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Optimality of pairwise blocked definitive screening designs

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Abstract Definitive screening designs are a new class of three-level designs which are shown superior to the classical central composite designs in response surface methodology. They can be constructed by inserting conference matrices into their fold-over structures. How to block definitive screening designs in an optimal way is of practical importance, and lacks systematic theoretical research up to now. Pairwise blocking schemes are usually adopted which assign each pair of fold-over runs into the same block. In this paper, the optimality of such pairwise blocking schemes is thoroughly studied in theory. It is shown that under the linear model consisting of main effects, quadratic effects and block effects, pairwise blocked definitive screening designs are universally optimal for the main effects among all balanced blocking schemes. Moreover, such blocked designs are proved to have the same generalized wordlength pattern and are also shown optimal under the generalized minimum aberration criterion.

Keywords Blocking · Definitive screening design · Optimality · Generalized minimum aberration · Fold-over

1 Introduction

Jones and Nachtsheim (2011) proposed a new class of small three-level designs for definitive screening, called definitive screening designs (DSDs). Such designs possess many advantages for identifying both the main and quadratic effects. For example, the estimates of main effects are unbiased with quadratic effects and two-factor interactions, and all quadratic effects are estimable in models consisting of any number of

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main and quadratic effect terms. Later, Xiao et al. (2012) used the conference matrices to construct DSDs with orthogonal main effects, which was recommended by Jones and Nachtsheim (2013). Throughout, we focus on the DSDs constructed based on conference matrices.

Blocking, a fundamental technique in design of experiments, can effectively eliminate the effects of the nuisance variations. How to block DSDs in an optimal way is a problem of practical importance. Lin (2014b) considered all schemes that block a DSD into $2^q (q \geq 1)$ blocks of equal size, and selected the optimal one under the generalized minimum aberration criterion by an algorithm. From the results of computer search, he observed that the optimal blocking schemes follow a common rule, but provided no confirmation in theory. In this paper, the common rule is referred to as *pairwise blocking*. Pairwise blocking schemes assign each pair of fold-over runs in a DSD into the same block. A theoretical insight into these blocking schemes shows that pairwise blocked DSDs are universally optimal for the main effects among all balanced blocking schemes, under the linear model consisting of main effects, quadratic effects and block effects. Furthermore, we find that all pairwise blocked DSDs have the same treatment and block wordlength patterns, and are optimal under the generalized minimum aberration criterion with respect to a combined generalized wordlength pattern.

The rest of the paper is unfolded as follows. Section 2 gives the definition of pairwise blocking schemes for DSDs. Section 3 studies the optimality of pairwise blocked DSDs for estimating the main effects under the linear model consisting of main effects, quadratic effects and block effects. Section 4 shows that pairwise blocked DSDs are optimal under the generalized minimum aberration criterion with respect to a combined generalized wordlength pattern. Section 5 concludes this paper with some remarks.

2 Pairwise blocking schemes for DSDs

We first review the definition of conference matrices (Goethals and Seidel 1967). For a matrix $\mathbf{A}$, let $\mathbf{A}[i, :]$, $\mathbf{A}[:, j]$ and $\mathbf{A}[i, j]$ denote its ith row, jth column and (i, j)th entry, respectively. For an even number m, a conference matrix of order m, denoted by $\mathbf{C}_m$, is an $m \times m$ matrix with diagonal entries $\mathbf{C}_m[i, i] = 0$, $i = 1, \ldots, m$, and off-diagonal entries $\mathbf{C}_m[i, j] \in \{1, -1\}$, $i \neq j$, such that $\mathbf{C}_m^T \mathbf{C}_m = (m-1)\mathbf{I}_m$. Here $\mathbf{I}_m$ is the m-order identity matrix and $\mathbf{C}_m^T$ is the transpose of $\mathbf{C}_m$. Conference matrices can be algebraically constructed for $m = 0 \pmod 4$ and have been found by computer program when $m = 2, 6, 10, 14, 18, 26, 30, 38, 42, 46, 50, 54$ and so on. See Xiao et al. (2012) for details. Note that $\mathbf{C}_m^T \mathbf{C}_m = (m-1)\mathbf{I}_m$ implies $\mathbf{C}_m^{-1} = (m-1)^{-1}\mathbf{C}_m^T$. We have $\mathbf{C}_m \mathbf{C}_m^T = \mathbf{C}_m^T \mathbf{C}_m = (m-1)\mathbf{I}_m$.

Based on a conference matrix $\mathbf{C}_m$, a DSD for investigating m factors is constructed as

$$\mathbf{D} = \begin{pmatrix} \mathbf{C}_m \\ -\mathbf{C}_m \\ \mathbf{0}_{1\times m} \end{pmatrix}, \tag{1}$$

where $\mathbf{0}_{1\times m}$ is a $1 \times m$ matrix of zeros (Xiao et al. 2012). Each column of $\mathbf{D}$ represents a three-level factor and each row is an experimental run.

Suppose the number of blocks, k, divides m. Let $n = m/k$. We need to assign the runs of $\mathbf{D}$ into k blocks. A blocking scheme is called *balanced* if all blocks are of equal size.

For the similar arguments of Lin (2014b), throughout we only consider balanced blocking schemes in the following fashion. First divide the $2m$ nonzero runs of $\mathbf{D}$ into k blocks evenly and then add one zero run in each block. The resulting design, denoted by $\mathbf{D}^b$, is called a balanced blocked DSD and can be written as

$$\mathbf{D}^b = \left(\begin{array}{c:c} \mathbf{C}_m & \mathbf{b}_1 \\ -\mathbf{C}_m & \mathbf{b}_2 \\ \hdashline \mathbf{0}_{k\times m} & \mathbf{b}_0 \end{array}\right), \tag{2}$$

where the last column $(\mathbf{b}_1^T, \mathbf{b}_2^T, \mathbf{b}_0^T)^T$ represents the block factor. More specifically, $(\mathbf{b}_1^T, \mathbf{b}_2^T)^T$ consists of $2n$ 1's, $2n$ 2's, ..., $2n$ k's, and $\mathbf{b}_0 = (1, 2, \ldots, k)^T$. Any balanced blocking scheme for a DSD is uniquely determined by the vector $(\mathbf{b}_1^T, \mathbf{b}_2^T)$.

Since any DSD contains a fold-over structure $(\mathbf{C}_m^T, -\mathbf{C}_m^T)^T$, a natural way for blocking is to let each fold-over pair fall into the same block, i.e. $\mathbf{b}_1 = \mathbf{b}_2$. Such schemes are called *pairwise* blocking schemes and the corresponding $\mathbf{D}^b$'s are called pairwise blocked DSDs. From computer search, Lin (2014b) observed that pairwise blocked DSDs are optimal among all balanced blocking schemes when $k = 2^q\,(q \geq 1)$ under the generalized minimum aberration criterion. In the subsequence, the optimality of such blocked designs is thoroughly studied in theory.

Example 1 Suppose $m = 12$ and $k = 3$. The conference matrix $\mathbf{C}_{12}$ can be found in Appendix of Xiao et al. (2012), given by

$$\mathbf{C}_{12} = \begin{pmatrix}
0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & -1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 \\
1 & 1 & -1 & 0 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 0 & 1 & -1 & 1 & 1 & 1 & -1 & -1 \\
1 & 1 & 1 & -1 & -1 & 0 & 1 & 1 & -1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & 0 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & -1 & -1 & -1 & 0 & 1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 0 & 1 & 1 & -1 \\
1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 0 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 0
\end{pmatrix}.$$

Let $\mathbf{b}_0 = (1, 2, 3)^T$, $\mathbf{b}_1 = (1, 1, 1, 1, 2, 1, 1, 3, 3, 3, 3, 2)^T$ and $\mathbf{b}_2 = (2, 3, 2, 2, 1, 2, 2, 1, 3, 3, 2, 3)^T$. Then, the balanced blocked DSD constructed by (2) is not pairwise blocked. By letting $\mathbf{b}_1 = \mathbf{b}_2 = (1, 1, 1, 1, 2, 2, 2, 2, 3, 3, 3, 3)^T$, we get a pairwise blocked DSD. If we take $\mathbf{b}_1 = \mathbf{b}_2 = (1, 2, 3, 4, 2, 1, 4, 3, 3, 2, 1, 4)^T$, another pairwise blocked DSD is obtained. For ease of later use, the three blocked DSDs obtained above are denoted by $\mathbf{D}_1^b$, $\mathbf{D}_2^b$, $\mathbf{D}_3^b$, respectively.

3 Universal optimality of pairwise blocked DSDs

In this section, we discuss the optimality of the pairwise blocked DSDs for estimating the main effects. Consider the linear model

$$y_{ij} = \alpha_0 + \sum_{l=1}^{m} \alpha_l x_{ijl} + \sum_{l=1}^{m} \alpha_{ll} x_{ijl}^2 + \gamma_i + \epsilon_{ij}, \tag{3}$$

where x_{ijl} is the lth factor's value of the jth run in the ith block and y_{ij} is the corresponding response, $i = 1, \ldots, k$, $j = 1, \ldots, 2n + 1$ and $l = 1, \ldots, m$. Here α_0 is the intercept, α_l is the main effect of the lth factor, α_{ll} is the quadratic effect of the lth factor, γ_i is the effect of the ith block with the zero-sum constraint $\sum_{i=1}^{k} \gamma_i = 0$, and ϵ_{ij}'s are the i.i.d. errors with mean zero and variance σ^2. The blocked DSD in (2) is saturated for estimating the intercept, main effects, quadratic effects and block effects in the model.

For the design $\mathbf{D}^b$ in (2), Model (3) can be written in the matrix form

$$\mathbf{Y} = \mathbf{1}_{2m+k}\alpha_0 + \mathbf{X}_1\boldsymbol{\alpha}_1 + \mathbf{X}_2\boldsymbol{\alpha}_2 + \boldsymbol{\Gamma}\boldsymbol{\gamma} + \boldsymbol{\epsilon}, \tag{4}$$

where $\mathbf{Y}$ is the vector of $2m + k$ responses, $\mathbf{1}_{2m+k}$ is the vector of $2m + k$ ones, $\boldsymbol{\alpha}_1 = (\alpha_1, \ldots, \alpha_m)^T$, $\boldsymbol{\alpha}_2 = (\alpha_{11}, \ldots, \alpha_{mm})^T$ and $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_k)^T$. Let $\mathbf{Q}_m = -\mathbf{I}_m + \mathbf{J}_m$ with $\mathbf{J}_m = \mathbf{1}_m\mathbf{1}_m^T$. Denote $\mathbf{B}_1$ and $\mathbf{B}_2$ as the incidence matrices corresponding to $\mathbf{b}_1$ and $\mathbf{b}_2$ in (2), respectively. We have $\mathbf{X}_1 = (\mathbf{C}_m^T, -\mathbf{C}_m^T, \mathbf{0}_{m\times k})^T$, $\mathbf{X}_2 = (\mathbf{Q}_m^T, \mathbf{Q}_m^T, \mathbf{0}_{m\times k})^T$ and $\boldsymbol{\Gamma} = (\mathbf{B}_1^T, \mathbf{B}_2^T, \mathbf{I}_k)^T$. Finally, $\boldsymbol{\epsilon}$ is the vector of errors.

For estimating the parameters in (4), $\gamma_k = -\sum_{i=1}^{k-1} \gamma_i$ is substituted by the zero-sum constraint. Let $\tilde{\boldsymbol{\gamma}} = (\gamma_1, \ldots, \gamma_{k-1})^T$, $\widetilde{\mathbf{B}}_1 = \mathbf{B}_1(\mathbf{I}_{k-1}, -\mathbf{1}_{k-1})^T$, $\widetilde{\mathbf{B}}_2 = \mathbf{B}_2(\mathbf{I}_{k-1}, -\mathbf{1}_{k-1})^T$ and $\widetilde{\boldsymbol{\Gamma}} = \boldsymbol{\Gamma}(\mathbf{I}_{k-1}, -\mathbf{1}_{k-1})^T$. Then Model (4) reduces to an unconstrained model

$$\mathbf{Y} = \mathbf{1}_{2m+k}\alpha_0 + \mathbf{X}_1\boldsymbol{\alpha}_1 + \mathbf{X}_2\boldsymbol{\alpha}_2 + \widetilde{\boldsymbol{\Gamma}}\tilde{\boldsymbol{\gamma}} + \boldsymbol{\epsilon}. \tag{5}$$

It is apparent that $\mathbf{D}^b$ is pairwise blocked if and only if $\mathbf{B}_1 = \mathbf{B}_2$, or equivalently $\widetilde{\mathbf{B}}_1 = \widetilde{\mathbf{B}}_2$.

The Fisher's information matrix for $\boldsymbol{\alpha}_1$ in Model (4) is

$$\mathbf{M}_{\boldsymbol{\alpha}_1}(\mathbf{D}^b) = \mathbf{X}_1^T\mathbf{X}_1 - \mathbf{X}_1^T\mathbf{X}_{(-1)}\left(\mathbf{X}_{(-1)}^T\mathbf{X}_{(-1)}\right)^{-1}\mathbf{X}_{(-1)}^T\mathbf{X}_1, \tag{6}$$

where $\mathbf{X}_{(-1)} = (\mathbf{1}_{2m+k}, \mathbf{X}_2, \widetilde{\boldsymbol{\Gamma}})$.

The goal is to find the balanced blocked DSDs with maximum information matrix. According to Sect. 5.1 of Pukelsheim (1993), we shall try to find $\mathbf{D}^b$'s which maximize $\phi(\mathbf{M}_{\boldsymbol{\alpha}_1}(\mathbf{D}^b))$, where $\phi(\cdot)$ is an optimality function. Typically, an optimality function $\phi(\cdot)$ satisfies the following four conditions.

(i) Isotonic to the Loewner ordering: if $\mathbf{M}_1 \geq \mathbf{M}_2$, then $\phi(\mathbf{M}_1) \geq \phi(\mathbf{M}_2)$.
(ii) Concavity: $\phi((1-\lambda)\mathbf{M}_1 + \lambda\mathbf{M}_2) \geq (1-\lambda)\phi(\mathbf{M}_1) + \lambda\phi(\mathbf{M}_2)$ for any scalar $\lambda \in (0, 1)$.
(iii) Positive homogeneity: $\phi(\delta\mathbf{M}) = \delta\phi(\mathbf{M})$ for any scalar $\delta \geq 0$.

(iv) Permutation invariant: $\phi(\mathbf{PMP}^T) = \phi(\mathbf{M})$ for any permutation matrix $\mathbf{P}$.

Here a symmetric matrix $\mathbf{M} > 0$ means $\mathbf{M}$ is positive definite and $\mathbf{M} \geq 0$ means $\mathbf{M}$ is nonnegative definite. For two symmetric matrices $\mathbf{M}_1$ and $\mathbf{M}_2$, $\mathbf{M}_1 \geq \mathbf{M}_2$ means $\mathbf{M}_1 - \mathbf{M}_2 \geq 0$. The commonly used optimality functions include A, D, E and T-optimality functions. A design $\mathbf{D}^b_*$ is said to be ϕ-optimal if it achieves the maximum of $\phi(\mathbf{M}_{\boldsymbol{\alpha}_1}(\mathbf{D}^b))$ among all possible $\mathbf{D}^b$'s. It is *universally optimal* if it achieves the maximum of $\phi(\mathbf{M}_{\boldsymbol{\alpha}_1}(\mathbf{D}^b))$ for any ϕ.

In the following we will show the optimality of pairwise blocked DSDs for estimating the main effects $\boldsymbol{\alpha}_1$ in Model (4). We first give a simple but very useful lemma, whose proof is omitted.

Lemma 1 *If* $b \neq -\frac{a}{m}$, *we have* $(a\mathbf{I}_m + b\mathbf{J}_m)^{-1} = \frac{1}{a}\mathbf{I}_m - \frac{b}{a(a+mb)}\mathbf{J}_m$.

For estimating $\boldsymbol{\alpha}_1$, the theorem below shows that pairwise blocked DSDs are universally optimal among all balanced blocked DSDs and are the only universally optimal ones. The proof is given in Appendix.

Theorem 1 *Given m and k, the design* $\mathbf{D}^b$ *is universally optimal among all balanced blocked DSDs for estimating* $\boldsymbol{\alpha}_1$ *under Model* (4) *if and only if it is a pairwise blocked DSD.*

From the definition of $\mathbf{C}_m$, it is easy to see that the main effects are orthogonal to each other and all quadratic effects for any DSD in (1). It would be nice if the block factor would not affect the estimates of main effects either. The following result shows that only pairwise blocking schemes satisfy such requirement. Its proof is postponed in Appendix.

Proposition 1 *The main effects are orthogonal to block effects if and only if* $\mathbf{D}^b$ *is a pairwise blocked DSD.*

4 Minimum aberration of pairwise blocked DSDs

Besides universal optimality, the popular generalized minimum aberration criterion is considered in this section. The standard framework for finding optimal blocked factorial designs is using generalized minimum aberration criterion with respect to the split generalized wordlength pattern, i.e. treatment wordlength pattern and block wordlength pattern. Treatment factors are categorized into qualitative and quantitative factors. If treatment factors are qualitative, refer to Chen and Cheng (1999) and Ai and Zhang (2004) for details. If both qualitative and quantitative factors are involved, Lin (2014a) proposed a new split generalized wordlength pattern modified from the β wordlength pattern (Cheng and Ye 2004) to search for optimal blocked orthogonal arrays. Lin (2014b) used the same method to select optimal balanced blocking schemes for a DSD with $2^q (q \geq 1)$ blocks based on a combined generalized wordlength pattern. In this section, we will show that pairwise blocked DSDs have minimum aberration among all balanced blocked DSDs with respect to the combined generalized wordlength pattern.

First we briefly review the combined generalized wordlength pattern defined in Lin (2014b). Let $F_1, \ldots, F_m$ denote the m three-level quantitative factors in a balanced blocked DSD $\mathbf{D}^b$ and F_{m+1} denote the block factor with k blocks. Recall that k divides m and $n = m/k$. For convenience of presentation, recode the levels of F_i as $-1 \to 0, 0 \to 1$ and $1 \to 2$, for $i = 1, \ldots, m$. Recode the levels of F_{m+1} as $1 \to 0, 2 \to 1, \ldots, k \to k-1$. Define $\mathcal{T}_0 = \{0, 1, 2\}^m$, $\mathcal{T}_1 = \{0, 1, \ldots, k-1\}$, and $\mathcal{T} = \mathcal{T}_0 \times \mathcal{T}_1$.

For each factor F_i with s_i levels, let $C_0^i(x), C_1^i(x), \ldots, C_{s_i-1}^i(x)$ be the orthogonal polynomial contrasts satisfying

$$\sum_{x \in \{0,1,\ldots,s_i-1\}} C_u^i(x) C_v^i(x) = \begin{cases} 0 & \text{if } u \neq v, \\ s_i & \text{if } u = v, \end{cases}$$

where $C_j^i(x)$ is a polynomial of degree j for $j = 0, 1, \ldots, s_i - 1$. In particular, for the three-level factors F_i, $1 \leq i \leq m$, we have $C_0^i(x) = 1$, $C_1^i(x) = \sqrt{3/2}(x-1)$ and $C_2^i(x) = 3\sqrt{2}/2(x-1)^2 - \sqrt{2}$. For each run $\mathbf{x} = (x_1, \ldots, x_{m+1})$ of $\mathbf{D}^b$ and any $\mathbf{t} = (t_1, \ldots, t_{m+1}) \in \mathcal{T}$, define $C_{\mathbf{t}}(\mathbf{x}) = \prod_{i=1}^{m+1} C_{t_i}^i(x_i)$. Then the indicator function of $\mathbf{D}^b$ is

$$F_{\mathbf{D}^b}(\mathbf{x}) = \sum_{\mathbf{t} \in \mathcal{T}} b_{\mathbf{t}} C_{\mathbf{t}}(\mathbf{x}), \tag{7}$$

where the coefficient of $C_{\mathbf{t}}$ is uniquely determined by

$$b_{\mathbf{t}} = \frac{1}{k3^m} \sum_{\mathbf{x} \in \mathbf{D}^b} C_{\mathbf{t}}(\mathbf{x}). \tag{8}$$

Especially, we have $b_{\mathbf{0}} = (k3^m)^{-1}(2m+k)$.

If $b_{\mathbf{t}} \neq 0$, then $\mathbf{t} = (t_1, \ldots, t_{m+1})$ is called a word. A word $\mathbf{t}$ is said to be a pure-type word if $t_{m+1} = 0$. Otherwise $\mathbf{t}$ is a mixed-type word. Denote by w_t the set of all pure-type words and w_b the set of all mixed-type words. Define $\|\mathbf{t}\| = \sum_{i=1}^m t_i$, the sum of the first m elements in $\mathbf{t}$. The treatment wordlength pattern W_t and the block wordlength pattern W_b are given as follows.

$$W_t = (\beta_{1,0}, \beta_{2,0}, \ldots, \beta_{2m,0}), \text{ where } \beta_{i,0} = \sum_{\mathbf{t} \in w_t, \|\mathbf{t}\| = i} \left(\frac{b_{\mathbf{t}}}{b_{\mathbf{0}}}\right)^2, \tag{9}$$

$$W_b = (\beta_{1,1}, \beta_{2,1}, \ldots, \beta_{2m,1}), \text{ where } \beta_{i,1} = \sum_{\mathbf{t} \in w_b, \|\mathbf{t}\| = i} \left(\frac{b_{\mathbf{t}}}{b_{\mathbf{0}}}\right)^2. \tag{10}$$

The combined wordlength pattern is defined as

$$W = (\beta_{1,0}, \beta_{1,1}, \beta_{2,0}, \beta_{3,0}, \beta_{2,1}, \beta_{4,0}, \ldots), \tag{11}$$

where $\beta_{i,1}$ is between $\beta_{2i-1,0}$ and $\beta_{2i,0}$ for $i \leq m$ and $\beta_{i,1}$ is before $\beta_{i+1,1}$ for $i \geq m+1$. The order of components in (11) is determined by comparing the importance of $\beta_{i,1}$, $\beta_{2i-1,0}$ and $\beta_{2i,0}$. Among the three, $\beta_{2i-1,0}$ is the most important because $\beta_{2i-1,0} \neq 0$ could result in the aliasing between $(i-1)$-order effects and i-order effects. Since the aliasing between treatment effects (resulting in $\beta_{2i,0} > 0$) can be de-aliased through a follow-up design, but the confounding between treatment effects and block effects (resulting $\beta_{i,1} > 0$) cannot be de-confounded, $\beta_{i,1}$ is considered more important than $\beta_{2i,0}$. The generalized minimum aberration criterion is to find the balanced blocked DSDs which sequentially minimize the components in the combined wordlength pattern W.

Let $\mathbf{Z}_b$ be the $(2m+k) \times (k-1)$ matrix whose columns are labeled by all nonzero elements of $\mathcal{T}_1$ and the column labeled by $t_{m+1} \in \mathcal{T}_1$ is

$$\left(C_{t_{m+1}}^{m+1}(\mathbf{D}^b[1, m+1]), \ldots, C_{t_{m+1}}^{m+1}(\mathbf{D}^b[2m+k, m+1])\right)^T.$$

For any $\mathbf{t} \in \mathcal{T}_0$, we also denote $\|\mathbf{t}\| = \sum_{i=1}^m t_i$. For $j = 1, \ldots, 2m$, let $\mathbf{Z}_j$ be the $(2m+k) \times \sum_{l=0}^{\lfloor j/2 \rfloor} \binom{m}{l}\binom{m-l}{j-2l}$ matrix whose columns are labeled by all elements of the set $\{\mathbf{t} \in \mathcal{T}_0 : \|\mathbf{t}\| = j\}$ and the column labeled by $\mathbf{t} = (t_1, \ldots, t_m)$ is

$$\left(\prod_{i=1}^m C_{t_i}^i(\mathbf{D}^b[1, i]), \ldots, \prod_{i=1}^m C_{t_i}^i(\mathbf{D}^b[2m+k, i])\right)^T,$$

where $\lfloor x \rfloor$ is the largest integer not exceeding x. From (8)–(10) and the definitions of $\mathbf{Z}_j$ and $\mathbf{Z}_b$, the following lemma can be obtained directly.

Lemma 2 *For a balanced blocked DSD $\mathbf{D}^b$, we have*

$$\beta_{j,0}(\mathbf{D}^b) = (2m+k)^{-2}\mathrm{tr}\,(\mathbf{Z}_j^T \mathbf{1}_{2m+k}\mathbf{1}_{2m+k}^T \mathbf{Z}_j), \quad (12)$$

$$\beta_{j,1}(\mathbf{D}^b) = (2m+k)^{-2}\mathrm{tr}\,(\mathbf{Z}_j^T \mathbf{Z}_b \mathbf{Z}_b^T \mathbf{Z}_j), \quad (13)$$

where $\mathrm{tr}(\mathbf{A})$ *is the trace of a matrix* $\mathbf{A}$.

From Lemma 2, it is clear that once a DSD $\mathbf{D}$ and the number of blocks k are given, all balanced blocking schemes have the same treatment wordlength pattern W_t, since $\mathbf{Z}_j$ depends only on the first m columns of $\mathbf{D}^b$. Furthermore, we find that W_t is constant for all possible $\mathbf{C}_m$'s used in $\mathbf{D}^b$, when m and k are fixed. See the following lemma, whose proof is given in Appendix.

Lemma 3 *Given m and k, the treatment wordlength pattern W_t in (9) is independent of the choice of $\mathbf{C}_m$ used in $\mathbf{D}^b$. Especially, we have $\beta_{i,0}(\mathbf{D}^b) = 0$ for odd i and $\beta_{2,0}(\mathbf{D}^b) = (2m+k)^{-2}2m(k-m+3)^2$.*

Now to find the optimal balanced blocked DSDs under the generalized minimum aberration criterion with respect to the combined wordlength pattern W in (11), we need only to find the balanced blocked DSDs which sequentially minimize the block wordlength pattern W_b. We shall show that for given m and k, among all balanced blocked DSDs, the pairwise blocked DSDs are optimal. For any two balanced blocked designs $\mathbf{D}^b$ and $\mathbf{D}_*^b$, $\mathbf{D}_*^b$ is said to have less aberration than $\mathbf{D}^b$ with respect to W_b, if $\beta_{r,1}(\mathbf{D}_*^b) < \beta_{r,1}(\mathbf{D}^b)$, where r is the smallest integer such that $\beta_{r,1}(\mathbf{D}_*^b) \neq \beta_{r,1}(\mathbf{D}^b)$.

We first show that pairwise blocked DSDs are superior than those not pairwise blocked by comparing their $\beta_{1,1}$'s.

Theorem 2 $\beta_{1,1}(\mathbf{D}^b) = 0$ *if and only if* $\mathbf{D}^b$ *is a pairwise blocked DSD.*

The Proof of Theorem 2 is postponed in Appendix. It shows that any pairwise blocked DSD has less aberration than those not pairwise blocked with respect to W_b. Moreover, we find that for any two different pairwise blocked DSDs $\mathbf{D}^b$ and $\widetilde{\mathbf{D}}^b$, their block wordlength patterns are the same. A detailed proof of the following is given in Appendix.

Theorem 3 *For given* m *and* k*, all pairwise blocked DSDs share the same block wordlength pattern* W_b *in* (10)*. Especially, we have* $\beta_{i,1} = 0$ *for odd* i*.*

According to Theorem 3, there is no difference between any two pairwise blocked DSDs in the sense of generalized minimum aberration criterion when m and k are given. By Lemma 3, Theorems 2 and 3, we obtain that pairwise blocked DSDs are the only optimal balanced blocked DSDs under the generalized minimum aberration with respect to the combined wordlength pattern W in (11).

Theorem 4 *A balanced blocked DSD is optimal under the generalized minimum aberration criterion with respect to the combined wordlength pattern* W *in* (11) *if and only if it is a pairwise blocked DSD.*

Example 2 (Example 1 continued). Consider the treatment and block wordlength patterns of the three balanced blocked DSDs $\mathbf{D}_1^b$, $\mathbf{D}_2^b$ and $\mathbf{D}_3^b$ in Example 1. They share the same $W_t = (0, 1.185, 0, 196.370, \ldots)$. For $\mathbf{D}_1^b$, we have $\beta_{1,1}(\mathbf{D}_1^b) = 1.358 > 0$. Contrarily, the two pairwise blocked DSDs, $\mathbf{D}_2^b$ and $\mathbf{D}_3^b$, enjoy the same $W_b = (0, 18.370, 0, 325.185, \ldots)$.

5 Concluding remarks

In this paper, we investigate the optimality of a special class of balanced blocked DSDs, called pairwise blocked DSDs. Different from Lin (2014b), the number of blocks k here can be any divisor of m. Two optimality criteria are considered. We show that under Model (4), only pairwise blocked DSDs are universally optimal for estimating the main effects. Moreover, with respect to the combined wordlength pattern W, pairwise blocked DSDs are the only generalized minimum aberration balanced blocked DSDs. Note that our conclusion takes not only different balanced blocking schemes, but also different choices of $\mathbf{C}_m$, into consideration.

For estimating all parameters under Model (4), pairwise blocked DSDs are not universally optimal and we have tried other optimality criteria. It can be proved that, given m and k, all balanced blocked DSDs are common in the sense of D-optimality. For A, E and T-optimality, some examples show that pairwise blocked DSDs are not always optimal.

Although pairwise blocked DSDs are proved to be equivalent optimal for estimating the main effects or under the generalized minimum aberration criterion, they still have many possibilities. It is worth to distinguish the pairwise blocked DSDs under some criteria stricter and find the optimal ones.

Since a conference matrix is a special case of a weighing matrix, Georgiou et al. (2013) replaced the conference matrix in the DSD with a weighing matrix to construct efficient screening designs. Note that for any design with a fold-over structure, pairwise blocking schemes can always be defined. So it is possible to generalize the results of this paper to those weighing matrix-based screening designs and we leave it for a future work.

Appendix

Proof of Theorem 1 Note that $\mathbf{C}_m^T\mathbf{C}_m = \mathbf{C}_m\mathbf{C}_m^T = (m-1)\mathbf{I}_m$, $\mathbf{Q}_m^T\mathbf{Q}_m = \mathbf{I}_m + (m-2)\mathbf{J}_m$, $\mathbf{J}_m^T(\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2) = \mathbf{0}_{m\times(k-1)}$, $\widetilde{\mathbf{\Gamma}}^T\widetilde{\mathbf{\Gamma}} = (2n+1)(\mathbf{I}_{k-1} + \mathbf{J}_{k-1})$, $\widetilde{\mathbf{B}}_1^T\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2^T\widetilde{\mathbf{B}}_2 = 2n(\mathbf{I}_{k-1} + \mathbf{J}_{k-1})$. From (6), we have

$$
\begin{aligned}
\mathbf{M}_{\boldsymbol{\alpha}_1}(\mathbf{D}^b) &= \mathbf{X}_1^T\mathbf{X}_1 - \mathbf{X}_1^T\mathbf{X}_{(-1)}\left(\mathbf{X}_{(-1)}^T\mathbf{X}_{(-1)}\right)^{-1}\mathbf{X}_{(-1)}^T\mathbf{X}_1 \\
&= 2\mathbf{C}_m^T\mathbf{C}_m - \left(\mathbf{0}_{m\times 1}, \mathbf{0}_{m\times m}, \mathbf{C}_m^T(\widetilde{\mathbf{B}}_1 - \widetilde{\mathbf{B}}_2)\right)\left(\mathbf{X}_{(-1)}^T\mathbf{X}_{(-1)}\right)^{-1} \\
&\quad \times \left(\mathbf{0}_{m\times 1}, \mathbf{0}_{m\times m}, \mathbf{C}_m^T(\widetilde{\mathbf{B}}_1 - \widetilde{\mathbf{B}}_2)\right)^T \\
&= 2(m-1)\mathbf{I}_m - \mathbf{C}_m^T(\widetilde{\mathbf{B}}_1 - \widetilde{\mathbf{B}}_2)\mathbf{\Delta}^{-1}(\widetilde{\mathbf{B}}_1 - \widetilde{\mathbf{B}}_2)^T\mathbf{C}_m, \qquad (14)
\end{aligned}
$$

where $\mathbf{\Delta}^{-1}$ is the bottom right $(k-1)\times(k-1)$ submatrix of $(\mathbf{X}_{(-1)}^T\mathbf{X}_{(-1)})^{-1}$ and

$$
\begin{aligned}
\mathbf{X}_{(-1)}^T\mathbf{X}_{(-1)} &= (\mathbf{1}_{2m+k}, \mathbf{X}_2, \widetilde{\mathbf{\Gamma}})^T(\mathbf{1}_{2m+k}, \mathbf{X}_2, \widetilde{\mathbf{\Gamma}}) \\
&= \begin{pmatrix} 2m+k & 2(m-1)\mathbf{1}_m^T & \mathbf{0}_{1\times(k-1)} \\ 2(m-1)\mathbf{1}_m & 2\mathbf{Q}_m^T\mathbf{Q}_m & \mathbf{Q}_m^T(\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2) \\ \mathbf{0}_{(k-1)\times 1} & (\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2)^T\mathbf{Q}_m & \widetilde{\mathbf{\Gamma}}^T\widetilde{\mathbf{\Gamma}} \end{pmatrix}.
\end{aligned}
$$

We first show that $\mathbf{\Delta} > 0$. To see this, using the block-wise matrix inversion technique and Lemma 1, we have

$$
\begin{aligned}
\mathbf{\Delta} &= \widetilde{\mathbf{\Gamma}}^T\widetilde{\mathbf{\Gamma}} - \left(\mathbf{0}_{(k-1)\times 1}, (\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2)^T\mathbf{Q}_m\right)\begin{pmatrix} 2m+k & 2(m-1)\mathbf{1}_m^T \\ 2(m-1)\mathbf{1}_m & 2\mathbf{Q}_m^T\mathbf{Q}_m \end{pmatrix}^{-1} \\
&\quad \times \left(\mathbf{0}_{(k-1)\times 1}, (\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2)^T\mathbf{Q}_m\right)^T \\
&= (2n+1)(\mathbf{I}_{k-1} + \mathbf{J}_{k-1}) - (\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2)^T\mathbf{Q}_m \\
&\quad \times \left(2\mathbf{Q}_m^T\mathbf{Q}_m - \frac{4(m-1)^2}{2m+k}\mathbf{1}_m\mathbf{1}_m^T\right)^{-1}\mathbf{Q}_m^T(\widetilde{\mathbf{B}}_1 + \widetilde{\mathbf{B}}_2)
\end{aligned}
$$

$$
\begin{aligned}
&= (2n+1)(\mathbf{I}_{k-1}+\mathbf{J}_{k-1}) - (\widetilde{\mathbf{B}}_1+\widetilde{\mathbf{B}}_2)^T \\
&\quad \times \left(2\mathbf{I}_m + \left(2m-4-\frac{4(m-1)^2}{2m+k}\right)\mathbf{J}_m\right)^{-1} (\widetilde{\mathbf{B}}_1+\widetilde{\mathbf{B}}_2) \\
&= (2n+1)(\mathbf{I}_{k-1}+\mathbf{J}_{k-1}) - 2^{-1}(\widetilde{\mathbf{B}}_1+\widetilde{\mathbf{B}}_2)^T(\widetilde{\mathbf{B}}_1+\widetilde{\mathbf{B}}_2) \\
&= (2n+1)(\mathbf{I}_{k-1}+\mathbf{J}_{k-1}) - \left(\widetilde{\mathbf{B}}_1^T\widetilde{\mathbf{B}}_1+\widetilde{\mathbf{B}}_2^T\widetilde{\mathbf{B}}_2\right) + 2^{-1}(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2)^T(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2) \\
&= \mathbf{I}_{k-1}+\mathbf{J}_{k-1} + 2^{-1}(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2)^T(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2) > 0.
\end{aligned}
$$

Thus, by formula (14), for a pairwise blocked DSD $\mathbf{D}_*^b$ and any balanced blocked DSD $\mathbf{D}^b$, we have

$$\mathbf{M}_{\boldsymbol{\alpha}_1}(\mathbf{D}_*^b) - \mathbf{M}_{\boldsymbol{\alpha}_1}(\mathbf{D}^b) = \mathbf{C}_m^T(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2)\boldsymbol{\Delta}^{-1}(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2)^T\mathbf{C}_m \geq 0,$$

which implies that $\mathbf{D}_*^b$ is universally optimal for estimating $\boldsymbol{\alpha}_1$. Moreover, since $\boldsymbol{\Delta}^{-1} > 0$ and $\mathbf{C}_m$ is nonsingular, $\mathbf{C}_m^T(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2)\boldsymbol{\Delta}^{-1}(\widetilde{\mathbf{B}}_1-\widetilde{\mathbf{B}}_2)^T\mathbf{C}_m = \mathbf{0}_{m\times m}$ if and only if $\widetilde{\mathbf{B}}_1 = \widetilde{\mathbf{B}}_2$, which implies that $\mathbf{D}^b$ is pairwise blocked. And shows that any universally optimal balanced blocked DSD for estimating $\boldsymbol{\alpha}_1$ is a pairwise blocked DSD. So the Proof of Theorem 1 is complete. □

Proof of Proposition 1 From the Proof of Theorem 1, we have $\mathbf{X}_1^T\widetilde{\boldsymbol{\Gamma}} = \mathbf{C}_m^T(\widetilde{\mathbf{B}}_1 - \widetilde{\mathbf{B}}_2) = \mathbf{0}_{m\times(k-1)}$ if and only if $\widetilde{\mathbf{B}}_1 = \widetilde{\mathbf{B}}_2$. The conclusion follows. □

Proof of Lemma 3 Write $\mathbf{Z}_j$ as $(\mathbf{Z}_{j,1}^T, \mathbf{Z}_{j,2}^T, \mathbf{Z}_{j,0}^T)^T$, where the submatrices $\mathbf{Z}_{j,1}$, $\mathbf{Z}_{j,2}$ and $\mathbf{Z}_{j,0}$ have m, m and k rows, respectively. Note that $\mathbf{Z}_{j,1}$ and $\mathbf{Z}_{j,2}$ depend on the choice of $\mathbf{C}_m$. It is easy to obtain that when j is odd, $\mathbf{Z}_{j,2} = -\mathbf{Z}_{j,1}$ and $\mathbf{Z}_{j,0} = \mathbf{0}$; when j is even, $\mathbf{Z}_{j,2} = \mathbf{Z}_{j,1}$. According to Lemma 2, when j is odd, $\beta_{j,0}(\mathbf{D}^b) = 0$ and when j is even,

$$
\begin{aligned}
\beta_{j,0}(\mathbf{D}^b) &= (2m+k)^{-2}\mathrm{tr}\left(\mathbf{Z}_j\mathbf{Z}_j^T\mathbf{1}_{2m+k}\mathbf{1}_{2m+k}^T\right) \\
&= (2m+k)^{-2}\mathrm{tr}\left(\begin{pmatrix} \mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T & \mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T & \mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T \\ \mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T & \mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T & \mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T \\ \mathbf{Z}_{j,0}\mathbf{Z}_{j,1}^T & \mathbf{Z}_{j,0}\mathbf{Z}_{j,1}^T & \mathbf{Z}_{j,0}\mathbf{Z}_{j,0}^T \end{pmatrix}\mathbf{1}_{2m+k}\mathbf{1}_{2m+k}^T\right).
\end{aligned}
$$

Next, we are ready to show that $\beta_{j,0}(\mathbf{D}^b)$ is independent of the choice of $\mathbf{C}_m$ for even j. It suffices to show that $\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T$ and $\mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T$ do not change according to different $\mathbf{C}_m$'s. For any $\mathbf{C}_m$, define $\mathbf{A}_1 = \sqrt{3/2}\mathbf{C}_m$ and $\mathbf{A}_2 = -3\sqrt{2}/2\mathbf{I}_m + \sqrt{2}/2\mathbf{J}_m$. By the definition of $\mathbf{Z}_j$, for any $\mathbf{t} = (t_1, \ldots, t_m) \in \{\mathbf{t} \in \mathcal{T}_0 : \|\mathbf{t}\| = j$, there are $j/2$ compoments of $\mathbf{t}$ is $2\}$, the column of $\mathbf{Z}_{j,0}$ labeled by $\mathbf{t}$ is $(-\sqrt{2})^{j/2}\mathbf{1}_k$, and the column of $\mathbf{Z}_{j,1}$ labeled by $\mathbf{t}$ is the element-wise product of all the ith columns of $\mathbf{A}_2$, where $1 \leq i \leq m$ and $t_i = 2$. For any $\mathbf{t} = (t_1, \ldots, t_m) \in \{\mathbf{t} \in \mathcal{T}_0 : \|\mathbf{t}\| = j$, at least one $t_i = 1, 1 \leq i \leq m\}$, the column of $\mathbf{Z}_{j,0}$ labeled by $\mathbf{t}$ is $\mathbf{0}_{k\times 1}$, and the column of $\mathbf{Z}_{j,1}$ labeled by $\mathbf{t}$ is the element-wise product of all the ith columns of $\mathbf{A}_2$ and all the lth columns of $\mathbf{A}_1$, where $1 \leq i, l \leq m$, $t_i = 2$ and $t_l = 1$.

Thus $\mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T = a\mathbf{1}_{m\times k}$, where a is a constant which is independent of the choice of $\mathbf{C}_m$.

Now let us focus on $\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T$. For $1 \le u, v \le m$ and $u \ne v$, the uth diagonal entry and the (u, v)th entry of $\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T$ are actually

$$\sum_{\mathbf{t}\in\mathcal{T}_0, \|\mathbf{t}\|=j} \left(\prod_{l:t_l=1} \mathbf{A}_1[u,l]^2 \prod_{i:t_i=2} \mathbf{A}_2[u,i]^2 \right)$$

and

$$\sum_{\mathbf{t}\in\mathcal{T}_0, \|\mathbf{t}\|=j} \left(\prod_{l:t_l=1} \mathbf{A}_1[u,l]\mathbf{A}_1[v,l] \prod_{i:t_i=2} \mathbf{A}_2[u,i]\mathbf{A}_2[v,i] \right),$$

respectively. Denote by $\odot$ the element-wise product. Using the fact that $\mathbf{C}_m\mathbf{C}_m^T = (m-1)\mathbf{I}_m$, it can be derived that

$$\begin{pmatrix} \mathbf{A}_1[u,:] \odot \mathbf{A}_1[u,:] \\ \mathbf{A}_2[u,:] \odot \mathbf{A}_2[u,:] \end{pmatrix}$$

consists of one column as $(0, 2)^T$ and $m-1$ columns as $(3/2, 1/2)^T$, and

$$\begin{pmatrix} \mathbf{A}_1[u,:] \odot \mathbf{A}_1[v,:] \\ \mathbf{A}_2[u,:] \odot \mathbf{A}_2[v,:] \end{pmatrix}$$

consists of two columns as $(0, -1)^T$, $(m-2)/2$ columns as $(3/2, 1/2)^T$ and $(m-2)/2$ columns as $(-3/2, 1/2)^T$. Thus it follows that $\mathbf{Z}_{j,1}^T\mathbf{Z}_{j,1} = a_1\mathbf{I}_m + a_2\mathbf{J}_m$, where a_1 and a_2 are constants which are independent of the choice of $\mathbf{C}_m$. Especially, by straightforward calculations, we have $\beta_{2,0}(\mathbf{D}^b) = (2m+k)^{-2}2m(k-m+3)^2$. The proof of Lemma 3 is complete. □

Proof of Theorem 2 Directly, we have $\mathbf{Z}_1 = (\sqrt{3/2}\mathbf{C}_m^T, -\sqrt{3/2}\mathbf{C}_m^T, \mathbf{0}_{k\times m}^T)^T$. Suppose $\mathbf{Z}_b = (\mathbf{Z}_{b1}^T, \mathbf{Z}_{b2}^T, \mathbf{Z}_{b0}^T)^T$, where $\mathbf{Z}_{b1}$, $\mathbf{Z}_{b2}$ and $\mathbf{Z}_{b0}$ are $m\times(k-1)$, $m\times(k-1)$ and $k\times(k-1)$ submatrices of $\mathbf{Z}_b$, respectively. Then by Lemma 2,

$$\begin{aligned}\beta_{1,1}(\mathbf{D}^b) &= (2m+k)^{-2}\text{tr}\left(3/2\mathbf{C}_m^T(\mathbf{Z}_{b1}-\mathbf{Z}_{b2})(\mathbf{Z}_{b1}-\mathbf{Z}_{b2})^T\mathbf{C}_m\right)\\ &= 2^{-1}(2m+k)^{-2}3(m-1)\text{tr}\left((\mathbf{Z}_{b1}-\mathbf{Z}_{b2})(\mathbf{Z}_{b1}-\mathbf{Z}_{b2})^T\right).\end{aligned}$$

So $\beta_{1,1}(\mathbf{D}^b) = 0$ if and only if $\mathbf{Z}_{b1} = \mathbf{Z}_{b2}$, which is equivalent to $\mathbf{b}_1 = \mathbf{b}_2$ in (2), i.e. $\mathbf{D}^b$ is pairwise blocked. □

Proof of Theorem 3 Let

$$\mathbf{D}_*^b = \left(\begin{array}{c|c} \mathbf{C}_m & \mathbf{b} \\ -\mathbf{C}_m & \mathbf{b} \\ \hline \mathbf{0}_{k\times m} & \mathbf{b}_0 \end{array}\right), \widetilde{\mathbf{D}}_*^b = \left(\begin{array}{c|c} \mathbf{C}_m & \tilde{\mathbf{b}} \\ -\mathbf{C}_m & \tilde{\mathbf{b}} \\ \hline \mathbf{0}_{k\times m} & \mathbf{b}_0 \end{array}\right)$$

be two pairwise blocked DSDs. Then there exists an m-order permutation matrix $\mathbf{P}$ such that $\tilde{\mathbf{b}} = \mathbf{P}\mathbf{b}$. Let $\mathbf{Z}_j = (\mathbf{Z}_{j,1}^T, \mathbf{Z}_{j,2}^T, \mathbf{Z}_{j,0}^T)^T$ be the corresponding matrices defined in the proof of Lemma 3, $j = 1, \ldots, 2m$. And let $\mathbf{Z}_b = (\mathbf{Z}_{b1}^T, \mathbf{Z}_{b1}^T, \mathbf{Z}_{b0}^T)^T$ and $\widetilde{\mathbf{Z}}_b = (\widetilde{\mathbf{Z}}_{b1}^T, \widetilde{\mathbf{Z}}_{b2}^T, \widetilde{\mathbf{Z}}_{b0}^T)^T$ be the corresponding matrices defined in the Proof of Theorem 2 for $\mathbf{D}^b$ and $\widetilde{\mathbf{D}}^b$, respectively. Then we have $\widetilde{\mathbf{Z}}_{b0} = \mathbf{Z}_{b0}$ and $\widetilde{\mathbf{Z}}_{b1} = \mathbf{P}\mathbf{Z}_{b1}$.

From the Proof of Lemma 3, when j is odd, $\mathbf{Z}_{j,2} = -\mathbf{Z}_{j,1}$, and when j is even, $\mathbf{Z}_{j,2} = \mathbf{Z}_{j,1}$. Thus, by (13) we have $\beta_{j,1}(\mathbf{D}_*^b) = \beta_{j,1}(\widetilde{\mathbf{D}}_*^b) = 0$, when j is odd.

Now we will show that $\beta_{j,1}(\widetilde{\mathbf{D}}_*^b) = \beta_{j,1}(\mathbf{D}_*^b)$ and $\beta_{j,1}(\mathbf{D}_*^b)$ is independent of the choice of $\mathbf{C}_m$, when j is even. According to (13),

$$\begin{aligned} \beta_{j,1}(\widetilde{\mathbf{D}}_*^b) &= (2m+k)^{-2}\mathrm{tr}\left(\widetilde{\mathbf{Z}}_j^T\widetilde{\mathbf{Z}}_b\widetilde{\mathbf{Z}}_b^T\widetilde{\mathbf{Z}}_j\right) \\ &= (2m+k)^{-2}\mathrm{tr}\left(\begin{pmatrix} \mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T\mathbf{P}^T & \mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T\mathbf{P}^T & \mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T \\ \mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T\mathbf{P}^T & \mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T\mathbf{P}^T & \mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T \\ \mathbf{Z}_{j,0}\mathbf{Z}_{j,1}^T\mathbf{P}^T & \mathbf{Z}_{j,0}\mathbf{Z}_{j,1}^T\mathbf{P}^T & \mathbf{Z}_{j,0}\mathbf{Z}_{j,0}^T \end{pmatrix}\mathbf{Z}_b\mathbf{Z}_b^T\right). \end{aligned}$$

In the Proof of Lemma 3, we have shown that $\mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T = a\mathbf{1}_{m\times k}$ and $\mathbf{Z}_{j,1}^T\mathbf{Z}_{j,1} = a_1\mathbf{I}_m + a_2\mathbf{J}_m$, where a, a_1 and a_2 are constants independent of the choice of $\mathbf{C}_m$. Since $\mathbf{P}$ is a permutation matrix and $\mathbf{P}\mathbf{P}^T = \mathbf{I}_m$, we further have $\mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T\mathbf{P}^T = \mathbf{Z}_{j,1}\mathbf{Z}_{j,1}^T$ and $\mathbf{P}\mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T = \mathbf{Z}_{j,1}\mathbf{Z}_{j,0}^T$. The conclusion follows. □

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