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Some optimal criteria of model-robustness for two-level non-regular fractional factorial designs

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Abstract We present some optimal criteria to evaluate model-robustness of non-regular two-level fractional factorial designs. Our method is based on minimizing the sum of squares of all the off-diagonal elements in the information matrix, and considering expectation under appropriate distribution functions for unknown contamination of the interaction effects. By considering uniform distributions on the symmetric support, our criteria can be expressed as linear combinations of $B_s(d)$ characteristic, which is used to characterize the generalized minimum aberration. We give some empirical studies for 12-run non-regular designs to evaluate our method.

Keywords Non-regular designs · Fractional factorial designs · Robustness · Affinely full-dimensional factorial designs · D-optimality

1 Introduction

The most commonly used designs for two-level factorial experiments are regular fractional factorial designs. This is because properly chosen regular fractional factorial designs have many desirable properties such as being orthogonal and balanced. In addition, we can easily consider important concepts such as resolution and aberration for the regular fractional factorial designs in applications. For example, under the hierarchical assumption, i. e, lower-order effects are more important than higher-order effects and effects of the same order are equally important, a minimum aberration criterion by Fries and Hunter (1980) seems natural and widely used. As another reason

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for using regular designs, an elegant theory based on the linear algebra over $\mathbb{F}_2$ is well established for regular two-level fractional factorial designs. See Mukerjee and Wu (2006) for example. The only drawback of using regular fractional factorial designs is that its run size must be a power of 2. Therefore if the run size of the design is restricted not to be a power of 2 by some cost or manufacturing limitations, we must consider non-regular fractional factorial designs. See Xu et al. (2009) for recent developments in non-regular fractional factorial designs.

One approach of optimal selection for non-regular designs is various extension of the minimum aberration criterion to non-regular designs. For example, Deng and Tang (1999) proposed a generalized minimum aberration criterion, which is a natural extension of the minimum aberration criterion from regular to non-regular designs. Tang and Deng (1999) also proposed a minimum G_2 aberration criterion, which is a simpler version of the generalized minimum aberration criterion. To justify these criteria, one approach is to evaluate these criteria from the viewpoint of model-robustness. For example, Cheng et al. (1999) shows that the designs with the minimum aberration have a good property of model-robustness. Similarly, Cheng et al. (2002) also investigates the generalized minimum aberration criterion from the viewpoint of model-robustness. In this paper, we follow these works and give a new criterion for model-robustness. Our new criterion is obtained as an extension of the approach by Cheng et al. (2002). We consider contamination of two- and three-factor interaction effects for estimating the main effects, whereas Cheng et al. (2002) only considers contamination of the two-factor interaction effects.

Another approach of choosing non-regular fractional factorial designs is proposed recently by Aoki and Takemura (2009). Aoki and Takemura (2009) defines a new class of two-level non-regular fractional factorial designs, called an affinely full-dimensional factorial design. The design points in the design of this class are not contained in any affine hyperplane in the vector space over $\mathbb{F}_2$. Aoki and Takemura (2009) also investigates the property of this class from the viewpoint of D-optimality. However, the arguments of Aoki and Takemura (2009) are restricted to the models of the main effects, and the property of this class in the case of the presence of the interaction effects is not yet obtained. In this paper, we also investigate the relation between our new criteria and the affinely full-dimensional factorial designs.

The construction of this paper is as follows. In Sect. 2, we give necessary definitions and notations for our criteria. We also review the generalized minimum aberration criterion and the affinely full-dimensional factorial designs briefly. In Sect. 3, we give definitions of our optimal criteria. One of the important contributions of this paper is to show the relation between our criteria and the generalized minimal aberration criterion. For this point, we give a general method to handle this problem and evaluate values for some cases. We also give empirical studies for 12-run non-regular designs.

2 Preliminaries

First we give necessary definitions and notations for our criteria. We use some of notations by Cheng et al. (2002). We also review the generalized minimum aberration criterion and affinely full-dimensional factorial designs.

2.1 Definition of $B_s(d)$ characteristic

Suppose there are m controllable factors with two levels. We represent an n-run design d by $X(d) \in \{-1, +1\}^{n\times m}$, an $n \times m$ matrix of -1's and $+1$'s. The (i, j)th element of $X(d)$, $x_{ij}(d)$, is the level of the jth factor in the ith run. Let $S = \{j_1, \ldots, j_s\} \subseteq \{1, \ldots, m\}$. Let $\boldsymbol{x}_S(d)$ be the component-wise product of the j_1th, ..., j_sth columns of $X(d)$. The ith element of $\boldsymbol{x}_S(d)$ can be written as $\prod_{j\in S} x_{ij}(d)$. Note that for any two subsets $S, T \subset \{1, \ldots, m\}$, the component-wise product of $\boldsymbol{x}_S(d)$ and $\boldsymbol{x}_T(d)$, say $\boldsymbol{x}_S(d) \odot \boldsymbol{x}_T(d)$, is written as $\boldsymbol{x}_S(d) \odot \boldsymbol{x}_T(d) = \boldsymbol{x}_{S\triangle T}(d)$, where $S\triangle T = (S \cup T) \setminus (S \cap T)$. We denote the cardinality of $S \subset \{1, \ldots, m\}$ by $|S|$. Then $|S| = s$ for $S = \{j_1, \ldots, j_s\}$. Define $j_S(d)$ as the sum of all the elements of $\boldsymbol{x}_S(d)$, i.e., $j_S(d) = \sum_{i=1}^{n} \prod_{j\in S} x_{ij}(d)$. For $s = 1, \ldots, m$, we define

$$B_s(d) = \frac{1}{n^2} \sum_{S:\ |S|=s} (j_S(d))^2.$$

$\{B_s(d), s = 1, \ldots, m\}$ is the key item in this paper. We call it $B_s(d)$ characteristic.

2.2 Generalized minimum aberration and affinely full-dimensional factorial designs

Now we give a relation between $B_s(d)$ characteristic and the generalized minimum aberration criterion and affinely full-dimensional factorial designs.

First we note that the set of $j_S(d)$ values over all the possible $S \subseteq \{1, \ldots, m\}$ has all the information of the design d. In fact, Tang (2001) shows that a design d is uniquely determined by the set of $j_S(d)$ values. Another basic fact is relation between $j_S(d)$ values and the coefficients in the indicator function of d defined by Fontana et al. (2000). From the definition of the indicator function, $j_S(d)/n = b_S/b_\phi$ holds, where b_S and b_ϕ are the coefficients of the term corresponding to S and the constant term, respectively, in the indicator function of d. See Fontana et al. (2000) for detail.

On the other hand, $B_s(d)$ characteristic has the information of the aberration of designs. For example, if two levels are equireplicated for each factor of the design d, $B_1(d) = 0$ holds. For the orthogonal designs, $B_2(d) = 0$ holds. If d is a regular design, $B_3(d) = 0$ holds for designs of the resolution IV, $B_3(d) = B_4(d) = 0$ holds for designs of the resolution V, and so on. Considering these facts and the hierarchical assumption, Tang and Deng (1999) defined the generalized minimum aberration criterion as to sequentially minimize $B_1(d), B_2(d), \ldots, B_m(d)$.

We also give the relation of the $j_S(d)$ values and the affinely full-dimensional factorial design. Note that, for regular designs, each $j_S(d)/n$ is $+1$, -1 or 0. By definition, $|j_S(d)/n| = 1$ implies an aliasing relation, whereas $|j_S(d)/n| = 0$ implies an orthogonality. For non-regular designs, on the other hand, $|j_S(d)/n|$ can be strictly between 0 and 1, leading to a partial aliasing relation. The affinely full-dimensional factorial design can be characterized as the design satisfying $0 \le |j_S(d)/n| < 1$ for all $S \subseteq \{1, \ldots, m\}$. See Lemma 2.2 of Aoki and Takemura (2009) for detail.

From these considerations, the relation between the generalized minimum aberration criterion and the affinely full-dimensionality is shown to some extent. Since $B_s(d)$

characteristic is the squared total of $j_S(d)/n$ for all S satisfying $|S| = s$, minimizing $B_s(d)$ coincides with minimizing each $j_S(d)$ for $|S| = s$ to some extent. The difference is that the generalized minimum aberration criterion considers sequentially minimizing $B_1(d), B_2(d), \ldots, B_m(d)$, whereas the affinely full-dimensionality considers simultaneous control that each $|j_S(d)/n|$ is strictly less than 1. The aim of this paper is to investigate this relation from the viewpoint of the model-robustness.

3 Optimal criteria for model-robustness

To evaluate the model-robustness of the designs, one approach is to consider the estimation capacity defined by Cheng et al. (1999). Though the original definition by Cheng et al. (1999) is restricted to the regular designs, this concept is generalized by Cheng et al. (2002) to non-regular designs. In this paper, we generalize their works and give general model-robustness criteria.

When we choose fractional factorial designs, we can rely on various optimal criteria such as D-optimality based on the information matrix if the model to be considered is known. On the other hand, if the model is unknown, which is more realistic situation, we have to evaluate the model-robustness. In this paper, we consider the situation where (i) all the main effects are of primary interest and their estimates are required, (ii) the experimenters suppose that there are f active two-factor interaction effects and g active three-factor interaction effects, but which of two- and three-factor interactions are active is unknown and (iii) all the four-factor and higher-order interactions are negligible. This situation is a natural extension of the setting of Cheng et al. (2002), where the case of $g = 0$ for equireplicated designs. Another important case is $f = \binom{m}{2}$, meaning that (i) all the main and the two-factor interaction effects are of interest and their estimates are required, (ii) there are g active three-factor interactions, but which of the three-factor interactions are active is unknown and (iii) all the four-factor and higher-order interactions are negligible. The aim of our model-robustness criteria is to evaluate the influence of contamination of active interaction effects on the parameter estimation.

3.1 $D_{f,g}$-criterion and $S^2_{f,g}$-criterion

First we derive an information matrix in our settings. Let $\mathcal{P}$ be the set of all the $\binom{m}{2}$ subsets of the size two of $\{1, \ldots, m\}$. Similarly, let $\mathcal{Q}$ be the set of all the $\binom{m}{3}$ subsets of the size three of $\{1, \ldots, m\}$. We have

$$\mathcal{P} = \{\{1, 2\}, \{1, 3\}, \ldots, \{m-1, m\}\},$$
$$\mathcal{Q} = \{\{1, 2, 3\}, \{1, 2, 4\}, \ldots, \{m-2, m-1, m\}\}$$

and define

$$|\mathcal{P}| = \binom{m}{2} = F, \quad |\mathcal{Q}| = \binom{m}{3} = G$$

for later use. Let $\mathcal{F} \subset \mathcal{P}$ and $\mathcal{G} \subset \mathcal{Q}$ be f active two-factor interactions and g active three-factor interactions, respectively. We write $|\mathcal{F}| = f$ and $|\mathcal{G}| = g$. Though we suppose that $\mathcal{F}$ and $\mathcal{G}$ are unknown, it is natural to restrict the models to be considered to satisfy the following hierarchical assumption.

Definition 1 $\mathcal{F}$ and $\mathcal{G}$ are called *hierarchically consistent* if

$$(i_1, i_2, i_3) \in \mathcal{G} \implies (i_1, i_2), (i_1, i_3), (i_2, i_3) \in \mathcal{F}.$$

For given $\mathcal{F}$ and $\mathcal{G}$, we consider a linear model

$$\boldsymbol{y} = \mu \mathbf{1}_n + X(d)\boldsymbol{\beta}_1 + Y_{\mathcal{F}}(d)\boldsymbol{\beta}_2 + Z_{\mathcal{G}}(d)\boldsymbol{\beta}_3 + \boldsymbol{\varepsilon},$$

where $\boldsymbol{y}$ is the $n \times 1$ vector of observations, μ is an unknown parameter of the general mean, $X(d)$ is the $n \times m$ matrix defined in Sect. 2.1, $\boldsymbol{\beta}_1$ is the $m \times 1$ vector of the main effects, $Y_{\mathcal{F}}(d)$ is an $n \times f$ matrix consisting of the f columns $\boldsymbol{x}_S(d)$, $S \in \mathcal{F}$, $\boldsymbol{\beta}_2$ is the $f \times 1$ vector of the active two-factor interactions, $Z_{\mathcal{G}}(d)$ is an $n \times g$ matrix consisting of the g columns $\boldsymbol{x}_S(d)$, $S \in \mathcal{G}$, $\boldsymbol{\beta}_3$ is the $g \times 1$ vector of the active three-factor interactions and $\boldsymbol{\varepsilon}$ is an $n \times 1$ random vector satisfying $E(\boldsymbol{\varepsilon}) = \mathbf{0}$, $var(\boldsymbol{\varepsilon}) = \sigma^2 I_n$. Let $X_{\mathcal{F},\mathcal{G}} = [\mathbf{1}_n \vdots X(d) \vdots Y_{\mathcal{F}}(d) \vdots Z_{\mathcal{G}}(d)]$. Then the information matrix for the observations of d is written as

$$M_{\mathcal{F},\mathcal{G}}(d) = \frac{1}{n} X_{\mathcal{F},\mathcal{G}}(d)' X_{\mathcal{F},\mathcal{G}}(d)$$

$$= \begin{bmatrix} 1 & \frac{1}{n}\mathbf{1}_n' X(d) & \frac{1}{n}\mathbf{1}_n' Y_{\mathcal{F}}(d) & \frac{1}{n}\mathbf{1}_n' Z_{\mathcal{G}}(d) \\ \frac{1}{n} X(d)'\mathbf{1}_n & \frac{1}{n} X(d)'X(d) & \frac{1}{n} X(d)'Y_{\mathcal{F}}(d) & \frac{1}{n} X(d)'Z_{\mathcal{G}}(d) \\ \frac{1}{n} Y_{\mathcal{F}}(d)'\mathbf{1}_n & \frac{1}{n} Y_{\mathcal{F}}(d)'X(d) & \frac{1}{n} Y_{\mathcal{F}}(d)'Y_{\mathcal{F}}(d) & \frac{1}{n} Y_{\mathcal{F}}(d)'Z_{\mathcal{G}}(d) \\ \frac{1}{n} Z_{\mathcal{G}}(d)'\mathbf{1}_n & \frac{1}{n} Z_{\mathcal{G}}(d)'X(d) & \frac{1}{n} Z_{\mathcal{G}}(d)'Y_{\mathcal{F}}(d) & \frac{1}{n} Z_{\mathcal{G}}(d)'Z_{\mathcal{G}}(d) \end{bmatrix}. \quad (1)$$

If $\{\mathcal{F}, \mathcal{G}\}$ is known, we can rely on various optimal criteria based on $M_{\mathcal{F},\mathcal{G}}(d)$ to choose d. For example, D-optimal criterion is to choose the design that maximize $\det M_{\mathcal{F},\mathcal{G}}(d)$. For the case that $\{\mathcal{F}, \mathcal{G}\}$ is unknown, it is natural to consider the average performance over all possible combinations of f two-factor interaction effects and g three-factor interaction effects. To clarify the arguments, we consider probability functions over the set of all the subsets of, $\mathcal{P}$, $\mathcal{Q}$, i.e., $2^{\mathcal{P}}$, $2^{\mathcal{Q}}$, and consider the expectation of $\det M_{\mathcal{F},\mathcal{G}}(d)$ with respect to this probability function. If we have no prior information, it is natural to consider the uniform distribution

$$p(\mathcal{F}, \mathcal{G}) = \begin{cases} \text{Const}, & \text{if } \mathcal{F} \text{ and } \mathcal{G} \text{ are hierarchically consistent} \\ 0, & \text{otherwise.} \end{cases}$$

Consequently, we can use the expectation $D_{f,g} = E_p[\det M_{\mathcal{F},\mathcal{G}}(d)]$ to evaluate the model-robustness. We call this a $D_{f,g}$-optimal criterion.

However, there is a problem that the calculation of $\det M_{\mathcal{F},\mathcal{G}}(d)$ is difficult. For this problem, we follow the approach by Cheng et al. (2002) and consider minimizing

$E_p[\mathrm{tr}(M_{\mathcal{F},\mathcal{G}}(d))^2]$ instead of maximizing $E_p[\det M_{\mathcal{F},\mathcal{G}}(d)]$. Note that the calculation of $\mathrm{tr}(M_{\mathcal{F},\mathcal{G}}(d))^2$ is considerably easier than that of $\det M_{\mathcal{F},\mathcal{G}}(d)$. It is also known that minimizing $\mathrm{tr}(M_{\mathcal{F},\mathcal{G}}(d))^2$ is a good surrogate for maximizing $\det M_{\mathcal{F},\mathcal{G}}(d)$. See Cheng (1996) for example. In addition, since all the diagonal elements of $M_{\mathcal{F},\mathcal{G}}(d)$ are 1, minimizing $E_p[\mathrm{tr}(M_{\mathcal{F},\mathcal{G}}(d))^2]$ is equivalent to minimizing the expectation of the sum of squares of all the off-diagonal elements of $M_{\mathcal{F},\mathcal{G}}(d)$. We write this value as

$$S^2_{f,g} = E_p[\text{sum of squares of all the off-diagonal elements of } M_{\mathcal{F},\mathcal{G}}(d)]$$

and define our criterion.

Definition 2 $S^2_{f,g}$-optimal criterion is to choose designs that minimize $S^2_{f,g}$.

3.2 Calculation of $S^2_{f,g}$ values

To evaluate the $S^2_{f,g}$ value, we have to calculate all the off-diagonal elements of $M_{\mathcal{F},\mathcal{G}}(d)$. We consider each block in the partitioned matrix (1) separately. First we see that the sum of squares of all the elements of $(1/n)\mathbf{1}_n' X(d)$ is $\sum_{i=1}^m (j_{\{i\}}(d))^2/n^2 = B_1(d)$ by definition. Similarly, the sum of squares of all the off-diagonal elements of $(1/n)X(d)'X(d)$ is $2\sum_{S\in\mathcal{P}}(j_S(d))^2/n^2 = 2B_2(d)$ by definition. Since the calculations of all the other blocks depend on the probability function $p(\mathcal{F},\mathcal{G})$, we have the following expression.

$$\begin{aligned} S^2_{f,g} = {} & 2B_1(d) + 2B_2(d) + 2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_S(d))^2\right] + 2E_p\left[\frac{1}{n^2}\sum_{i=1}^m\sum_{S\in\mathcal{F}}(j_{\{i\}\triangle S}(d))^2\right] \\ & + E_p\left[\frac{1}{n^2}\sum_{\substack{S,T\in\mathcal{F}\\ S\neq T}}\sum (j_{S\triangle T}(d))^2\right] + 2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{G}}(j_S(d))^2\right] \\ & + 2E_p\left[\frac{1}{n^2}\sum_{i=1}^m\sum_{S\in\mathcal{G}}(j_{\{i\}\triangle S}(d))^2\right] + 2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}\sum_{T\in\mathcal{G}}(j_{S\triangle T}(d))^2\right] \\ & + E_p\left[\frac{1}{n^2}\sum_{\substack{S,T\in\mathcal{G}\\ S\neq T}}\sum (j_{S\triangle T}(d))^2\right] \end{aligned} \tag{2}$$

Now all we have to do is to evaluate the expectations of (2) for specific values of f, g and $p(\mathcal{F},\mathcal{G})$. In this paper, we only consider the cases that $p(\mathcal{F},\mathcal{G})$ is the uniform distribution on the symmetric support for the factors $\{1,\ldots,m\}$. For these cases, $S^2_{f,g}$ is expressed as a linear combination of $B_1(d), B_2(d), \ldots, B_6(d)$. Note that $B_6(d)$ only arises in the last term of (2) as the contribution of $(j_{S\triangle T}(d))^2$ where S and T are disjoint. Though the uniform assumption on the symmetric support is natural, there are various important situations where the support of $p(\mathcal{F}, \mathcal{G})$ is asymmetric. For this point, we consider shortly in Sect. 4.

Unfortunately, it seems very difficult to derive $S^2_{f,g}$ values for general f, g values. One of the simpler problems, evaluation of $S^2_{f,1}$, is also difficult. In this paper, we obtain the results on some specific cases.

3.2.1 Calculation of $S^2_{f,0}$

First we consider the situation that all the three-factor interaction effects are negligible. This situation is considered in Cheng et al. (2002) for equireplicated designs and therefore our result is an extension of their result. In this case, the relation (2) becomes

$$S^2_{f,0} = 2B_1(d) + 2B_2(d) + 2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_S(d))^2\right] + 2E_p\left[\frac{1}{n^2}\sum_{i=1}^{m}\sum_{S\in\mathcal{F}}(j_{\{i\}\triangle S}(d))^2\right] + E_p\left[\frac{1}{n^2}\sum_{\substack{S,T\in\mathcal{F}\\ S\neq T}}\sum(j_{S\triangle T}(d))^2\right], \quad (3)$$

and we consider the uniform distribution on $\mathcal{P}$,

$$p(\mathcal{F}) = \frac{1}{\binom{F}{f}}.$$

The result is summarized as follows.

Theorem 1 *$S^2_{f,0}$ is written as $S^2_{f,0} = \sum_{s=1}^{4} a_s B_s(d)$, where*

$$a_1 = 2\left(1 + \frac{f(m-1)}{F}\right), \quad a_2 = 2\left(1 + \frac{f}{F} + \frac{f(f-1)}{F(F-1)}(m-2)\right),$$
$$a_3 = \frac{6f}{F} \quad \text{and} \quad a_4 = \frac{6f(f-1)}{F(F-1)}.$$

We give the proof in Appendix A. Note that the result except for a_1 is also given in Cheng et al. (2002). From Theorem 1, we see the following result.

Proposition 1 *The relation $a_1 > a_2 > a_3 > a_4$ holds for $m > 3$ for Theorem 1.*

We give the proof in Appendix B. Proposition 1 implies a consistency of the $S^2_{f,0}$-criterion and the generalized minimum aberration criterion. We see the optimal designs for these two criteria can be reversed by empirical studies for 12-run designs of 5 factors in Sect. 3.3.

3.2.2 Calculation of $S^2_{F,g}$

Next we consider the situation that all the two-factor interactions are active, i.e., the case of $f = F$. In this case, since $\mathcal{F} = \mathcal{P}$, we consider the uniform distribution on $\mathcal{Q}$ as

$$p(\mathcal{G}) = \frac{1}{\binom{G}{g}}.$$

The result is summarized as follows.

Theorem 2 *$S^2_{F,g}$ is written as $S^2_{F,g} = \sum_{s=1}^{6} a_s B_s(d)$, where*

$$\begin{aligned}
a_1 &= 2m + \frac{g(m-1)(m-2)}{G},\\
a_2 &= 2m + \frac{2g(m-2)}{G} + \frac{g(g-1)(m-2)(m-3)}{G(G-1)},\\
a_3 &= 6 + \frac{2g}{G} + \frac{6g(m-3)}{G},\\
a_4 &= 6 + \frac{8g}{G} + \frac{6g(g-1)(m-4)}{G(G-1)},\\
a_5 &= \frac{20g}{G} \quad \text{and}\\
a_6 &= \frac{20g(g-1)}{G(G-1)}.
\end{aligned}$$

We give the proof in Appendix C. From Theorem 2, we have the following result.

Proposition 2 *The relation $a_1 > a_2 > a_3 > a_4 > a_5 > a_6$ holds for $m > 5$ for Theorem 2.*

We give the proof in Appendix D. Proposition 2 implies a consistency of the $S^2_{F,g}$-criterion and the generalized minimum aberration criterion.

3.2.3 Calculation of $S^2_{3,1}$

Next we calculate $S^2_{3,1}$, which means the situation that there are one active three-factor interaction and three active two-factor interactions included in the three-factor interaction hierarchically. In this case, the joint probability function and its marginal probability functions are written as

$$p(\mathcal{F}, \mathcal{G}) = \begin{cases} \frac{1}{G}, & \text{if } \mathcal{F} \text{ and } \mathcal{G} \text{ are hierarchically consistent,}\\ 0, & \text{otherwise,} \end{cases}$$

$$p(\mathcal{G}) = \frac{1}{G}$$

and

$$p(\mathcal{F}) = \begin{cases} \frac{1}{G}, & \text{if there exists } \mathcal{G} \text{ such that } \mathcal{F} \text{ and } \mathcal{G} \text{ are hierarchically consistent} \\ 0, & \text{otherwise.} \end{cases}$$

The result is summarized as follows.

Theorem 3 *$S^2_{3,1}$ is written as $S^2_{3,1} = \sum_{s=1}^{4} a_s B_s(d)$, where*

$$\begin{aligned} a_1 &= 2\left(1 + \frac{9}{m}\right), \\ a_2 &= 2\left((m-1) + \frac{4(m-2)}{G}\right), \\ a_3 &= \frac{2(3m-5)}{G} \quad \text{and} \\ a_4 &= \frac{8}{G}. \end{aligned}$$

We give the proof in Appendix E. From Theorem 3, we have the following result.

Proposition 3 *The relation $a_2 > a_1 > a_3 > a_4$ holds for $m > 3$ for Theorem 3.*

We give the proof in Appendix F. Proposition 3 shows quite different tendency against Proposition 1 and Proposition 2, i.e., $a_1 < a_2$ holds. This fact implies an essential difference between the $S^2_{3,1}$-criterion and the generalized minimum aberration criterion, i.e., the $S^2_{3,1}$-criterion puts more importance on the orthogonality between the columns of $X(d)$ than the equireplicateness of two levels, which is mostly emphasized in the generalized minimum aberration criterion. Consequently, we can suppose the optimal designs for two criteria can be reversed. We investigate this point by empirical studies for 12-run designs of 5 factors in Sect. 3.3.

3.3 $S^2_{f,g}$-optimal designs for 12-run designs

To clarify the relation between the $S^2_{f,g}$-criterion and the generalized minimum aberration, we consider fractional factorial 12-run designs of 5 factors. We are also interested in the affinely full-dimensionality of the optimal designs. Note that all the fractional factorial designs with $n > 2^{m-1}$ are affinely full-dimensional since these designs cannot be a proper subset of any regular fractional factorial designs. See Aoki and Takemura (2009) for detail. Another reason that we consider 12-run designs is related to the existence of Hadamard matrix of order 12. Since the run size $n = 12$ is even, it is clear that the generalized minimum aberration criterion prefers the designs with equireplicated levels. It is also clear that we can easily construct orthogonal designs by choosing the columns of Hadamard matrices of order 12. See Deng et al. (2000) for example. From these considerations, we see that the optimal designs with the generalized minimum aberration satisfy $B_1(d) = B_2(d) = 0$. In fact, all the 12×5

Table 1 $S^2_{f,0}$- and $S^2_{3,1}$-optimal 12-run design of 5 factors

1	1	1	1	1
1	1	−1	−1	−1
1	−1	1	1	−1
1	−1	1	−1	1
1	−1	−1	1	1
−1	1	1	1	−1
−1	1	1	−1	1
−1	1	−1	1	1
−1	−1	1	1	1
−1	−1	1	−1	−1
−1	−1	−1	1	−1
−1	−1	−1	−1	1

Table 2 $S^2_{f,0}$, $f = 1, \ldots, 5$ and $S^2_{3,1}$ values for two deigns, d_h and d_s

	$S^2_{1,0}$	$S^2_{2,0}$	$S^2_{3,0}$	$S^2_{4,0}$	$S^2_{5,0}$	$S^2_{3,1}$
d_s	0.5556	0.9074	1.3333	1.8333	2.4074	1.7778
d_h	0.6667	1.4074	2.2222	3.1111	4.0741	2.6667

designs constructed from five columns (except for $\mathbf{1}_{12}$) of Hadamard matrices of order 12, say d_h, satisfy

$$B_1(d_h) = B_2(d_h) = 0, \quad B_3(d_h) = 1.1111, \quad B_4(d_h) = 0.5556.$$

We compare the $B_s(d)$ characteristics of the $S^2_{f,g}$-optimal designs with this value.

We enumerate all the fractional factorial designs of 5 factors with 12 runs and obtain $S^2_{f,0}$-optimal designs for $f = 1, \ldots, 5$ and $S^2_{3,1}$-optimal design. We have confirmed that all the optimal designs are equivalent to the design shown in Table 1 by permuting factors or levels and changing signs. This design satisfies the $S^2_{f,0}$-, $f = 1, \ldots, 5$ and $S^2_{3,1}$-optimality simultaneously. The $B_s(d)$ characteristics for this design, say d_s, are

$$B_1(d_s) = 0.138889, \quad B_2(d_s) = 0, \quad B_3(d_s) = 0.27778, \quad B_4(d_s) = 0.5556.$$

Since $B_1(d_s) > B_1(d_h)$, d_s does not have the generalized minimum aberration. We also see that d_s is an orthogonal design and $B_4(d_s) = B_4(d_h)$. The difference between the two designs in view of $B_s(d)$ characteristics lies in $B_1(d)$ and $B_3(d)$. We see that the generalized minimum aberration criterion puts the importance on $B_1(d)$, whereas the $S^2_{f,g}$-criteria consider the overall values. Table 2 shows the $S^2_{f,0}$, $f = 1, \ldots, 5$ and $S^2_{3,1}$ values for d_h and d_s.

We see that both d_h and d_s are affinely full-dimensional, and therefore not proper subsets of any regular fractional factorial designs. This fact implies that the simple strategies such as choosing 12 rows from regular 2^{5-1} fractional factorial designs to construct a 12-run design can cause a design of bad performance, in view of the generalized minimum aberration and model-robustness.

4 Discussion

We propose a general method to evaluate model-robustness for non-regular two-level designs. Though we suppose, in this paper, the four- and higher-factor interactions are negligible, which is considered to be a natural assumption in actual situations, we can easily generalize our method to incorporate higher-factor interactions.

It is also possible to calculate $S^2_{f,g}$ values for small f, g such as $S^2_{4,1}$, $S^2_{5,1}$ or $S^2_{5,2}$. Though the calculations will be rather complicated, they are indeed based on a simple counting. It is true that the assumption that the experimenters only have an information on the number of the interactions in the true model seems unnatural in actual situations. However, we think that the $S^2_{f,g}$ values for small f, g can be used to evaluate the model-robustness. Here we regard f and g as the degree of contamination of interactions.

Though we only consider the cases that $p(\mathcal{F}, \mathcal{G})$ is the uniform distribution on the symmetric support for the factors $\{1, \ldots, m\}$, there are various important situations where the support of $p(\mathcal{F}, \mathcal{G})$ is asymmetric. One of the examples for asymmetric cases is that (i) there are m_1 controllable factors and $m - m_1$ noise factors, (ii) all the main effects and two-factor interaction effects between the controllable factor and the noise factor are of primary interest and their estimates are required, (iii) all the two-factor interactions between two controllable factors are negligible. all the three- and higher-factor interactions are also negligible, and (iv) among the two-factor interactions between two noise factors, there are $f - m_1(m - m_1)$ active interactions. For this situation, it is the important problem to investigate the model-robustness of designs for the contamination of the two-factor interactions between two noise factors. However, for such asymmetric situation, $S^2_{f,g}$ values cannot be expressed as a linear combination of $B_s(d)$ characteristic. We postpone this attractive topic to future works.

Appendix A: Proof of Theorem 1

We evaluate the terms of (3) separately. First we have

$$E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_S(d))^2\right] = \frac{1}{\binom{F}{f}}\sum_{\mathcal{F}\subset\mathcal{P}}\sum_{S\in\mathcal{F}}\left(\frac{j_S(d)}{n}\right)^2$$

$$= \frac{1}{\binom{F}{f}}\frac{\binom{F}{f}f}{F}\sum_{S\in\mathcal{P}}\left(\frac{j_S(d)}{n}\right)^2 = \frac{f}{F}B_2(d).$$

Next from

$$\{i\}\triangle S = \begin{cases} S\setminus i, & \text{if } i\in S,\\ \{i, S\}, & \text{otherwise}\end{cases} \tag{4}$$

for $S \in \mathcal{F}$, we have

$$E_p\left[\frac{1}{n^2}\sum_{i=1}^{m}\sum_{S\in\mathcal{F}}(j_{\{i\}\triangle S}(d))^2\right]=\frac{1}{\binom{F}{f}}\sum_{\mathcal{F}\subset\mathcal{P}}\sum_{i=1}^{m}\sum_{S\in\mathcal{F}}\left(\frac{j_{\{i\}\triangle S}(d)}{n}\right)^2$$
$$=\frac{f}{F}\sum_{i=1}^{m}\sum_{S\in\mathcal{P}}\left(\frac{j_{\{i\}\triangle S}(d)}{n}\right)^2$$
$$=\frac{f}{F}\left((m-1)\sum_{i=1}^{m}\left(\frac{j_{\{i\}}(d)}{n}\right)^2+3\sum_{S\in\mathcal{Q}}\left(\frac{j_S(d)}{n}\right)^2\right)$$
$$=\frac{f}{F}((m-1)B_1(d)+3B_3(d)).$$

Similarly, for distinct $i, j, k, \ell \in \{1,\ldots,m\}$ we have

$$S\triangle T=\begin{cases}\{i,j\}, & \text{for } S=\{i,k\}, T=\{j,k\},\\ \{i,j,k,\ell\}, & \text{for } S=\{i,j\}, T=\{k,\ell\}.\end{cases} \tag{5}$$

Then it follows

$$E_p\left[\frac{1}{n^2}\sum_{\substack{S,T\in\mathcal{F}\\ S\neq T}}(j_{S\triangle T}(d))^2\right]=\frac{f(f-1)}{F(F-1)}\sum_{\substack{S,T\in\mathcal{P}\\ S\neq T}}\left(\frac{j_{S\triangle T}(d)}{n}\right)^2$$
$$=\frac{f(f-1)}{F(F-1)}(2(m-2)B_2(d)+6B_4(d))$$

by simple counting. From the above calculations, we have the theorem. □

Appendix B: Proof of Proposition 1

For $m > 3$, we have

$$a_1-a_2=\frac{2f(m-2)(F-f)}{F(F-1)}>0$$

and

$$a_3-a_4=\frac{6f(F-f)}{F(F-1)}>0.$$

From the relations

$$a_2-a_3=\frac{2}{F(F-1)}\{(m-2)f^2-(2F+m-4)f+F(F-1)\}$$

and

$$(2F+m-4)^2-4F(F-1)(m-2)=-(m-2)^2(m^3-m^2-5m-4)<0,$$

we have $a_2 > a_3$ for all f. Therefore we have shown the proposition. □

Appendix C: Proof of Theorem 2

From $\mathcal{F} = \mathcal{P}$ and simple counting, we have

$$2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_S(d))^2\right] = \frac{2}{n^2}\sum_{S\in\mathcal{P}}(j_S(d))^2 = 2B_2(d),$$

$$2E_p\left[\frac{1}{n^2}\sum_{i=1}^{m}\sum_{S\in\mathcal{F}}(j_{\{i\}\triangle S}(d))^2\right] = \frac{2}{n^2}\sum_{i=1}^{m}\sum_{S\in\mathcal{P}}(j_{\{i\}\triangle S}(d))^2$$
$$= 2((m-1)B_1+3B_3(d))$$

and

$$E_p\left[\frac{1}{n^2}\sum\sum_{\substack{S,T\in\mathcal{F}\\ S\neq T}}(j_{S\triangle T}(d))^2\right]$$
$$= \frac{1}{n^2}\sum\sum_{\substack{S,T\in\mathcal{P}\\ S\neq T}}(j_{S\triangle T}(d))^2 = 2(m-2)B_2(d)+6B_4(d).$$

Therefore (2) becomes

$$S^2_{f,g} = 2mB_1(d)+2mB_2(d)+6B_3(d)+6B_4(d)+2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{G}}(j_S(d))^2\right]$$
$$+2E_p\left[\frac{1}{n^2}\sum_{i=1}^{m}\sum_{S\in\mathcal{G}}(j_{\{i\}\triangle S}(d))^2\right]+2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}\sum_{T\in\mathcal{G}}(j_{S\triangle T}(d))^2\right]$$
$$+E_p\left[\frac{1}{n^2}\sum\sum_{\substack{S,T\in\mathcal{G}\\ S\neq T}}(j_{S\triangle T}(d))^2\right].$$

Now we consider the expectations above separately. From simple counting, we have

$$E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{G}}(j_S(d))^2\right] = \frac{g}{G}\sum_{S\in\mathcal{Q}}\left(\frac{j_S(d)}{n}\right)^2 = \frac{g}{G}B_3(d),$$

$$E_p\left[\frac{1}{n^2}\sum_{i=1}^{m}\sum_{S\in\mathcal{G}}(j_{\{i\}\triangle S}(d))^2\right] = \frac{g}{G}\sum_{i=1}^{m}\sum_{S\in\mathcal{Q}}\left(\frac{j_{\{i\}\triangle S}(d)}{n}\right)^2$$
$$= \frac{g}{G}((m-2)B_2(d)+4B_4(d))$$

from (4) for $S \in \mathcal{Q}$,

$$E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}\sum_{T\in\mathcal{G}}(j_{S\triangle T}(d))^2\right] = \frac{g}{G}\sum_{S\in\mathcal{P}}\sum_{T\in\mathcal{Q}}\left(\frac{j_{S\triangle T}(d)}{n}\right)^2$$
$$= \frac{g}{G}\left(\frac{(m-1)(m-2)}{2}B_1(d) + 3(m-3)B_3(d) + 10B_5(d)\right)$$

from

$$S\triangle T = \begin{cases} \{i_1\}, & \text{for } S=\{i_2,i_3\},\ T=\{i_1,i_2,i_3\} \\ \{i_1,i_2,i_3\}, & \text{for } S=\{i_3,i_4\},\ T=\{i_1,i_2,i_4\} \\ \{i_1,i_2,i_3,i_4,i_5\}, & \text{for } S=\{i_4,i_5\},\ T=\{i_1,i_2,i_3\} \end{cases}$$

for distinct $i_1,\ldots,i_5 \in \{1,\ldots,m\}$ and

$$E_p\left[\frac{1}{n^2}\sum\sum_{\substack{S,T\in\mathcal{G}\\ S\neq T}}(j_{S\triangle T}(d))^2\right] = \frac{g(g-1)}{G(G-1)}\sum\sum_{\substack{S,T\in\mathcal{Q}\\ S\neq T}}\left(\frac{j_{S\triangle T}(d)}{n}\right)^2$$
$$= \frac{g(g-1)}{G(G-1)}((m-2)(m-3)B_2(d) + 6(m-4)B_4(d) + 20B_6(d))$$

from

$$S\triangle T = \begin{cases} \{i_1,i_2\}, & \text{for } S=\{i_1,i_3,i_4\},\ T=\{i_2,i_3,i_4\} \\ \{i_1,i_2,i_3,i_4\}, & \text{for } S=\{i_1,i_2,i_5\},\ T=\{i_3,i_4,i_5\} \\ \{i_1,i_2,i_3,i_4,i_5,i_6\}, & \text{for } S=\{i_1,i_2,i_3\},\ T=\{i_4,i_5,i_6\} \end{cases}$$

for distinct $i_1,\ldots,i_6 \in \{1,\ldots,m\}$. From the above calculations, we have the theorem. □

Appendix D: Proof of Proposition 2

For $m > 5$, we have

$$a_1 - a_2 = \frac{g(m-2)(m-3)(G-g)}{G(G-1)} > 0,$$

$$a_3 - a_4 = \frac{6g(m-4)(G-g)}{G(G-1)} > 0$$

and

$$a_5 - a_6 = \frac{20g(G-g)}{G(G-1)} > 0.$$

For the relation between a_2 and a_3, we have

$$a_2 - a_3 = \frac{m-3}{G(G-1)}\{(m-2)g^2 - (4G+m-6)g + 2G(G-1)\}$$

and

$$\begin{aligned}
&(4G+m-6)^2 - 8G(G-1)(m-2) \\
&\quad = -8(m-4)G^2 + 16(m-4)G + (m-6)^2 \\
&\quad < -(m-4)(8G(G-2) - (m-4)) \\
&\quad < -(m-4)\left(8\frac{m^2(m-4)}{6}(G-2) - (m-4)\right) \\
&\quad = -\frac{(m-4)^2}{3}(4m^2(G-2) - 3) \\
&\quad < -\frac{(m-4)^2}{3}(4 \cdot 5^2 \cdot 8 - 3) < 0
\end{aligned}$$

since $G > m^2(m-4)/6$ holds for $m > 5$ and $m^2(G-2)$ is a monotone increasing function of m. Similarly, for the relation between a_4 and a_5, we have

$$a_4 - a_5 = \frac{6}{G(G-1)}\{(m-4)g^2 - (2G+m-6)g + G(G-1)\}$$

and

$$\begin{aligned}
&(2G+m-6)^2 - 4G(G-1)(m-4) \\
&\quad = -4(m-5)G^2 + 8(m-5)G + (m-6)^2 \\
&\quad < -(m-5)(4G(G-2) - (m-5)) \\
&\quad < -(m-5)\left(4\frac{m^2(m-5)}{6}(G-2) - (m-5)\right) \\
&\quad = -\frac{(m-5)^2}{3}(2m^2(G-2) - 3) \\
&\quad < -\frac{(m-5)^2}{3}(2 \cdot 5^2 \cdot 8 - 3) < 0
\end{aligned}$$

since $G > m^2(m-5)/6$ holds for $m > 5$ and $m^2(G-2)$ is a monotone increasing function of m. Therefore we have shown the proposition. □

Appendix E: Proof of Theorem 3

In this case, we write $\mathcal{G} = \{U\} \in \mathcal{Q}$ and $Z_{\mathcal{G}}(d) = \boldsymbol{x}_U(d)$. Then (2) becomes

$$\begin{aligned} S_{3,1}^2 = & 2B_1(d) + 2B_2(d) + 2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_S(d))^2\right] \\ & +2E_p\left[\frac{1}{n^2}\sum_{i=1}^m\sum_{S\in\mathcal{F}}(j_{\{i\}\triangle S}(d))^2\right] \\ & +E_p\left[\frac{1}{n^2}\sum\sum_{\substack{S,T\in\mathcal{F}\\ S\neq T}}(j_{S\triangle T}(d))^2\right] + 2E_p\left[\left(\frac{j_U(d)}{n}\right)^2\right] \\ & +2E_p\left[\frac{1}{n^2}\sum_{i=1}^m(j_{\{i\}\triangle U}(d))^2\right] + 2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_{S\triangle U}(d))^2\right]. \end{aligned} \tag{6}$$

We consider all the terms of (6) separately. From simple counting, we have

$$2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_S(d))^2\right] = 2\frac{m-2}{G}\sum_{S\in\mathcal{P}}\left(\frac{j_S(d)}{n}\right)^2 = \frac{2(m-2)}{G}B_2(d),$$

$$\begin{aligned} & 2E_p\left[\frac{1}{n^2}\sum_{i=1}^m\sum_{S\in\mathcal{F}}(j_{\{i\}\triangle S}(d))^2\right] \\ & = \frac{2}{G}\left(2\binom{m-1}{2}\sum_{i=1}^m\left(\frac{j_{\{i\}}(d)}{n}\right)^2 + (3+3(m-3))\sum_{S\in\mathcal{Q}}\left(\frac{j_S(d)}{n}\right)^2\right) \\ & = \frac{2(m-1)(m-2)}{G}B_1(d) + \frac{6(m-2)}{G}B_3(d) \end{aligned}$$

from (4) for $S \in \mathcal{F}$,

$$E_p\left[\frac{1}{n^2}\sum\sum_{\substack{S,T\in\mathcal{F}\\ S\neq T}}(j_{S\triangle T}(d))^2\right] = 2(m-2)\sum_{S\in\mathcal{P}}\left(\frac{j_S(d)}{n}\right)^2 = 2(m-2)B_2(d)$$

from (5) where $S \cap T \neq \emptyset$,

$$2E_p\left[\left(\frac{j_U(d)}{n}\right)^2\right] = \frac{2}{G}\sum_{U\in\mathcal{Q}}\left(\frac{j_U(d)}{n}\right)^2 = \frac{2}{G}B_3(d),$$

$$\begin{aligned}2E_p\left[\frac{1}{n^2}\sum_{i=1}^{m}(j_{\{i\}\triangle U}(d))^2\right] &= \frac{2}{G}\left((m-2)\sum_{S\in\mathcal{P}}\left(\frac{j_S(d)}{n}\right)^2 + 4\sum_{S:|S|=4}\left(\frac{j_S(d)}{n}\right)^2\right)\\ &= \frac{2(m-2)}{G}B_2(d) + \frac{8}{G}B_4(d)\end{aligned}$$

from (4) for $S = U \in \mathcal{Q}$ and

$$2E_p\left[\frac{1}{n^2}\sum_{S\in\mathcal{F}}(j_{S\triangle U}(d))^2\right] = \frac{2}{G}\frac{3G}{m}\sum_{i=1}^{m}\left(\frac{j_{\{i\}}(d)}{n}\right)^2 = \frac{6}{m}B_1(d)$$

from $S \subset U$ and $S\triangle U = U \setminus S$. From the above calculations, we have the theorem. □

Appendix F: Proof of Proposition 3

For $m > 3$, we have

$$\begin{aligned}a_2 - a_1 &= \frac{2}{mG}((m^2-2m-9)G + 4m(m-2))\\ &= \frac{m-2}{3G}(m^3-3m^2-7m+33) > 0,\end{aligned}$$

$$\begin{aligned}a_1 - a_3 &= \frac{2}{mG}((m+9)G - m(3m-5))\\ &= \frac{1}{3G}(m^3+6m^2-28m+23) > 0\end{aligned}$$

and

$$a_3 - a_4 = \frac{2}{G}(3m-9) > 0.$$

Therefore we have shown the proposition. □

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References

Aoki, S., Takemura, A. (2009). Some characterizations of affinely full-dimensional factorial designs. *Journal of Statistical Planning and Inference, 139*, 3525–3532.

Cheng, C. S. (1996). Optimal design: Exact theory. In S. Ghosh, C. R. Rao (Eds.), *Handbook of statistics* (Vol. 13, pp. 977–1006). Amsterdam: North-Holland.

Cheng, C. S., Steinberg, D. M., Sun, D. X. (1999). Minimum aberration and model robustness for two-level factorial designs. *Journal of Royal Statistics Society Series B, 61*, 85–93.

Cheng, C. S., Deng, L. Y., Tang, B. (2002). Generalized minimum aberration and design efficiency for nonregular fractional factorial designs. *Statistica Sinica, 12*, 991–1000.

Deng, L. Y., Tang, B. (1999). Generalized resolution and minimum aberration criteria for Plackett–Burman and other nonregular factorial designs. *Statistica Sinica, 9*, 1071–1082.

Deng, L. Y., Li, Y., Tang, B. (2000). Catalogue of small runs nonregular designs from Hadamard matrices with generalized minimum aberration. *Communications in Statistics—Theory and Methods, 29*, 1379–1395.

Fontana, R., Pistone, G., Rogantin, M. P. (2000). Classification of two-level factorial fractions. *Journal of Statistical Planning and Inference, 87*, 149–172.

Fries, A., Hunter, W. G. (1980). Minimum aberration 2^{k-p} designs. *Technometrics, 22*, 601–608.

Mukerjee, R., Wu, C. F. J. (2006). A modern theory of factorial designs. In *Springer series in statistics*. New York: Springer.

Tang, B. (2001). Theory of J-characteristics for fractional factorial designs and projection justification of minimum G_2-aberration. *Biometrika, 88*, 401–407.

Tang, B., Deng, L. Y. (1999). Minimum G_2-aberration for nonregular fractional factorial designs. *Annals of Statistics, 27*, 1914–1926.

Xu, H., Phoa, F. K. H., Wong, W. K. (2009). Recent developments in nonregular fractional factorial designs. *Statistics Surveys, 3*, 18–46.