$ is the $i$th largest eigenvalue of the corresponding matrix.*
*Further, if both $A$ and $B$ are positive semidefinite matrices, then*

**Table A.1**
Comparison of the first-order efficiencies among $D_{\text{Type I}}$, $D_{\text{Type II}}$ and $D_{\text{JN}}$.

| $m$ | $m_2$ | $m_3$ | $D_{\text{Type II}}$ | | | $D_{\text{Type I}}$ | | | $D_{\text{JN}}$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Runs | $\text{D}_{\text{eff}}$ | $\text{A}_{\text{eff}}$ | Runs | $\text{D}_{\text{eff}}$ | $\text{A}_{\text{eff}}$ | Runs | $\text{D}_{\text{eff}}$ | $\text{A}_{\text{eff}}$ |
| 8 | 1 | 6 | 16 | 0.892 | 0.878 | 18 | 0.818 | 0.804 | 18 | 0.818 | 0.804 |
| 8 | 2 | 5 | 16 | 0.899 | 0.876 | 18 | 0.836 | 0.813 | 18 | 0.836 | 0.813 |
| 8 | 3 | 4 | 16 | 0.910 | 0.882 | 18 | 0.856 | 0.825 | 18 | 0.856 | 0.824 |
| 8 | 4 | 3 | 16 | 0.925 | 0.895 | 18 | 0.881 | 0.847 | 18 | 0.882 | 0.849 |
| 8 | 5 | 2 | 16 | 0.945 | 0.919 | 18 | 0.910 | 0.878 | 18 | 0.910 | 0.878 |
| 8 | 6 | 1 | 16 | 0.970 | 0.952 | 18 | 0.944 | 0.922 | 18 | 0.944 | 0.922 |
| 12 | 1 | 10 | 24 | 0.924 | 0.917 | 26 | 0.865 | 0.858 | 26 | 0.865 | 0.858 |
| 12 | 2 | 9 | 24 | 0.926 | 0.914 | 26 | 0.872 | 0.861 | 26 | 0.872 | 0.861 |
| 12 | 3 | 8 | 24 | 0.929 | 0.914 | 26 | 0.881 | 0.865 | 26 | 0.880 | 0.864 |
| 12 | 4 | 7 | 24 | 0.933 | 0.915 | 26 | 0.890 | 0.870 | 26 | 0.890 | 0.871 |
| 12 | 5 | 6 | 24 | 0.939 | 0.919 | 26 | 0.899 | 0.877 | 26 | 0.900 | 0.877 |
| 12 | 6 | 5 | 24 | 0.946 | 0.926 | 26 | 0.910 | 0.886 | 26 | 0.910 | 0.887 |
| 12 | 7 | 4 | 24 | 0.954 | 0.935 | 26 | 0.923 | 0.899 | 26 | 0.923 | 0.899 |
| 12 | 8 | 3 | 24 | 0.963 | 0.947 | 26 | 0.936 | 0.913 | 26 | 0.936 | 0.913 |
| 12 | 9 | 2 | 24 | 0.974 | 0.961 | 26 | 0.951 | 0.931 | 26 | 0.951 | 0.931 |
| 12 | 10 | 1 | 24 | 0.986 | 0.979 | 26 | 0.967 | 0.952 | 26 | 0.967 | 0.952 |
| 16 | 1 | 14 | 32 | 0.942 | 0.938 | 34 | 0.893 | 0.889 | 34 | 0.893 | 0.889 |
| 16 | 2 | 13 | 32 | 0.942 | 0.936 | 34 | 0.897 | 0.890 | 34 | 0.897 | 0.890 |
| 16 | 3 | 12 | 32 | 0.944 | 0.934 | 34 | 0.902 | 0.892 | 34 | 0.902 | 0.892 |
| 16 | 4 | 11 | 32 | 0.945 | 0.934 | 34 | 0.906 | 0.894 | 34 | 0.906 | 0.894 |
| 16 | 5 | 10 | 32 | 0.948 | 0.935 | 34 | 0.912 | 0.897 | 34 | 0.912 | 0.897 |
| 16 | 6 | 9 | 32 | 0.951 | 0.937 | 34 | 0.917 | 0.902 | 34 | 0.917 | 0.902 |
| 16 | 7 | 8 | 32 | 0.954 | 0.939 | 34 | 0.923 | 0.905 | 34 | 0.923 | 0.905 |
| 16 | 8 | 7 | 32 | 0.958 | 0.943 | 34 | 0.929 | 0.910 | 34 | 0.929 | 0.910 |
| 16 | 9 | 6 | 32 | 0.962 | 0.948 | 34 | 0.936 | 0.917 | 34 | 0.936 | 0.917 |
| 16 | 10 | 5 | 32 | 0.967 | 0.953 | 34 | 0.943 | 0.925 | 34 | 0.943 | 0.924 |
| 20 | 1 | 18 | 40 | 0.953 | 0.950 | 42 | 0.912 | 0.909 | 42 | 0.912 | 0.909 |
| 20 | 2 | 17 | 40 | 0.953 | 0.949 | 42 | 0.914 | 0.910 | 42 | 0.914 | 0.910 |
| 20 | 3 | 16 | 40 | 0.954 | 0.947 | 42 | 0.917 | 0.911 | 42 | 0.917 | 0.911 |
| 20 | 4 | 15 | 40 | 0.955 | 0.947 | 42 | 0.920 | 0.912 | 42 | 0.920 | 0.912 |
| 20 | 5 | 14 | 40 | 0.956 | 0.946 | 42 | 0.923 | 0.913 | 42 | 0.923 | 0.913 |
| 20 | 6 | 13 | 40 | 0.957 | 0.947 | 42 | 0.926 | 0.915 | 42 | 0.928 | 0.916 |
| 20 | 7 | 12 | 40 | 0.959 | 0.948 | 42 | 0.930 | 0.917 | 42 | 0.930 | 0.917 |
| 20 | 8 | 11 | 40 | 0.961 | 0.949 | 42 | 0.933 | 0.920 | 42 | 0.934 | 0.920 |
| 20 | 9 | 10 | 40 | 0.963 | 0.951 | 42 | 0.937 | 0.923 | 42 | 0.937 | 0.923 |
| 20 | 10 | 9 | 40 | 0.965 | 0.953 | 42 | 0.941 | 0.926 | 42 | 0.941 | 0.927 |

*(iii)*

$$|A+B| \geq |A| + |B|.$$

*(iv)*

$$0 \leq tr(AB) \leq \lambda_{\max}(A) \cdot tr(B).$$

*(v)* *if $A-B$ is positive semidefinite, then*

$$tr(A) \geq tr(B).$$

*(vi)* *if both $A$ and $B$ are positive definite, then*
*$A-B$ is positive semidefinite if and only if $B^{-1}-A^{-1}$ is positive semidefinite.*

**Lemma 2** (*Kantorovich-Type Inequality* Marshall et al., 2009). *If $0 < m \leq a_i \leq M$, $i = 1, 2, \ldots, n$, then*

$$\left(\frac{1}{n}\sum_{i=1}^{n} a_i\right)\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{a_i}\right) \leq \frac{(M+m)^2}{4mM}.$$

**Lemma 3.** *Let $(C_3, C_2)_{m\times(m_3+m_2)}$ be a submatrix of an $m \times m$ conference matrix $C$, and let $C_2^*$ be generated by changing 0's of $C_2$ to $\pm 1$'s. Then,*

*(i)* *all entries of $C_3' C_2^*$ are $\pm 1$'s, and*
*(ii)* *all nondiagonal elements of $C_2^{*\prime} C_2^*$ are 0's and $\pm 2$'s.*
*Further, if $C$ is skew-symmetric, and $C_2^*$ is generated by changing 0's of $C_2$ to 1's, then*

*(iii)* $(C + I_m)'(C + I_m) = mI_m$, *and*
*(iv)* $C_2^{*\prime} C_2^* = mI_{m_2}$.

**Lemma 4** (*Lemma 7.10 Hedayat et al., 1999*). *Let $s$ be a prime power, and $Q = (q_{ij})_{s\times s}$ with $q_{ij} = \chi(\alpha_i - \alpha_j)$, for $i, j = 0, 1, \ldots, s-1$, has the following properties:*

*(i)* *$Q$ is skew-symmetric if $s \equiv 3 (\mathrm{mod}\, 4)$;*
*(ii)* $QJ_s = J_sQ = \mathbf{0}$;
*(iii)* $QQ' = sI_s - J_s$;

*where $J_s$ is the $s \times s$ matrix of ones and $\mathbf{0}$ is a matrix of zeros.*

**Proofs of Proposition 1–Proposition 7.** For any matrix $D_{n\times m}$, $D'D = (\alpha_{ij})_{m\times m}$. Due to

$$J_2(D'D) = \sum_{1\le i<j\le m} |\alpha_{ij}|,$$

then Propositions 1–7 can be obtained by some tedious algebra based on Lemma 3. Therefore, we omit the detailed proofs.

**Proof of Theorem 1.** By Construction 2, we have $O_k'O_k = 2^k I_{2^k}$. Now we prove $C_k'O_k = O_k'C_k$ by induction as the preparation of the orthogonality of $C_k$. Clearly, $C_1'O_1 = O_1'C_1$. Suppose $C_a'O_a = O_a'C_a$ holds for $k = a$ and consider

$$C_{a+1}'O_{a+1} = \begin{pmatrix} C_a'O_a - O_a'O_a & C_a'O_a + O_a'O_a \\ C_a'O_a + O_a'O_a & O_a'O_a - C_a'O_a \end{pmatrix};$$

$$O_{a+1}'C_{a+1} = \begin{pmatrix} O_a'C_a - O_a'O_a & O_a'C_a + O_a'O_a \\ O_a'C_a + O_a'O_a & O_a'O_a - O_a'C_a \end{pmatrix}.$$

The result $C_k'O_k = O_k'C_k$ follows by induction.

Further, we have $C_1'C_1 = I_2$ and

$$\begin{aligned} C_k'C_k &= \begin{pmatrix} C_{k-1}' & -O_{k-1}' \\ O_{k-1}' & C_{k-1}' \end{pmatrix}\begin{pmatrix} C_{k-1} & O_{k-1} \\ -O_{k-1} & C_{k-1} \end{pmatrix} \\ &= \begin{pmatrix} C_{k-1}'C_{k-1} + O_{k-1}'O_{k-1} & \mathbf{0} \\ \mathbf{0} & C_{k-1}'C_{k-1} + O_{k-1}'O_{k-1} \end{pmatrix} \\ &= \begin{pmatrix} C_{k-1}'C_{k-1} + 2^{k-1}I_{2^{k-1}} & \mathbf{0} \\ \mathbf{0} & C_{k-1}'C_{k-1} + 2^{k-1}I_{2^{k-1}} \end{pmatrix}. \end{aligned}$$

Then, we have $C_k'C_k = (2^k - 1)I_{2^k}$ by induction. Continuing to use induction, we can obtain $C_k + C_k' = \mathbf{0}$, that is, $C_k$ is a skew-symmetric matrix. Therefore, we complete the proof.

**Proof of Theorem 2.** $D_{\text{Type I}}$ has $2m+2$ rows and $m_2 + m_3$ columns ($m_2 + m_3 \le m$), and its model matrix $X$ for the first-order model (2) can be expressed as

$$X = \begin{pmatrix} \mathbf{1}_m & C_3^* & C_2^* \\ \mathbf{1}_m & -C_3^* & -C_2^* \\ 1 & \mathbf{0}_{m_3}' & \mathbf{1}_{m_2}' \\ 1 & \mathbf{0}_{m_3}' & -\mathbf{1}_{m_2}' \end{pmatrix},$$

where $C^* = (C_3^*, C_2^*)$ is generated by Construction 3. Then, we have

$$\begin{aligned} X'X &= 2\begin{pmatrix} m+1 & \mathbf{0}_{m_3}' & \mathbf{0}_{m_2}' \\ \mathbf{0}_{m_3} & C_3^{*\prime}C_3^* & C_3^{*\prime}C_2^* \\ \mathbf{0}_{m_2} & C_2^{*\prime}C_3^* & C_2^{*\prime}C_2^* + J_{m_2} \end{pmatrix} \\ &= 2\begin{pmatrix} m+1 & \mathbf{0}_{m_3}' & \mathbf{0}_{m_2}' \\ \mathbf{0}_{m_3} & (m-1)I_{m_3} & C_3^{*\prime}C_2^* \\ \mathbf{0}_{m_2} & C_2^{*\prime}C_3^* & mI_{m_2} + J_{m_2} \end{pmatrix}. \end{aligned} \tag{B.1}$$

By calculation, we have

$$|X'X| = 2^{m_2+m_3+1}(m+1)(m-1)^{m_3}\left|mI_{m_2} + J_{m_2} - \frac{1}{m-1}C_2^{*\prime}C_3^*C_3^{*\prime}C_2^*\right|.$$

Let $G_1$ be the $m \times m_2$ matrix of the last $m_2$ columns of $\widetilde{C}$ in Construction 3; then, $C_2^*$ can be written as $C_2^* = G_1 + G_2$, where each column of $G_2$ consists of only one 1 and $m-1$ 0's. Based on the column orthogonality of the conference matrix, we have

$\frac{1}{m-1}C_2^{*\prime}C_3^*C_3^{*\prime}C_2^* = (G_1+G_2)'C_3^*(C_3^{*\prime}C_3^*)^{-1}C_3^{*\prime}(G_1+G_2) = G_2'C_3^*(C_3^{*\prime}C_3^*)^{-1}C_3^{*\prime}G_2$. Using Lemma 1(i), we obtain

$$\begin{aligned} 0 &= \lambda_{\min}\left(C_3^*\left(C_3^{*\prime}C_3^*\right)^{-1}C_3^{*\prime}\right) \\ &\le \lambda\left(\frac{1}{m-1}C_2^{*\prime}C_3^*C_3^{*\prime}C_2^*\right) \\ &\le \lambda_{\max}\left(C_3^*\left(C_3^{*\prime}C_3^*\right)^{-1}C_3^{*\prime}\right) = 1. \end{aligned} \tag{B.2}$$

Let $Q = mI_{m_2} - \frac{1}{m-1}C_2^{*\prime}C_3^*C_3^{*\prime}C_2^*$. Combining (B.2) and Lemma 1 (ii), we have $m-1 \le \lambda(Q) \le m$. By applying Lemma 1 (iii), we have

$$\begin{aligned} |X'X| &\ge 2^{m_2+m_3+1}(m+1)(m-1)^{m_3}\left(|Q| + \left|J_{m_2}\right|\right) \\ &\ge 2^{m_2+m_3+1}(m+1)(m-1)^{m_3}\,|Q|. \end{aligned}$$

By Lemma 2 and $tr\,(Q) = m_2\left(m - m_3/\,(m-1)\right)$, we have

$$|Q| = \prod_{i=1}^{m_2}\lambda_i(Q) \ge \left(\frac{m_2}{\frac{1}{\lambda_1(Q)} + \cdots + \frac{1}{\lambda_{m_2}(Q)}}\right)^{m_2} \ge \left(\frac{4m\left(m^2-m-m_3\right)}{(2m-1)^2}\right)^{m_2}. \tag{B.3}$$

Thus, we have

$$\begin{aligned} D_{\mathrm{eff}}(D_{\mathrm{Type\ I}}) &\ge \left(1 - \frac{2}{m+1}\right)^{\frac{m_3}{m_3+m_2+1}}\left(1 - \frac{4m^2-3m+4mm_3+1}{(m+1)(2m-1)^2}\right)^{\frac{m_2}{m_3+m_2+1}} \\ &\ge \left(1 - \frac{2}{m+1}\right)^{\frac{m_3}{m_3+m_2+1}}\left(1 - \frac{2}{m}\right)^{\frac{m_2}{m_3+m_2+1}} \\ &\ge 1 - \frac{2}{m}. \end{aligned}$$

Hence, we obtain the lower bound of the first-order D-efficiency for $D_{\mathrm{Type\ I}}$.

Next, we turn to the first-order A-efficiency for $D_{\mathrm{Type\ I}}$. From (B.1), we have

$$tr(X'X)^{-1} = 1/(2m+2) + 1/2 \cdot tr(A^{-1}), \tag{B.4}$$

where

$$\begin{aligned} A &= \begin{pmatrix} (m-1)\,I_{m_3} & C_3^{*\prime}C_2^* \\ C_2^{*\prime}C_3^* & mI_{m_2} + J_{m_2} \end{pmatrix}, \\ A^{-1} &= \begin{pmatrix} \frac{1}{m-1}I_{m_3} + \frac{1}{(m-1)^2}C_3^{*\prime}C_2^*B^{-1}C_2^{*\prime}C_3^* & * \\ * & B^{-1} \end{pmatrix}, \\ B &= Q + J_{m_2}. \end{aligned}$$

Then, we obtain

$$\begin{aligned} & tr\left(A^{-1}\right) \\ &= \frac{m_3}{m-1} + \frac{1}{(m-1)^2}\cdot tr\left(B^{-1}C_2^{*\prime}C_3^*C_3^{*\prime}C_2^*\right) + tr\left(B^{-1}\right) \\ &\le \frac{m_3}{m-1} + \frac{1}{(m-1)^2}\cdot tr\left(B^{-1}\right)\lambda_{\max}(C_2^{*\prime}C_3^*C_3^{*\prime}C_2^*) + tr\left(B^{-1}\right)\ \ (\text{Lemma 1 (iv)}) \\ &\le \frac{m_3}{m-1} + \frac{m}{m-1}\cdot tr\left(B^{-1}\right)\ (\text{refer to (B.2)}) \\ &\le \frac{m_3}{m-1} + \frac{m}{m-1}\cdot tr\left(Q^{-1}\right)\ \ (\text{Lemma 1 (v) and (vi)}) \\ &\le \frac{m_3}{m-1} + \frac{m_2(2m-1)^2}{4\,(m-1)\left(m^2-m-m_3\right)}\ \ (\text{refer to (B.3)}). \end{aligned} \tag{B.5}$$

Thus, we have

$$
\begin{aligned}
& A_{\mathrm{eff}}(\text{Type I}) \\
& \geq 1-\frac{\left(4 m_3+1\right) m_2+8\left(m^2-m-m_3\right) m_3 /(m-1)+2(2 m-1)^2 m_2 /(m-1)}{4\left(m^2-m-m_3\right)\left(1+m_3\left(1+\frac{2}{m-1}\right)\right)+(2 m-1)^2 m_2\left(1+\frac{2}{m-1}\right)} \\
& \geq 1-\frac{8 m_3 / m_2\left(m^2-m-m_3\right)+8 m^2-7 m+4 m m_3-4 m_3+1}{(m+1)(2 m-1)^2} \\
& \left(or \geq 1-\frac{8\left(m^2-m-m_3\right)+m_2 / m_3\left(8 m^2-7 m+4 m m_3-4 m_3+1\right)}{4\left(m^2-m-m_3\right)(m+1)}\right) \\
& \geq 1-\frac{6}{m+1} .
\end{aligned}
$$

Therefore, we complete the proof.

**Proof of Theorem 3.** $D_{\text{Type II}}$ has $2m$ rows and $m_2+m_3$ columns ($m_2+m_3 \leq m$), and its model matrix $X$ for the first-order model (2) can be expressed as

$$
X=\begin{pmatrix} \mathbf{1}_m & C_3^* & C_2^* \\ \mathbf{1}_m & -C_3^* & -C_2^* \end{pmatrix}.
$$

where $C^*=(C_3^*, C_2^*)$ is generated by Construction 3. Then, we have

$$
\begin{aligned}
X^{\prime} X & =2\begin{pmatrix} m & \mathbf{0}_{m_3}^{\prime} & \mathbf{0}_{m_2}^{\prime} \\ \mathbf{0}_{m_3} & C_3^{*\prime} C_3^* & C_3^{*\prime} C_2^* \\ \mathbf{0}_{m_2} & C_2^{*\prime} C_3^* & C_2^{*\prime} C_2^* \end{pmatrix} \\
& =2\begin{pmatrix} m & \mathbf{0}_{m_3}^{\prime} & \mathbf{0}_{m_2}^{\prime} \\ \mathbf{0}_{m_3} & (m-1) I_{m_3} & C_3^{*\prime} C_2^* \\ \mathbf{0}_{m_2} & C_2^{*\prime} C_3^* & m I_{m_2} \end{pmatrix} .
\end{aligned} \tag{B.6}
$$

By calculation, we have

$$
|X^{\prime} X| = 2^{m_2+m_3+1} m(m-1)^{m_3}\left|m I_{m_2}-\frac{1}{m-1} C_2^{*\prime} C_3^* C_3^{*\prime} C_2^*\right| .
$$

Employing $Q=m I_{m_2}-\frac{1}{m-1} C_2^{*\prime} C_3^* C_3^{*\prime} C_2^*$ and $|Q| \geq\left(\frac{4 m\left(m^2-m-m_3\right)}{(2 m-1)^2}\right)^{m_2}$, we have

$$
\begin{aligned}
D_{\mathrm{eff}}(D_{\text{Type II}}) & \geq\left(1-\frac{1}{m}\right)^{\frac{m_3}{m_3+m_2+1}}\left(1-\frac{4 m_3+1}{(2 m-1)^2}\right)^{\frac{m_2}{m_3+m_2+1}} \\
& \geq\left(1-\frac{1}{m}\right)^{\frac{m_3}{m_3+m_2+1}}\left(1-\frac{1}{m-1}\right)^{\frac{m_2}{m_3+m_2+1}} \\
& \geq 1-\frac{1}{m-1} .
\end{aligned}
$$

Therefore, we obtain the lower bound of the first-order D-efficiency for $D_{\text{Type II}}$.

Next, we discuss the first-order A-efficiency for $D_{\text{Type II}}$. By (B.6), we have

$$
tr(X^{\prime} X)^{-1}=1/(2\ m)+1/2 \cdot tr(A^{-1}),
$$

where

$$
A=\begin{pmatrix} (m-1) I_{m_3} & C_3^{*\prime} C_2^* \\ C_2^{*\prime} C_3^* & m I_{m_2} \end{pmatrix}, A^{-1}=\begin{pmatrix} \frac{1}{m-1} I_{m_3}+\frac{1}{(m-1)^2} C_3^{*\prime} C_2^* Q^{-1} C_2^{*\prime} C_3^* & * \\ * & Q^{-1} \end{pmatrix} .
$$

Then, similar to (B.5), we have

$$
tr\left(A^{-1}\right) \leq \frac{m_3}{m-1}+\frac{m_2(2 m-1)^2}{4(m-1)\left(m^2-m-m_3\right)} .
$$

Thus, we have

$$
\begin{aligned}
&A_{\mathrm{eff}}(\text{Type II}) \\
&\geq 1-\frac{4\left(m^2-m-m_3\right)m_3/(m-1)+m_2\left(4m_3+1+(2m-1)^2/(m-1)\right)}{4\left(m^2-m-m_3\right)\left(1+m_3\left(1+\frac{1}{m-1}\right)\right)+(2m-1)^2m_2\left(1+\frac{1}{m-1}\right)} \\
&\geq 1-\frac{4\left(m^2-m-m_3\right)m_3/m_2+4m^2-3m+4mm_3-4m_3}{m(2m-1)^2} \\
&\left(or \geq 1-\frac{4\left(m^2-m-m_3\right)+m_2/m_3\left(4m^2-3m+4mm_3-4m_3\right)}{4m\left(m^2-m-m_3\right)}\right) \\
&\geq 1-\frac{3}{m}.
\end{aligned}
$$

Therefore, we complete the proof.

**Proof of Theorem 4.** By Lemma 4 and some algebraic calculations, we can obtain Theorem 4 directly, so we omit the detailed proofs.

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