# A UNIFIED FRAMEWORK FOR MINIMUM ABERRATION

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Abstract: Minimum aberration is a popular method of selecting fractional factorial designs. Numerous extensions to the original methods have benefited fields of experimental design such as multi-stratum designs, multi-group designs, and multi-platform designs. However, most of these extensions are ad hoc, developed on case-by-case bases without strong statistical justifications or a unified rationale. As such, we provide a new perspective on minimum aberration using a Bayesian approach. Our theory includes a unified framework for minimum aberration and is easily applied to many situations. Furthermore, it enables experimenters to derive their own aberration criteria. Several theoretical results and three numerical illustrations are provided.

Key words and phrases: Bayesian, Fractional factorial, Multi-stratum, Multiplatform, Multi-group, Mixed-level, Blocking, Split-plot, Strip-plot.

#### 1. Introduction

Minimum aberration is a well established field. The first aberration criterion was proposed by Fries and Hunter (1980) and is popular for assessing fractional factorial designs. It is especially beneficial when experimenters have little knowledge about the potentially important factorial effects. This criterion was originally developed to evaluate *regular* fractional factorial designs with *unstructured experimental units*; refer to Wu and Hamada (2009) and Cheng (2014) for a comprehensive review.

Several modifications of the aberration criterion of Fries and Hunter (1980) have been proposed, including those for nonregular designs, block designs, and split-plot designs (Dean et al., 2015). Sitter, Chen, and Feder (1997), Chen and Cheng (1999), and Cheng and Wu (2002) developed aberration criteria for blocked two-level regular fractional factorial designs. Cheng, Li, and Ye (2004) proposed a version for blocked two-level nonregular fractional factorial designs. Lin (2014) extended the results in Cheng, Li, and Ye (2004) to blocked mixed-level orthogonal arrays. In addition to block designs, minimum aberration has been used or modified for split-plot designs as well. Huang, Chen, and Voelkel (1998), Bingham and Sitter (1999), and Bingham, Schoen, and Sitter (2004) used it to compare twolevel split-plot designs. Tichon, Li, and Mcleod (2012) considered selecting split-plot designs under five scenarios, each associated with a modified aberration criterion. Yang and Lin (2017) used the same approach as that of Lin (2014) to develop an aberration criterion for mixed-level split-plot designs. An aberration criterion is mathematically formulated by a *wordlength pattern*, which requires an order of desirability among pertinent words. In the literature, however, most wordlength patterns are ad hoc modifications of that of Fries and Hunter (1980) and lack strong statistical justifications. For block designs, one needs to argue an order between *block defining words* and *treatment defining words*, while three distinct orders were individually proposed by Sitter, Chen, and Feder (1997), Chen and Cheng (1999), and Cheng and Wu (2002). Apart from the difficulty of judging an appropriate order, the lengths of defining words do not provide enough information for ranking designs in many situations, such as blocked nonregular designs. This is because designs that can estimate the same number of models may have different estimation efficiencies, not to mention to account for the structures of experimental units.

We develop a unified theory of aberration criteria for various scenarios in the literature based on a statistically meaningful framework. Moreover, our theory yields a systematic method allowing experimenters to derive aberration criteria appropriate for specific experimental conditions. Another work relevant to ours is that of Cheng and Tang (2005), who adopt the notion of *minimizing contamination*. However, Cheng and Tang (2005) studied two-level factorial designs with unstructured experimental units. Our theory, based on a Bayesian approach, has a sound statistical rationale and can be used to assess and compare mixed-level fractional factorial designs with experimental units that have complex structures.

In our work, the treatment factors are allowed to have multiple groups, in the sense that those in the same group are assumed to have (nearly) equal importance on the response. This setting has been considered in the literature, for example, with *control factors* and *noise factors* in robust parameter designs (Taguchi, 1987). Zhu (2003) studied two-level factorial designs with multiple groups of treatment factors. Tichon, Li, and Mcleod (2012) investigated optimal split-plot designs with two groups of treatment factors, separately corresponding to the whole-plot and subplot strata. Recently, an application of multi-group treatment factors was studied in *multi-platform* experiments (Sadeghi, Qian, and Arora, 2016, 2017), where the *sliced fac*tor itself is in one group and has higher importance than the other factors. Li, Zhou, and Zhang (2015) and Li, Mee, and Zhou (2018) proposed new aberration criteria for factorial designs with multiple groups of treatment factors. We discuss applying our work to multi-platform experiments in Section S5 of the Supplementary Material.

The remainder of this paper is organized as follows. Section 2 provides necessary preliminaries. Section 3 gives the theoretical results of our work and introduces a general aberration criterion with some applications. Section 4 illustrates minimum aberration designs under three settings: unstructured units, blocked mixed-level orthogonal arrays, and three-stage manufacturing processes. Finally, Section 5 concludes this paper. All proofs are deferred to the Supplementary Material.

# 2. Preliminaries

#### 2.1 Unit factors and block structures

The experimental units considered in this study have a structure, hereafter referred to as a *block structure*. Many common block structures, such as block designs, split-plot designs, strip-plot designs, and block strip-plot designs, belong to a specific class of block structures: *simple block structures* (Nelder, 1965a,b). A larger class of block structures, covering simple block structures and most block structures commonly encountered in practice, is that of *orthogonal block structures* (Speed and Bailey, 1982; Bailey, 1985); refer to Bailey (2008) and Cheng (2014) for details.

We denote the number of experimental units by N. A block structure can be described by a set of *unit factors* defined on the experimental units. An  $n_{\mathcal{F}}$ -level unit factor  $\mathcal{F}$  can be thought of as a partition of the N units into  $n_{\mathcal{F}}$  disjoint subsets. Each subset is called an  $\mathcal{F}$ -class and consists of units that have the same level of  $\mathcal{F}$ . A unit factor is said to be *uniform* if all of its classes are of the same size. For two different unit factors  $\mathcal{F}_1$  and  $\mathcal{F}_2$ , we say that  $\mathcal{F}_1$  is *nested in* (or *finer than*)  $\mathcal{F}_2$ , denoted by  $\mathcal{F}_1 \prec \mathcal{F}_2$ , if two units in the same  $\mathcal{F}_1$ -class implies that they are in the same  $\mathcal{F}_2$ -class. The expression  $\mathcal{F}_1 \preceq \mathcal{F}_2$  stands for either  $\mathcal{F}_1 \prec \mathcal{F}_2$  or  $\mathcal{F}_1 = \mathcal{F}_2$ . The finest unit factor, denoted by  $\mathcal{E}$ , has N levels, with each class consisting of one single unit. On the other hand,  $\mathcal{U}$  denotes the unit factor that has a single level with all units in the same class. A split-plot design has the block structure  $\{\mathcal{U}, \mathcal{P}, \mathcal{E}\}$ , where  $\mathcal{P}$  partitions the N units into  $n_{\mathcal{P}}$  whole-plots. We always include  $\mathcal{U}$  and  $\mathcal{E}$  into every block structure. A set of unstructured units can be treated as having the block structure  $\{\mathcal{U}, \mathcal{E}\}$ .

In this study, we consider block structures that satisfy conditions (i), (ii), (iii), (v), and (vi) in Definition 12.4 of Cheng (2014, p. 233), which cover orthogonal block structures. To save space, these five conditions, denoted by (S1.1)-(S1.5), and their importance for the theoretical results in our work are given in Section S1 of the Supplementary Material. Note that the block structures of most experiments encountered in practice, such as blocked, split-plot, or strip-plot factorial experiments, satisfy (S1.1)-(S1.5).

#### 2.2 Treatment factorial effects

Suppose there are *n* treatment factors with levels  $p_1, ..., p_n$ , and denote  $\prod_{i=1}^n p_i$  by  $\Xi$ . Let  $\beta_0$  be the intercept and  $\beta_1, ..., \beta_{\Xi-1}$  be the  $\Xi - 1$  factorial effects. Denote the  $\Xi \times 1$  vector of all  $\beta_j$  by  $\boldsymbol{\beta}$ . Let  $\boldsymbol{\alpha}$  be the  $\Xi \times 1$  vector of the effects of all  $\Xi$  treatment combinations. Then,  $\boldsymbol{\alpha}$  can be expressed as  $\boldsymbol{\alpha} = \mathbf{P}\boldsymbol{\beta}$ , where  $\mathbf{P}$  is a  $\Xi \times \Xi$  full model matrix for a complete factorial experiment with  $\mathbf{P}^T \mathbf{P} = \mathbf{I}_{\Xi}$ . It follows that  $\mathbf{P}^{-1} = \mathbf{P}^T$  and  $\boldsymbol{\beta} = \mathbf{P}^T \boldsymbol{\alpha}$ .

The matrix **P** can be systematically constructed based on Kurkjian and Zelen (1962) as follows. For each factor i = 1, ..., n, define a  $p_i \times p_i$ orthogonal matrix **P**<sub>i</sub>, with the first column proportional to the all-one vector. Then, let the remaining  $p_i - 1$  columns define  $p_i - 1$  treatment contrasts of the main effects of factor *i*. If  $p_1 = 3$ , for example, a choice of **P**<sub>1</sub> is  $\begin{bmatrix} 1/\sqrt{3} & -1/\sqrt{2} & 1/\sqrt{6} \\ 1/\sqrt{3} & 0 & -2/\sqrt{6} \\ 1/\sqrt{3} & 1/\sqrt{2} & 1/\sqrt{6} \end{bmatrix}$ , in which the first column represents

the intercept, the second column represents the linear main effect, and the third column represents the quadratic main effect. Once  $\mathbf{P}_1, ..., \mathbf{P}_n$  have been constructed, one can obtain  $\mathbf{P}$  by

$$\mathbf{P} = \mathbf{P}_1 \otimes \cdots \otimes \mathbf{P}_n, \tag{2.1}$$

where  $\otimes$  denotes the Kronecker product operator.

The components of  $\boldsymbol{\beta}$  can be divided into  $2^n$  groups in terms of the treatment factors involved. Let S be a subset of  $\{1, ..., n\}$ , where the empty set is denoted by  $\phi$ . Each S represents one such group and corresponds to certain  $\beta_j$ . For example,  $S = \phi$  corresponds to the intercept,  $S = \{i\}$  corresponds to the  $p_i - 1$  main effects of factor i, and  $S = \{i_1, ..., i_k\}$  corresponds to the  $(p_{i_1} - 1) \cdots (p_{i_k} - 1)$  k-factor interactions among factors  $i_1, ..., i_k$ .

We adopt a Bayesian framework for  $\boldsymbol{\beta}$ . To specify the prior distribution of  $\boldsymbol{\beta}$ , we assume that  $\boldsymbol{\beta}$  comprises uncorrelated random variables and follows a zero-mean multivariate normal distribution with  $\operatorname{var}(\beta_l) = \operatorname{var}(\beta_j)$  if both  $\beta_l$  and  $\beta_j$  are associated with the same S. Hence, there are at most  $2^n$ distinct values of  $\operatorname{var}(\beta_i)$ . These values are denoted by  $v_S$ , for  $S \subseteq \{1, ..., n\}$ . Furthermore, we require

$$v_S \ge v_{S'} \text{ if } S \subset S'. \tag{2.2}$$

This requirement, referred to as the property of *nested decreasing interaction variances* in Kerr (2001), is consistent with the *effect heredity principle* (Yates, 1935; Wu and Hamada, 2009, p. 172). This Bayesian framework is inspired by Mitchell, Morris, and Ylvisaker (1995), Kerr (2001), Joseph (2006), and Joseph and Delaney (2007). A common technique of their approaches is to induce the prior distribution of  $\boldsymbol{\beta}$  from  $\boldsymbol{\alpha}$ , where  $\boldsymbol{\alpha}$  is assumed to be a realization of a stationary Gaussian process. Some results of the prior distribution of  $\beta$  are given in Section S2 of the Supplementary Material.

#### 2.3 Statistical model

Suppose N experimental units have a block structure  $\mathfrak{B} = \{\mathcal{F}_0, \mathcal{F}_1, ..., \mathcal{F}_m\}$ , where  $\mathcal{F}_0 = \mathcal{U}$  and  $\mathcal{F}_m = \mathcal{E}$ . For each  $\mathcal{F}_i \in \mathfrak{B}$ , let  $\mathbf{X}_{\mathcal{F}_i}$  be an  $N \times n_{\mathcal{F}_i}$ *incidence* matrix that describes the relationship between the units and the levels of  $\mathcal{F}_i$ . Each entry of  $\mathbf{X}_{\mathcal{F}_i}$  is zero or one such that the ljth entry of  $\mathbf{X}_{\mathcal{F}_i}$  is one if and only if the lth unit is in the jth  $\mathcal{F}_i$ -class.

Under a fractional factorial design d with N treatment combinations, let

$$\mathbf{y} = \mathbf{U} oldsymbol{eta} + \sum_{i=0}^m \mathbf{X}_{\mathcal{F}_i} oldsymbol{\gamma}^{\mathcal{F}_i},$$

where  $\mathbf{y}$  is a vector of responses,  $\mathbf{U}$  is the  $N \times \Xi$  full model matrix under d (composed of N corresponding rows from  $\mathbf{P}$ ), and  $\boldsymbol{\gamma}^{\mathcal{F}_i} = (\gamma_1^{\mathcal{F}_i}, \dots, \gamma_{n_{\mathcal{F}_i}}^{\mathcal{F}_i})^T$ with  $\gamma_j^{\mathcal{F}_i}$  being the effect of the *j*th level of unit factor  $\mathcal{F}_i$  (e.g., block effects, whole-plot effects, and subplot effects). We assume that the  $\gamma_j^{\mathcal{F}_i}$  are uncorrelated, with each  $\gamma_j^{\mathcal{F}_i}$  following a zero-mean normal distribution with variance  $\sigma_{\mathcal{F}_i}^2$ , and that they are independent of  $\boldsymbol{\beta}$ . Then, the conditional distribution of y given  $\beta$  is the multivariate normal distribution

$$\mathbf{y}|\boldsymbol{\beta} \sim \mathrm{N}(\mathbf{U}\boldsymbol{\beta}, \sum_{i=0}^{m} \sigma_{\mathcal{F}_{i}}^{2} \mathbf{X}_{\mathcal{F}_{i}} \mathbf{X}_{\mathcal{F}_{i}}^{T}).$$
 (2.3)

Let  $\mathbf{V} = \sum_{i=0}^{m} \sigma_{\mathcal{F}_i}^2 \mathbf{X}_{\mathcal{F}_i} \mathbf{X}_{\mathcal{F}_i}^T$ . If  $\mathfrak{B}$  satisfies conditions (S1.1)–(S1.5), then  $\mathbf{V}$  has m+1 eigenspaces  $W_{\mathcal{F}_0}, \ldots, W_{\mathcal{F}_m}$ , with one eigenspace associated with each of the m+1 unit factors. Here,  $W_{\mathcal{F}_0} = W_{\mathcal{U}}$  is the one-dimensional space consisting of all the vectors with constant entries, and each other eigenvector defines a unit contrast (Cheng, 2014, p. 237). It follows that  $\sum_{i=0}^{m} \mathbf{P}_{W_{\mathcal{F}_i}} = \mathbf{I}_N$ , where  $\mathbf{P}_{W_{\mathcal{F}_i}}$  is the orthogonal projection matrix onto  $W_{\mathcal{F}_i}$ . Let the corresponding eigenvalues be  $\xi_{\mathcal{F}_0}, \ldots, \xi_{\mathcal{F}_m}$ . Here,  $W_{\mathcal{F}_i}$  and  $\xi_{\mathcal{F}_i}$  are called a *stratum* and stratum variance, respectively. It can be shown that  $\xi_{\mathcal{F}_i} \leq \xi_{\mathcal{F}_j}$  if  $\mathcal{F}_i \leq \mathcal{F}_j$  (Cheng, 2014, p. 246). The case where  $\gamma_1^{\mathcal{F}_i}, \ldots, \gamma_{n_{\mathcal{F}_i}}^{\mathcal{F}_i}$ are unknown constants (fixed effects) can be treated by letting  $\sigma_{\mathcal{F}_i}^2 = \infty$ , leading to  $\xi_{\mathcal{F}_j} = \infty$  if  $\mathcal{F}_i \leq \mathcal{F}_j$ .

A systematic method to construct  $\mathbf{P}_{W_{\mathcal{F}}}$  is as follows. Define  $V_{\mathcal{F}}$  as the column space of  $\mathbf{X}_{\mathcal{F}}$ , for each  $\mathcal{F} \in \mathfrak{B}$ . The orthogonal projection matrix onto  $V_{\mathcal{F}}$  is  $\mathbf{P}_{V_{\mathcal{F}}} = \mathbf{X}_{\mathcal{F}}(\mathbf{X}_{\mathcal{F}}^T\mathbf{X}_{\mathcal{F}})^{-1}\mathbf{X}_{\mathcal{F}}^T$ . It can be shown that  $\mathbf{P}_{W_{\mathcal{F}}} =$  $\mathbf{P}_{V_{\mathcal{F}}} - \sum_{\mathcal{G} \in \mathfrak{B}: \mathcal{F} \prec \mathcal{G}} \mathbf{P}_{W_{\mathcal{G}}}$ . Thus, one can obtain every  $\mathbf{P}_{W_{\mathcal{F}}}$  by starting from  $\mathbf{P}_{W_{\mathcal{U}}} = \frac{1}{N} \mathbf{1}_N \mathbf{1}_N^T$ . More details can be found in Cheng (2014, p. 243).

#### 3. A general aberration criterion

In this section, we propose an aberration criterion for design assessment and selection based on the Bayesian approach. This criterion is capable of handling mixed-level treatment factors, as well as complex structures of experimental units. In addition, it is easily modified according to experimenters' beliefs about important factorial effects. Sections 3.1 to 3.3 illustrate its three common applications.

From (2.2) and (2.3), the posterior distribution  $\boldsymbol{\beta}|\mathbf{y}$  is multivariate normal with a mean vector and the covariance matrix  $\operatorname{cov}(\boldsymbol{\beta}|\mathbf{y}) = \Sigma_{\boldsymbol{\beta}} - \Sigma_{\boldsymbol{\beta}} \mathbf{U}^T (\mathbf{U}\Sigma_{\boldsymbol{\beta}} \mathbf{U}^T + \mathbf{V})^{-1} \mathbf{U}\Sigma_{\boldsymbol{\beta}}$ , where  $\Sigma_{\boldsymbol{\beta}}$  is the (prior) covariance matrix of  $\boldsymbol{\beta}$ . Let  $\mathbf{M} = \operatorname{cov}(\boldsymbol{\beta}|\mathbf{y})^{-1}$ . A commonly used design selection criterion, *Bayesian D-optimality*, maximizes det[ $\mathbf{M}$ ]. However, while the D-optimality has a good statistical interpretation, it is not easily manageable. A good surrogate for the D-optimality, referred to as the (M.S)-optimality due to Eccleston and Hedayat (1974), first maximizes tr[ $\mathbf{M}$ ], and then minimizes tr[ $\mathbf{M}^2$ ] among the designs that maximize tr[ $\mathbf{M}$ ].

For each  $S \subseteq \{1, ..., n\}$ , let  $\mathbf{U}_S$  be composed of the columns in  $\mathbf{U}$ associated with S. If  $S = \{1, 2\}$  with  $p_1 = 2$  and  $p_2 = 3$ , for example, then  $\mathbf{U}_S$  consists of (2-1)(3-1) = 2 columns, each representing a treatment contrast of the two-factor interaction between factors 1 and 2 under the given design.

Define

$$\begin{split} \Phi_1(d; \boldsymbol{\xi}, \mathbf{v}) &= \sum_{i=0}^m \sum_{S \subseteq \{1, \dots, n\}} \frac{v_S}{\xi_{\mathcal{F}_i}} \mathrm{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right], \\ \Phi_2(d; \boldsymbol{\xi}, \mathbf{v}) &= \sum_{i=0}^m \frac{1}{\xi_{\mathcal{F}_i}^2} \mathrm{tr} \left[ (\boldsymbol{\Sigma}_\beta \mathbf{U}^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U})^2 \right] \\ &+ 2 \sum_{0 \le l < s \le m} \frac{1}{\xi_{\mathcal{F}_l} \xi_{\mathcal{F}_s}} \mathrm{tr} \left[ (\boldsymbol{\Sigma}_\beta \mathbf{U}^T \mathbf{P}_{W_{\mathcal{F}_l}} \mathbf{U}) (\boldsymbol{\Sigma}_\beta \mathbf{U}^T \mathbf{P}_{W_{\mathcal{F}_s}} \mathbf{U}) \right], \end{split}$$

where  $\mathbf{v}$  and  $\boldsymbol{\xi}$  are the vectors of  $v_S$  and  $\xi_{\mathcal{F}_i}$ , respectively. We have the following result for the Bayesian (M.S)-optimality.

**Theorem 1.** The Bayesian (M.S)-optimality involves first maximizing  $\Phi_1(d; \boldsymbol{\xi}, \mathbf{v})$ , and then minimizing  $\Phi_2(d; \boldsymbol{\xi}, \mathbf{v})$  among the designs that maximize  $\Phi_1(d; \boldsymbol{\xi}, \mathbf{v})$ .

To obtain a more structured form of  $\Phi_1(d; \boldsymbol{\xi}, \mathbf{v})$ , we need Lemmas 1 and 2 in Section S3 of the Supplementary Material, which jointly state that tr  $[\mathbf{U}_S^T \mathbf{U}_S]$  does not depend on the choice of designs and orthogonal-column bases of the column space of **P**. We summarize these the following theorem.

**Theorem 2.** For an  $S \subseteq \{1, ..., n\}$ ,  $tr[\mathbf{U}_S^T \mathbf{U}_S]$  is a constant for any choice of N-run designs, as well as for any choice of orthogonal-column bases in **P**.

With Theorem 2 and the property  $\sum_{i=0}^{m} \mathbf{P}_{W_{\mathcal{F}_i}} = \mathbf{I}_N$ , maximizing  $\Phi_1(d; \boldsymbol{\xi}, \mathbf{v})$ 

is reduced to minimizing

$$\Phi_1^*(d;\boldsymbol{\xi}, \mathbf{v}) = \sum_{i=0}^{m-1} \sum_{S \subseteq \{1,\dots,n\}} v_S\left(\frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}}\right) \operatorname{tr}\left[\mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S\right]$$

by replacing  $\mathbf{P}_{W_{\mathcal{F}_m}}$  with  $\mathbf{I}_N - \sum_{i=0}^{m-1} \mathbf{P}_{W_{\mathcal{F}_i}}$ .

In addition to the choice of designs,  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  and  $\Phi_2(d; \boldsymbol{\xi}, \mathbf{v})$  depend on unknown parameters  $\mathbf{v}$  and  $\boldsymbol{\xi}$ . The following result serves as a useful tool for searching for optimal designs with respect to minimizing  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$ for all *feasible*  $\mathbf{v}$  and  $\boldsymbol{\xi}$ . Here,  $\mathbf{v}$  and  $\boldsymbol{\xi}$  are said to be feasible if  $\mathbf{v}$  satisfies (2.2) and  $\mathcal{F}_i \prec \mathcal{F}_j$  implies  $\xi_{\mathcal{F}_i} \leq \xi_{\mathcal{F}_j}$ .

**Theorem 3.** Suppose  $\mathfrak{B}$  is a block structure satisfying conditions (S1.1)–(S1.5). Then, a necessary and sufficient condition for a design to minimize  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  for all feasible  $\mathbf{v}$  and  $\boldsymbol{\xi}$  is that it minimizes

$$\sum_{S \in \mathfrak{S}} \sum_{i: \mathcal{F}_i \in \mathfrak{G}} tr \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right],$$

for all nonempty subsets  $\mathfrak{S} \subseteq 2^{\{1,\dots,n\}} \setminus \{\phi\}$  and  $\mathfrak{G} \subseteq \mathfrak{B} \setminus \{\mathcal{F}_m\}$ , such that

$$S \in \mathfrak{S}, S' \in 2^{\{1,\dots,n\}} \setminus \{\phi\}, \text{ and } S' \subset S \Rightarrow S' \in \mathfrak{S}, \tag{3.4}$$

$$\mathcal{F} \in \mathfrak{G}, \mathcal{F}' \in \mathfrak{B}, \text{ and } \mathcal{F} \prec \mathcal{F}' \Rightarrow \mathcal{F}' \in \mathfrak{G}.$$
 (3.5)

We illustrate Theorem 3 using a simple scenario. Suppose n = 2 and  $\mathfrak{B} = \{\mathcal{F}_0, \mathcal{F}_1, \mathcal{F}_2\}$  with  $\mathcal{F}_2 \prec \mathcal{F}_1 \prec \mathcal{F}_0$ . The subsets of  $2^{\{1,2\}} \setminus \{\phi\} =$  $\{\{1\}, \{2\}, \{1,2\}\}$  that all satisfy (3.4) are  $\mathfrak{S}_1 = \{\{1\}\}, \mathfrak{S}_2 = \{\{2\}\}, \mathfrak{S}_3 =$  {{1}, {2}},  $\mathfrak{S}_4 = \{\{1\}, \{2\}, \{1, 2\}\}$ . Likewise, the subsets of  $\mathfrak{B} \setminus \{\mathcal{F}_2\}$  that all satisfy (3.5) are  $\mathfrak{G}_1 = \{\mathcal{F}_0\}, \mathfrak{G}_2 = \{\mathcal{F}_0, \mathcal{F}_1\}$ . By Theorem 3, if a design minimizes  $\sum_{S \in \mathfrak{S}_i} \sum_{j: \mathcal{F}_j \in \mathfrak{G}_l} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_j}} \mathbf{U}_S \right]$ , for i = 1, ..., 4 and l = 1, 2, then it minimizes  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  for all feasible  $\mathbf{v}$  and  $\boldsymbol{\xi}$ .

Theorem 3 extends Theorem 5.1 in Chang and Cheng (2018) in two ways. First, Chang and Cheng (2018) limit their theory to two-level designs, whereas here we deal with mixed-level treatment factors. Second, Theorem 3 provides a sufficient and necessary condition for a design to be optimal for all feasible  $\mathbf{v}$  and  $\boldsymbol{\xi}$ , whereas Theorem 5.1 in Chang and Cheng (2018) requires the values of  $\mathbf{v}$ .

Similarly to Chang and Cheng (2018), Theorem 3 is able to eliminate inferior designs. For two designs  $d_1$  and  $d_2$ , if  $\sum_{S \in \mathfrak{S}} \sum_{i:\mathcal{F}_i \in \mathfrak{G}} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right]$ of  $d_1$  is no greater than that of  $d_2$  under every combination of  $\mathfrak{S}$  and  $\mathfrak{G}$ , with strict inequality for at least one combination, then  $d_2$  is worse than  $d_1$ , and is said to be *inadmissible*. Eliminating inadmissible designs yields a considerable reduction of designs that need to be considered. If there remains one design (up to isomorphism), it minimizes  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  for all feasible  $\mathbf{v}$  and  $\boldsymbol{\xi}$ . Usually, using  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  is enough to distinguish designs. If more than one nonisomorphic design remains, we can assess them using either  $\Phi_2(d; \boldsymbol{\xi}, \mathbf{v})$  or the actual Bayesian D-optimal criterion. In the remainder of this section, we illustrate equivalent forms of minimizing  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  under several specific scenarios. Some are reduced to well-known aberration criteria. To define an aberration criterion, one needs a desirability order about the importance of factorial effects. This can be achieved under appropriate settings of the values of  $\mathbf{v}$ .

If it is known that the  $2^n$  subsets of  $\{1, ..., n\}$  can be divided into Jgroups  $\mathfrak{H}_1, ..., \mathfrak{H}_J$ , such that  $v_S = v_{S'}$  for S, S' in the same group and  $v_S > v_{S'}$ for  $S \in \mathfrak{H}_l$  and  $S' \in \mathfrak{H}_{l'}$  with l < l', then, because  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  is linear in  $v_S$ 's, the following wordlength pattern is induced:

$$\sum_{i=0}^{m-1} \left\{ \left( \frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}} \right) \left( \sum_{S \in \mathfrak{H}_1} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right], \dots, \sum_{j \in \mathfrak{H}_J} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right] \right) \right\}.$$
(3.6)

An aberration criterion can be defined as sequentially minimizing this wordlength pattern. Since tr  $\left[\mathbf{U}_{S}^{T}\mathbf{P}_{W_{\mathcal{F}_{i}}}\mathbf{U}_{S}\right] = \operatorname{tr}\left[\mathbf{U}_{S}\mathbf{U}_{S}^{T}\mathbf{P}_{W_{\mathcal{F}_{i}}}\right]$ , it follows from the proof of Lemma 2 (in the Supplementary Material) that (3.6) does not depend on orthogonal bases in **P**.

If, on the other hand, the information about important factorial effects is vague, then the effect hierarchy principle in Wu and Hamada (2009, p. 172) is often assumed, especially for screening experiments (Dean and Lewis, 2006). Under the Bayesian framework, this principle is basically consistent with choosing  $\mathfrak{H}_l = \{S \subseteq \{1, ..., n\} : |S| = l\}$ , for l = 1, ..., n; or equivalently,

(i) 
$$v_S = v_{S'}$$
 if  $|S| = |S'|$ ,  
(ii)  $v_S > v_{S'}$  if  $|S| < |S'|$ . (3.7)

It is obvious that (3.7) satisfies (2.2). By replacing " $S' \subset S$ " in (3.4) with " $v_{S'} \geq v_S$ ", we can establish another version of Theorem 3, tailored to the setting in (3.7).

**Theorem 4.** Suppose  $\mathfrak{B}$  is a block structure satisfying conditions (S1.1)–(S1.5). Then, under (3.7), a necessary and sufficient condition for a design to minimize  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$ , for all  $\mathbf{v}$  that satisfy (3.7) and feasible  $\boldsymbol{\xi}$ , is that it minimizes

$$\sum_{S \in \mathfrak{S}} \sum_{i: \mathcal{F}_i \in \mathfrak{G}} tr \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right],$$

for all nonempty subsets  $\mathfrak{G} \subseteq \mathfrak{B} \setminus \{\mathcal{F}_m\}$  satisfying (3.5), and  $\mathfrak{S} \subseteq 2^{\{1,\dots,n\}} \setminus \{\phi\}$  satisfying

$$S \in \mathfrak{S}, S' \in 2^{\{1,\dots,n\}} \setminus \{\phi\}, \text{ and } v_{S'} \ge v_S \Rightarrow S' \in \mathfrak{S}.$$

$$(3.8)$$

For n = 3, the nonempty subsets of  $2^{\{1,2,3\}} \setminus \{\phi\} = \{\{1\}, \{2\}, \{3\}, \{1,2\}, \{1,3\}, \{2,3\}, \{1,2,3\}\}$ that all satisfy (3.8) are  $\mathfrak{S}_k = \{S \subseteq \{1, ..., n\} : 0 < |S| \le k\}, k = 1, 2, 3,$ each corresponding to main effects, effects up to two-factor interactions, or effects up to the three-factor interaction. When (3.7) holds, with an additional requirement that  $v_S \gg v_{S'}$  if |S| < |S'| (i.e., lower-order effects are much more important than higherorder ones), minimizing  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  is equivalent to sequentially minimizing

$$\mathfrak{W} = \sum_{i=0}^{m-1} \left\{ \left( \frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}} \right) \left( \sum_{S:|S|=1} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right], \dots, \sum_{S:|S|=n} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right] \right) \right\}$$

The  $\mathfrak{W}$  can be regarded as a wordlength pattern and induces an aberration criterion for complex block structures. This criterion, not an ad hoc one, is developed based on good properties of a statistical model. If  $\boldsymbol{\xi}$  are known, their values can be inserted. Otherwise, based on Theorem 4, a design sequentially minimizes  $\mathfrak{W}$  for all feasible  $\boldsymbol{\xi}$  provided that it sequentially minimizes

$$\mathfrak{W}_{\mathfrak{G}} = \left( \sum_{i:\mathcal{F}_i \in \mathfrak{G}} \sum_{S:|S|=1} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right], \dots, \sum_{i:\mathcal{F}_i \in \mathfrak{G}} \sum_{S:|S|=n} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right] \right),$$

for all  $\mathfrak{G} \subseteq \mathfrak{B} \setminus \{\mathcal{F}_m\}$  satisfying (3.5).

Note that each  $\mathfrak{W}_{\mathfrak{G}}$  can be regarded as a wordlength pattern and induces an aberration criterion for the block structure  $\mathfrak{G} \cup \{\mathcal{F}_m\}$ , where all unit effects are fixed effects; that is,  $\xi_{\mathcal{F}} = \infty$  if  $\mathcal{F} \in \mathfrak{G}$ , because under the block structure  $\mathfrak{G} \cup \{\mathcal{F}_m\}$ ,

$$\lim_{\boldsymbol{\xi}_{\mathcal{F}}\to\infty:\mathcal{F}\in\mathfrak{G}}\Phi_{1}^{*}(d;\boldsymbol{\xi},\mathbf{v})\propto\sum_{i:\mathcal{F}_{i}\in\mathfrak{G}}\sum_{S\subseteq\{1,\ldots,n\}}v_{S}\mathrm{tr}\left[\mathbf{U}_{S}^{T}\mathbf{P}_{W_{\mathcal{F}_{i}}}\mathbf{U}_{S}\right].$$

Consequently, if a design has minimum aberration under each case of fixed

unit effects (i.e.,  $\mathfrak{W}_{\mathfrak{G}}$  with  $\mathfrak{G}$  satisfying (3.5)), then it has minimum aberration under random unit effects (i.e.,  $\mathfrak{W}$ ).

The aberration criterion induced by  $\mathfrak{W}$  can be applied to any block structure that satisfies conditions (S1.1)–(S1.5). In Sections 3.1 to 3.3, we introduce three common applications.

As a remark, if a finer hierarchy exists among  $\beta_j$  such that they can be divided into K groups  $\mathfrak{I}_1, ..., \mathfrak{I}_K$ , with those in the same group having equal variance and  $\operatorname{var}(\beta_j) > \operatorname{var}(\beta_{j'})$  for  $\beta_j \in \mathfrak{I}_l$  and  $\beta_{j'} \in \mathfrak{I}_{l'}$  with l < l', then a more flexible version of (3.6) is

$$\sum_{i=0}^{m-1} \left\{ \left( \frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}} \right) \left( \operatorname{tr} \left[ \mathbf{U}_1^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_1 \right], \dots, \operatorname{tr} \left[ \mathbf{U}_K^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_K \right] \right) \right\}, \quad (3.9)$$

where  $\mathbf{U}_l$  is composed of the columns in  $\mathbf{U}$  associated with the  $\beta_j$  belonging to  $\mathfrak{I}_l$ . This is useful in situations such as multi-platform experiments and experiments with quantitative treatment factors.

#### 3.1 Unstructured units

For unstructured experimental units, the block structures are denoted by  $\{\mathcal{F}_0, \mathcal{F}_1\}$  with  $\mathcal{F}_0 = \mathcal{U}$  and  $\mathcal{F}_1 = \mathcal{E}$ . Because  $W_{\mathcal{F}_0}$  is spanned by a vector of ones, we have  $\mathbf{P}_{W_{\mathcal{F}_0}} = \frac{1}{N} \mathbf{1}_N \mathbf{1}_N^T$  and  $\mathbf{P}_{W_{\mathcal{F}_1}} = \mathbf{I}_N - \mathbf{P}_{W_{\mathcal{F}_0}}$ . It follows that

sequentially minimizing  $\mathfrak{W}$  is equivalent to sequentially minimizing

$$\mathfrak{W}_{0} = \left(\sum_{S:|S|=1} (\mathbf{1}_{N}^{T}\mathbf{U}_{S})(\mathbf{1}_{N}^{T}\mathbf{U}_{S})^{T}, \dots, \sum_{S:|S|=n} (\mathbf{1}_{N}^{T}\mathbf{U}_{S})(\mathbf{1}_{N}^{T}\mathbf{U}_{S})^{T}\right).$$
(3.10)

As given by Cheng (2014, p. 340), the wordlength pattern of the generalized aberration criterion proposed by Xu and Wu (2001) takes the following form:  $\frac{\Xi}{N^2} \sum_{S:|S|=k} (\mathbf{1}_N^T \mathbf{U}_S) (\mathbf{1}_N^T \mathbf{U}_S)^T$ , for k = 1, ..., n. Thus, it is equivalent to sequentially minimizing  $\mathfrak{W}_0$ . Moreover, it follows from Theorem 4 that if a design minimizes  $\sum_{S:0<|S|\leq k} (\mathbf{1}_N^T \mathbf{U}_S) (\mathbf{1}_N^T \mathbf{U}_S)^T$  for all k = 1, ..., n, then it minimizes  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  for all  $\mathbf{v}$  satisfying (3.7); based on this, a generalized minimum aberration design must not be inadmissible. The following result implies that a design cannot minimize  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  for all  $\mathbf{v}$  satisfying (3.7) if it has replication.

**Theorem 5.** If an N-run design consists of m replicates, then

$$\sum_{k=0}^{n} \sum_{S:|S|=k} (\mathbf{1}_{N}^{T} \mathbf{U}_{S}) (\mathbf{1}_{N}^{T} \mathbf{U}_{S})^{T} = N + 2m.$$

Theorem 5 discloses a disadvantage of using designs with replicates in terms of estimating factorial effects. By Theorem 5, for two designs with the same run size, the one with more replicates has a larger value of  $\sum_{k=0}^{n} \sum_{S:|S|=k} (\mathbf{1}_{N}^{T} \mathbf{U}_{S}) (\mathbf{1}_{N}^{T} \mathbf{U}_{S})^{T}$ . Thus, it does not reach the necessary and sufficient condition in Theorem 4 and cannot minimize  $\Phi_{1}^{*}(d; \boldsymbol{\xi}, \mathbf{v})$  for all  $\mathbf{v}$  satisfying (3.7). This is not surprising because replicates do not provide any information about factorial effects.

#### **3.2** A chain of nested unit factors

In many real applications, the experimental units are partitioned by a chain of nested unit factors, such as block designs, split-plot designs, or split-split plot designs.

Without loss of generality, suppose the block structure is  $\{\mathcal{F}_0, \mathcal{F}_1, ..., \mathcal{F}_m\}$ with  $\mathcal{F}_i \prec \mathcal{F}_j$  if i > j, where block designs or split-plot designs correspond to m = 2 and split-split plot designs correspond to m = 3. Because the  $\mathfrak{G}$  that satisfy (3.5) are  $\{\mathcal{F}_0\}$ ,  $\{\mathcal{F}_0, \mathcal{F}_1\}$ ,...,  $\{\mathcal{F}_0, \mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_{m-1}\}$ , it follows from Theorem 4 that a design sequentially minimizes  $\mathfrak{W}$  for all feasible  $\boldsymbol{\xi}$ provided that it sequentially minimizes

$$\mathfrak{M}_{l} = \left(\sum_{i=0}^{l} \sum_{S:|S|=1} \operatorname{tr}\left[\mathbf{U}_{S}^{T} \mathbf{P}_{W_{\mathcal{F}_{i}}} \mathbf{U}_{S}\right], \dots, \sum_{i=0}^{l} \sum_{S:|S|=n} \operatorname{tr}\left[\mathbf{U}_{S}^{T} \mathbf{P}_{W_{\mathcal{F}_{i}}} \mathbf{U}_{S}\right]\right),$$

for all l = 0, 1, ..., m - 1.

For block or split-plot experiments, we have m = 2 and  $\mathcal{F}_1$  partitions the units into blocks or whole-plots. In this case, we have  $\mathbf{P}_{W_{\mathcal{F}_0}} = \frac{1}{N} \mathbf{1}_N \mathbf{1}_N^T$ ,  $\mathbf{P}_{W_{\mathcal{F}_1}} = \mathbf{P}_{V_{\mathcal{F}_1}} - \mathbf{P}_{W_{\mathcal{F}_0}}, \mathbf{P}_{W_{\mathcal{F}_2}} = \mathbf{I}_N - (\mathbf{P}_{W_{\mathcal{F}_0}} + \mathbf{P}_{W_{\mathcal{F}_1}})$ , and  $\mathfrak{W} = \sum_{i=0,1} \left\{ \left( \frac{1}{\xi_{\mathcal{F}_2}} - \frac{1}{\xi_{\mathcal{F}_i}} \right) \left( \sum_{S:|S|=1} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right], \dots, \sum_{S:|S|=n} \operatorname{tr} \left[ \mathbf{U}_S^T \mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{U}_S \right] \right) \right\}.$  Then, we have that if a design sequentially minimizes  $\mathfrak{W}_0$  and  $\mathfrak{W}_1$ , then it sequentially minimizes  $\mathfrak{W}$  for all feasible  $\boldsymbol{\xi}$ .

Under a block design,  $\mathfrak{W}_1$  defines an aberration criterion for models with fixed block effects. By letting

$$\mathfrak{W}_{1,i} = \left(\sum_{S:|S|=1} \operatorname{tr}\left[\mathbf{U}_{S}^{T}\mathbf{P}_{W_{\mathcal{F}_{i}}}\mathbf{U}_{S}\right], \dots, \sum_{S:|S|=n} \operatorname{tr}\left[\mathbf{U}_{S}^{T}\mathbf{P}_{W_{\mathcal{F}_{i}}}\mathbf{U}_{S}\right]\right), i = 0, 1,$$

we have  $\mathfrak{W}_1 = \mathfrak{W}_{1,0} + \mathfrak{W}_{1,1}$ . It can be seen that  $\mathfrak{W}_{1,0} = \frac{1}{N}\mathfrak{W}_0$ , which is proportional to the generalized wordlength pattern; also,  $\mathfrak{W}_{1,1}$  defines a wordlength pattern proportional to the *block wordlength pattern* in the literature (e.g., Cheng, Li, and Ye (2004)). Thus,  $\mathfrak{W}_1$  combines the treatment wordlength pattern and block wordlength pattern using  $\mathfrak{W}_1 = \mathfrak{W}_{1,0} + \mathfrak{W}_{1,1}$ , which differs from those in previous works, such as Chen and Cheng (1999); Cheng, Li, and Ye (2004); Lin (2014). For example, Cheng, Li, and Ye (2004) and Lin (2014) proposed aberration criteria for blocked nonregular designs by arguing two types of desirability between treatment defining words and block defining words. The two wordlength patterns in Cheng, Li, and Ye (2004) are proportional to

$$W_1 = (\delta_{1,0}, \delta_{2,0}, \delta_{1,1}, \delta_{3,0}, \delta_{4,0}, \delta_{2,1}, \delta_{5,0}, \delta_{6,0}, \delta_{3,1}, \delta_{7,0}, \dots),$$
$$W_2 = (\delta_{1,0}, \delta_{1,1}, \delta_{2,0}, \delta_{3,0}, \delta_{2,1}, \delta_{4,0}, \delta_{5,0}, \delta_{3,1}, \delta_{6,0}, \delta_{7,0}, \dots),$$

with  $\delta_{k,i} = \sum_{S:|S|=k} \operatorname{tr} \left[ \mathbf{U}_{S}^{T} \mathbf{P}_{W_{\mathcal{F}_{i}}} \mathbf{U}_{S} \right]$ . Those defined in Lin (2014) possess

the same patterns but are under (3.9) with  $\mathfrak{I}_l$  consisting of the  $\beta_j$  of the same polynomial degree l. It can be seen that  $\delta_{k,1}$  precedes  $\delta_{2k,0}$  in  $W_2$ , whereas  $\delta_{2k,0}$  precedes  $\delta_{k,1}$  in  $W_1$ . Because  $\mathfrak{W}_1 \propto \lim_{\xi_{\mathcal{F}_1}\to\infty} \mathfrak{W}$ , we expect  $\mathfrak{W}_1$  produce designs that are more similar to  $W_2$  than to  $W_1$  because  $W_2$ regards confounding treatments with blocks as more severe than  $W_1$  does. However, deciding to use  $W_1$  or  $W_2$  relies heavily on subjective judgment. In our work, the use of  $\mathfrak{W}_1$  is justified by the Bayesian (M.S)-optimality. In addition, it can be shown that  $\mathfrak{W}_1$  tends to maximize D-efficiency under certain fixed-effect models. More details can be found in Section S7 of the Supplementary Material. A numerical comparison of  $\mathfrak{W}_1$ ,  $W_1$ , and  $W_2$  is given in Section 4.2.

#### 3.3 Experiments with multiple processing stages

For experiments with multiple processing stages, the experimental units are partitioned into disjoint classes at each stage. For the treatment factors at some stage, their levels are randomly assigned to the classes of the partition, with the same level assigned to all units in the same class. Many industrial experiments have a sequence of processing stages (Mee and Bates, 1998; Butler, 2004; Bingham et al., 2008; Antolino et al., 2009a,b; Ranjan, Bingham, and Dean, 2009; Cheng and Tsai, 2011; Yuangyai and Lin, 2013). In an experiment with multiple processing stages, the partition of the experimental units at the *i*th stage defines a unit factor  $\mathcal{F}_i$ . As mentioned in Cheng and Tsai (2011), the resulting block structure may not satisfy conditions (S1.1)–(S1.5). Cheng and Tsai (2011) proved that if the  $\mathcal{F}_i$  (except  $\mathcal{U}$  and  $\mathcal{E}$ ) are uniform, mutually orthogonal, and are not nested in one another, then the resulting block structure satisfies the five conditions if and only if these  $\mathcal{F}_i$  define an orthogonal array of strength two.

Here, we consider block structures  $\mathfrak{B} = \{\mathcal{U}, \mathcal{E}, \mathcal{F}_1, ..., \mathcal{F}_h\}$ , where  $\mathcal{F}_1, ..., \mathcal{F}_h$ define an orthogonal array of strength two on the experimental units. Because  $\mathcal{E} \prec \mathcal{F}_1, ..., \mathcal{F}_h \prec \mathcal{U}$  and the  $\mathcal{F}_i$  are not nested in one another, the  $\mathfrak{G}$  that satisfy (3.5) are  $\{\mathcal{U}\}, \{\mathcal{U}, \mathcal{F}_i\}$  with  $1 \leq i \leq h, \{\mathcal{U}, \mathcal{F}_i, \mathcal{F}_j\}$  with  $1 \leq i, j \leq h, ..., \{\mathcal{U}, \mathcal{F}_1, ..., \mathcal{F}_h\}$ . There are  $2^h$  such subsets to be considered. It follows that  $\mathbf{P}_{W_{\mathcal{U}}} = \frac{1}{N} \mathbf{1}_N \mathbf{1}_N^T$  and  $\mathbf{P}_{W_{\mathcal{F}_i}} = \mathbf{P}_{V_{\mathcal{F}_i}} - \mathbf{P}_{W_{\mathcal{U}}}$  for i = 1, ..., h.

The *split-lot* designs in Mee and Bates (1998) belong to this category. Suppose 16 batches of material are to be arranged into four groups of equal size at each of three stages (h = 3). From Theorem 4, a design sequentially minimizes  $\mathfrak{W}$  for all feasible  $\boldsymbol{\xi}$  provided that it sequentially minimizes

$$\mathfrak{W}_{\mathfrak{I}} = \left( \sum_{\mathcal{F} \in \mathfrak{I}} \sum_{S:|S|=1} \operatorname{tr} \left[ \mathbf{U}_{S}^{T} \mathbf{P}_{W_{\mathcal{F}}} \mathbf{U}_{S} \right], \dots, \sum_{\mathcal{F} \in \mathfrak{I}} \sum_{S:|S|=n} \operatorname{tr} \left[ \mathbf{U}_{S}^{T} \mathbf{P}_{W_{\mathcal{F}}} \mathbf{U}_{S} \right] \right),$$
(3.11)

for all  $\mathfrak{I} = \{\mathcal{U}\}, \{\mathcal{U}, \mathcal{F}_1\}, \{\mathcal{U}, \mathcal{F}_2\}, \{\mathcal{U}, \mathcal{F}_3\}, \{\mathcal{U}, \mathcal{F}_1, \mathcal{F}_2\}, \{\mathcal{U}, \mathcal{F}_1, \mathcal{F}_3\}, \{\mathcal{U}, \mathcal{F}_2, \mathcal{F}_3\}, \{\mathcal{U}, \mathcal{F}_2, \mathcal{F}_3\}, \{\mathcal{U}, \mathcal{F}_2, \mathcal{F}_3\}, \{\mathcal{U}, \mathcal{F}_3, \mathcal{F}_3$ 

and  $\{\mathcal{U}, \mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3\}$ . Note that this is a scenario of orthogonal block structures but not simple block structures.

# 4. Examples: Minimum aberration designs under three scenarios

In this section, we apply the aberration criteria developed in Section 3 under (3.7) to three block structures. For the situations where **v** does not satisfy (3.7), it is easy to derive appropriate aberration criteria based on the results in Section 3 (e.g., (3.9)).

# 4.1 Eighteen-run nonregular designs

Suppose there are 18 unstructured experimental units. We have the block structure  $\{\mathcal{U}, \mathcal{E}\}$ . Consider a three-level 18-run orthogonal array of strength two in columns two to eight of Table 8C.2 of Wu and Hamada (2009), also given in Section S6 of the Supplementary Material. Many three-level 18-run nonregular designs with fewer factors can be obtained by deleting columns from the array.

For n = 3, Wang and Wu (1995) showed that there are three nonisomorphic designs. Xu and Wu (2001) gave their generalized wordlength patterns, which are (0, 0, 0.5), (0, 0, 1), (0, 0, 2). The first has generalized minimum aberration and, by Theorem 4, minimizes  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  for all  $\mathbf{v}$  satisfying (3.7). Moreover, because the sums of the generalized wordlengths of the three designs are 0.5, 1, and 2, respectively, it follows from  $(\mathbf{1}_N^T \mathbf{U}_{\phi})(\mathbf{1}_N^T \mathbf{U}_{\phi})^T =$  $\frac{N^2}{\Xi} = 12$  and Theorem 5 that  $\frac{3^3}{18^2}\{(18+2m)-12\} = l$  with l = 0.5, 1, 2 for the three designs. We have m = 0, 3, 9, respectively. Therefore, the first design does not have replicates, while the other two designs separately have 3 and 9 replicates.

For n = 4, Xu and Wu (2001) gave the generalized wordlength patterns of the only four nonisomorphic designs, which are (0, 0, 2, 1.5), (0, 0, 2.5, 1), (0, 0, 3.5, 0), and (0, 0, 3.5, 0). The first one has generalized minimum aberration and, by Theorem 4, minimizes  $\Phi_1^*(d; \boldsymbol{\xi}, \mathbf{v})$  for all  $\mathbf{v}$  satisfying (3.7). The sums of the generalized wordlengths are all equal to 3.5. By Theorem 5, we have  $\frac{3^4}{18^2}\{(18 + 2m) - 4\} = 3.5$ . Thus, m = 0 and these four designs have no replicates.

#### 4.2 Blocked mixed-level orthogonal arrays

Lin (2014) studied blocked mixed-level orthogonal arrays and listed several minimum aberration designs in terms of  $W_1$  and  $W_2$ . We consider a scenario in their study: 18-run blocked orthogonal arrays with three blocks of size six and four treatment factors, consisting of one two-level factor and three three-level factors. Each blocked orthogonal array is constructed by selecting five columns in Table 8C.2 of Wu and Hamada (2009), also given in Section S6 of the Supplementary Material, where one is the two-level column, one is a three-level column for blocking, and the others are three-level columns. There are  $7 \times C_3^6 = 140$  candidate designs.

A complete search shows that no design has minimum aberration with respect to both  $\mathfrak{W}_0$  and  $\mathfrak{W}_1$ . The minimum aberration design with respect to  $\mathfrak{W}_1$ , denoted by  $d^*$ , is constructed by selecting the eighth column for blocking, the first column for the two-level treatment factor, and the second, fourth, fifth columns for the three-level treatment factors. It has  $\mathfrak{W}_1 = (0, 0.125, 0.708, 1, 0.75, 0.042, 0)$ . Figure 1 gives the ranking of all 140 candidate designs in terms of  $\mathfrak{W}_1$ , where each point represents a design and the x-axis shows their rank values (average if tied, smaller the better). The black filled circle is  $d^*$ , with rank value one. The black filled square and black triangle represent those with minimum aberration in terms of  $W_1$  and  $W_2$ , respectively. We can see that the three minimum aberration designs under the three different aberration criteria do not coincide. As discussed in Section 3.2, the one obtained using  $W_2$  is closer to that using  $\mathfrak{W}_1$ . In addition,  $d^*$  has maximum D-efficiency under certain fixed-effects models. Refer to Section S7 of the Supplementary Material for details.



Figure 1: Comparison of  $\mathfrak{W}_1$ ,  $W_1$ , and  $W_2$ 

#### 4.3 Three-stage manufacturing process

Butler (2004) mentioned a three-stage manufacturing process with a few treatment factors in each stage. Suppose there are 36 experimental units and each stage consists of two three-level treatment factors. The 36 units are divided into six groups of equal size in each stage. We have the block structure { $\mathcal{U}, \mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{E}$ }, where each  $\mathcal{F}_i$  is a unit factor for one stage and partitions the 36 units into six classes. We also require that  $\mathcal{F}_1, \mathcal{F}_2$ , and  $\mathcal{F}_3$ define an orthogonal array of strength two that can be represented by the following Latin square (Wu and Hamada, 2009, p. 151):

А	В	С	D	Е	F	
В	С	F	А	D	Е	
С	F	В	Е	А	D	
D	Е	А	В	F	С	
Е	А	D	F	$\mathbf{C}$	В	
F	D	Е	С	В	А	

where each row, column, and letter represent a group of the first, second, and third stages, respectively. To reduce the computational burden, we assume that the interactions of the treatment factors across different stages are all negligible.

A complete search shows that the design given in Table 1 has minimum

aberration with respect to (3.11) for all  $\mathfrak{I} = \{\mathcal{U}\}, \{\mathcal{U}, \mathcal{F}_1\}, \{\mathcal{U}, \mathcal{F}_2\}, \{\mathcal{U}, \mathcal{F}_3\}, \{\mathcal{U}, \mathcal{F}_1, \mathcal{F}_2\}, \{\mathcal{U}, \mathcal{F}_1, \mathcal{F}_3\}, \{\mathcal{U}, \mathcal{F}_2, \mathcal{F}_3\}, \text{and } \{\mathcal{U}, \mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3\}, \text{with wordlength}$ patterns (0, 6), (16, 20), (16, 20), (16, 20), (32, 34), (32, 34), (32, 34), and (48, 48), respectively. Thus, it has minimum aberration with respect to  $\mathfrak{W}$  for all feasible  $\boldsymbol{\xi}$ . The three stages share the same design settings and balance, and are without replicates.

Stage 1		Stage 2		Stage 3	
0	0	0	0	0	0
0	1	0	1	0	1
1	0	1	0	1	0
1	2	1	2	1	2
2	1	2	1	2	1
2	2	2	2	2	2

Table 1: Minimum aberration design: Three-stage manufacturing process

## 5. Conclusion

We have developed a unified theory for aberration criteria using a Bayesian perspective. Our theory provides applications mixed-level/multi-group treatment factors, nonregular designs, and orthogonal block structures. Given design situations, experimenters can create suitable aberration criteria based on our theory. In addition, we provide a useful result to screen out inadmissible designs.

The block structures we consider require uniform unit factors. In real applications, however, this may not be feasible. For instance, this is impossible if the number of experimental units is not a multiple of the number of levels of some unit factor. Because this assumption is crucial to our theory, developing a more general theory is needed, and will be considered in future work.

## Supplementary Material

The online Supplementary Material contains all proofs and several additional explanations.

# Acknowledgments

We thank the referees for their helpful and constructive comments. This work was financially supported by the Ministry of Science and Technology (MOST) in Taiwan with grant number 107-2118-M-008-001-MY2, and the Young Scholar Fellowship Program (Einstein Program) under grant numbers 108-2636-M-008-004- and 109-2636-M-008-006-.

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