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An optimality criterion for supersaturated designs with quantitative factors

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ABSTRACT

A supersaturated design (SSD) is a factorial design in which the degrees of freedom for all its main effects exceed the total number of distinct factorial level-combinations (runs) of the design. Designs with quantitative factors, in which level permutation within one or more factors could result in different geometrical structures, are very different from designs with nominal ones which have been treated as traditional designs. In this paper, a new criterion is proposed for SSDs with quantitative factors. Comparison and analysis for this new criterion are made. It is shown that the proposed criterion has a high efficiency in discriminating geometrically nonisomorphic designs and an advantage in computation.

1. Introduction

Factorial designs are commonly used in scientific studies. In such studies, a number of fixed levels (settings) are selected for each factor, and some level-combinations are then chosen in an experiment. The factors can be nominal (qualitative) or quantitative. A nominal factor is a factor whose levels can be ordered free; whereas, a quantitative factor requires its levels to be in order. Thus, different types of data analysis methods are required. The purpose of analyzing an experiment with nominal factors is to investigate whether there exist differences in treatment means and if they do, which treatment means are different. Many methods, such as ANOVA or multiple comparison testing, are often used for treatment comparison. On the other hand, methods of response surface exploration are often used to deal with the data of experiments with quantitative factors. It is thus obvious that we need different criteria for design classification and design selection for different types of factors.

For designs with nominal factors, the design properties should be invariant to level permutation within factors. This is referred to as *combinatorial isomorphism*. Designs with nominal factors have received a great deal of attention in the literature, e.g. the maximum resolution (Box and Hunter, 1961), minimum aberration (Fries and Hunter, 1980), clear effects (Wu and Chen, 1992), and general minimum lower order confounding (Zhang et al., 2008) criteria for regular designs, and the minimum G_2-aberration (Tang and Deng, 1999), generalized minimum aberration (GMA, Deng and Tang, 1999; Ma and Fang, 2001; Xu and Wu, 2001), minimum moment aberration (Xu, 2003), discrete discrepancy (Fang et al., 2003), minimum projection uniformity (Hickernell and Liu, 2002), and minimum hybrid aberration (Pang and Liu, 2010) for nonregular designs. Note that all these criteria are invariant to level permutation and only applicable to designs with nominal factors.

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Table 1
Two combinatorially isomorphic designs each with six runs and three three-level factors.

Design I				Design II		
A	*B*	*C*		*A*	*B*	*C*
0	0	0		1	0	0
0	1	1		1	1	1
1	0	2	$\{0,1,2\} \leftrightarrow \{1,0,2\}$	0	0	2
1	2	0	on factor *A*	0	2	0
2	1	2		2	1	2
2	2	1		2	2	1

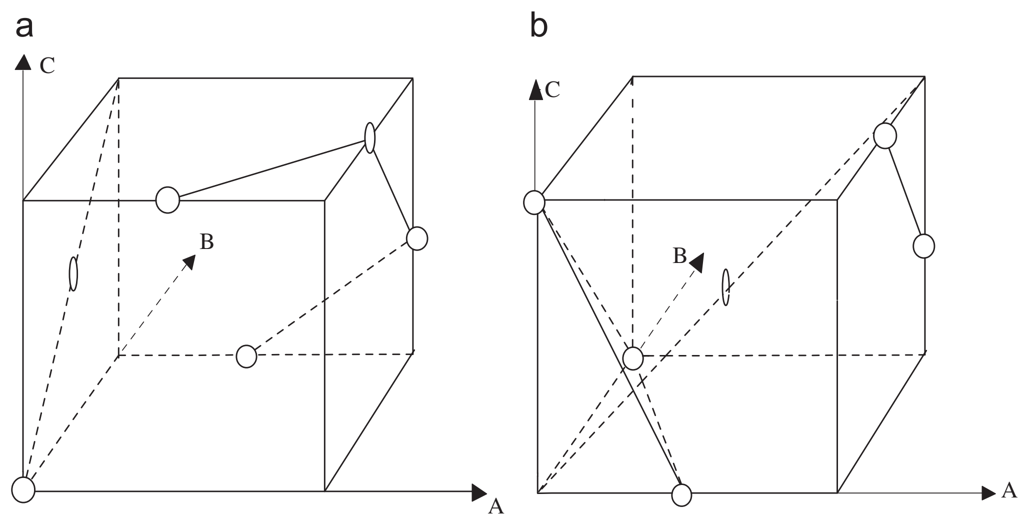

Fig. 1. Geometric structures for the two designs in Table 1. (a) Design I. (b) Design II.

For designs with quantitative factors, in which their level permutations could result in different data analysis, the above criteria may not be appropriate. Table 1 shows two designs with six runs and three three-level factors, where each column represents a factor and each row represents an experimental run. These designs are combinatorially isomorphic since one is obtained by applying the permutation $\{0,1,2\} \rightarrow \{1,0,2\}$ on factor *A* of the other. However, if these levels are quantitative, their geometric structures are apparently different as shown in Fig. 1. For example, there is a "central point" in Fig. 1(a) for Design I whilst no "central point" in Fig. 1(b) for Design II.

Supersaturated design (SSD) is a kind of factorial design in which the number of runs is insufficient to estimate all the main effects. It has recently received much interest mainly because of its potential in factor screening, namely, to efficiently identify a few active factors among many candidate factors at the initial step; see for example, Lin (1993, 1995, 2003). Multi-level and mixed-level SSDs arise, when two-level SSDs could not meet some specific experimental demands, see e.g. Liu and Lin (2009) for a motivating example and Sun et al. (2011) for some most recent construction results. There are many criteria specially defined for evaluating multi-level and mixed-level SSDs, such as, the $E(d^2)$ (Lu and Sun, 2001), $\chi^2(D)$ (Yamada and Matsui, 2002) and $E(f_{NOD})$ (Fang et al., 2003) criteria, see Section 2.3 below for the relevant definitions. Of course, these criteria are also invariant to level permutation within the factors and only applicable to SSDs with nominal factors.

Take the two designs in Table 1 as an example. It can be seen that they take the same values of $E(d^2)$, $E(f_{NOD})$ and $\chi^2(D)$, respectively, and cannot be discriminated under any of these criteria though they have the different geometric structures as shown in Fig. 1. It is thus desirable to have a new criterion to evaluate multi-level and mixed-level SSDs with quantitative factors.

In this paper, we propose a new criterion, specifically for SSDs with quantitative factors, to distinguish the geometrically nonisomorphic designs. Section 2 introduces some terminology and existing aberration criteria. The new criterion is proposed in Section 3. Section 4 provides some analysis and comparison results. Section 5 presents some concluding remarks.

2. The aberration criteria

In this section, we first review relevant notations and terminology, then discuss the β WLP and GMA criterion due to Cheng and Ye (2004), followed by the generalized WLP and GMA criterion due to Xu and Wu (2001). Existing criteria for SSDs and their relations are also reviewed here. A new criterion will be proposed in next section.

2.1. Notations and terminology

Let $\mathcal{D}$ be a design space of the full factorial design with n factors and v design points, denoted as $\mathcal{D}(v,s_1s_2\cdots s_n)$, where $v=s_1s_2\cdots s_n$, the levels of the ith factor are set at $G_i=\{0,1,\ldots,s_i-1\}, i=1,\ldots,n$. An n-factor design D with N runs is said to be in $\mathcal{D}$ if for any run $\mathbf{x}\in D$, $\mathbf{x}\in\mathcal{D}$, and we denote this design as $D(N,s_1s_2\cdots s_n)$. A design $D(N,s_1s_2\cdots s_n)$ is called *balanced* if all the levels occur equally often in each factor, and called *supersaturated* when $\sum_{i=1}^{n}(s_i-1)>N-1$. The following two definitions are due to Cheng and Ye (2004).

Definition 1. Let D be a design in the design space $\mathcal{D}$. The indicator function $F_D(\mathbf{x})$ of D is a function defined on $\mathcal{D}$ which calculates the number of appearances of point $\mathbf{x}$ in design D for $\mathbf{x}\in\mathcal{D}$.

Definition 2. Let D_1 and D_2 be two designs from the same design space $\mathcal{D}$. They are said to be *geometrically isomorphic* if one can be obtained from the other by relabeling the factors and/or reversing the level order of one or more factors.

It is clear that the indicator function $F_D(\mathbf{x})$ uniquely represents a design. Let $\mathcal{T}=G_1\times\cdots\times G_n$. For the ith factor of an n-factor design, define a set of orthogonal contrasts $P_0^i(x),P_1^i(x),\ldots,P_{s_i-1}^i(x)$ such that

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

Then an *orthonormal contrast basis* (OCB) on $\mathcal{D}$ is defined as

$$P_{\mathbf{t}}(\mathbf{x})=\prod_{i=1}^{n}P_{t_i}^i(x_i)$$

for $\mathbf{t}=(t_1,t_2,\ldots,t_n)\in\mathcal{T}$ and $\mathbf{x}=(x_1,x_2,\ldots,x_n)\in\mathcal{D}$. It is obvious that

$$\sum_{\mathbf{x}\in\mathcal{D}}P_{\mathbf{t}}(\mathbf{x})P_{\mathbf{u}}(\mathbf{x})=\begin{cases}0 & \text{if } \mathbf{t}\neq\mathbf{u},\\ v & \text{if } \mathbf{t}=\mathbf{u},\end{cases}$$

where $\mathbf{t}$ and $\mathbf{u}$ are the elements in the set $\mathcal{T}$. If $P_0^i(x)=1$ for all i, then we call $\{P_{\mathbf{t}}(\mathbf{x})\}$ a *statistical orthonormal contrast basis* (SOCB). When $P_j^i(x)$ is a polynomial of degree j for $j=0,1,\ldots,s_i-1$ and $i=1,2,\ldots,n$, the SOCB is called an *orthogonal polynomial basis* (OPB, see Draper and Smith, 1998, Chapter 22).

2.2. β wordlength pattern

For the indicator function $F_D(\mathbf{x})$ and OCB $\{P_{\mathbf{t}}(\mathbf{x}),\mathbf{t}\in\mathcal{T}\}$, Cheng and Ye (2004) showed that

$$F_D(\mathbf{x})=\sum_{\mathbf{t}\in\mathcal{T}}b_{\mathbf{t}}P_{\mathbf{t}}(\mathbf{x})$$

for all $\mathbf{x}\in\mathcal{D}$, and the coefficients $\{b_{\mathbf{t}},\mathbf{t}\in\mathcal{T}\}$ are uniquely determined as

$$b_{\mathbf{t}}=\frac{1}{v}\sum_{\mathbf{x}\in D}P_{\mathbf{t}}(\mathbf{x}). \tag{1}$$

Particularly, $b_{\mathbf{0}}=N/v$ with $\mathbf{0}=(0,0,\ldots,0)$. Then the β WLP and aberration criterion for factorial designs with quantitative factors can be defined as follows.

Definition 3. Let D be a $D(N,s_1s_2\ldots s_n)$ with quantitative factors in design space $\mathcal{D}$ and let $\{P_{\mathbf{t}}(\mathbf{x})\}$ be an OPB. The β WLP $(\beta_1(D),\ldots,\beta_K(D))$ is defined as

$$\beta_i(D)=\sum_{\|\mathbf{t}\|_1=i}(b_{\mathbf{t}}/b_{\mathbf{0}})^2. \tag{2}$$

The GMA criterion is to sequentially minimize β_i for $i=1,2,\ldots,K$, where $K=\sum_{i=1}^{n}(s_i-1)$ and $\|\mathbf{t}\|_1=\sum_{j=1}^{n}t_j$.

Remark 1. Note that in this definition, if we let $\{P_{\mathbf{t}}(\mathbf{x})\}$ be an SOCB, and replace $\beta_i(D)$ by

$$\alpha_i(D)=\sum_{\|\mathbf{t}\|_0=i}(b_{\mathbf{t}}/b_{\mathbf{0}})^2 \quad \text{for } i=1,2,\ldots,n, \tag{3}$$

where $\|\mathbf{t}\|_0=i$ represents the number of nonzero elements in $\mathbf{t}$, then we have the generalized WLP $(\alpha_1(D),\ldots,\alpha_n(D))$ and the GMA criterion due to Xu and Wu (2001) for designs with nominal factors. And this aberration criterion is invariant to level permutation as well as the choice of contrasts.

The only distinction between these two WLPs are the norms of $\mathbf{t}$ used in (2) and (3), which reflect the difference in ordering effects for quantitative and nominal factors. For a given design, the sum of its α_i's is the same as the sum of its β_i's. Cheng and Ye (2004) showed that this sum is a constant for designs that have the same run sizes and replication patterns. Furthermore, Cheng and Ye (2004, Corollary 4.1) proved that two designs with different β WLPs must be geometrically nonisomorphic. And for most cases, two geometrically nonisomorphic designs also have distinct β WLPs, see e.g. Tsai et al. (2006). Thus, the β WLP can be used to classify and select designs with quantitative factors.

2.3. *Existing criteria for SSDs and their relations*

SSDs are nonregular factorial designs, in which, orthogonality is not obtainable. Most existing criteria for SSDs measure the non-orthogonality combinatorially between two factors. We next review some existing criteria for multi-level and mixed-level SSDs.

For a design $D(N, s_1 \cdots s_n)$, define

$$\chi^2(i,j) = \sum_{u,v} (n_{uv}^{(ij)} - N/(s_i s_j))^2 / (N/(s_i s_j)),$$

where $n_{uv}^{(ij)}$ is the number of runs in which the ith and jth factors take the level-combination uv. Then the $\chi^2(D)$ criterion proposed by Yamada and Matsui (2002) is to minimize

$$\chi^2(D) = \sum_{1 \le i < j \le n} \chi^2(i,j).$$

And the $E(f_{NOD})$ criterion proposed by Fang et al. (2003) is to minimize

$$E(f_{NOD}) = \sum_{1 \le i < j \le n} (\chi^2(i,j) N/(s_i s_j)) \Big/ \binom{n}{2}.$$

When $s_1 = \cdots = s_n = s$, $E(f_{NOD})$ reduces to the $E(d^2)$ proposed by Lu and Sun (2001).

Note that Xu and Wu (2005) used the $\alpha_2(D)$ as a criterion for multi-level SSDs. Recently, Liu et al. (2006) generalized the $\chi^2(D)$ criterion to the so-called *minimum* χ^2 *criterion*, and provided statistical justification for both $\alpha_2(D)$ and $\chi^2(D)$. They showed that

$$\alpha_2(D) = \chi^2(D)/N, \qquad (4)$$

when D is a balanced design, and furthermore

$$\alpha_2(D) = \chi^2(D)/N = s^2 \binom{n}{2} E(f_{NOD}) \Big/ N^2 = s^2 \binom{n}{2} E(d^2) \Big/ N^2, \qquad (5)$$

when all factors have s levels. Obviously, all these criteria for SSDs attempt to minimize the aberration between two factors, and they are invariant to level permutation. Hence they are not applicable to designs with quantitative factors.

3. A new aberration criterion for SSDs

Since SSDs are typically used in factor screening experiments, i.e., to identify few active factors among many potential factors, the first- and second-order aberrations are dominated. We thus propose the γ WLP below to characterize such an important feature for quantitative factors.

Definition 4. Let D be a $D(N, s_1 s_2 \cdots s_n)$ with quantitative factors in design space $\mathcal{D}$ and let $\{P_{\mathbf{t}}(\mathbf{x})\}$ be an OPB. Then the new WLP $(\gamma_1(D), \ldots, \gamma_{K'}(D))$, called the γ *WLP*, is defined as

$$\gamma_i(D) = \sum_{\|\mathbf{t}\|_0 \le 2, \|\mathbf{t}\|_1 = i} (b_{\mathbf{t}}/b_{\mathbf{0}})^2, \quad i = 1, 2, \ldots, K', \qquad (6)$$

where $K' = \max\{s_i + s_j - 2 : i \ne j,\ i,j = 1, \ldots, n\}$, and $b_{\mathbf{t}}$ is defined in (1). The new GMA criterion is to sequentially minimize γ_i for $i = 1, 2, \ldots, K'$.

Example 1. For SSDs with quantitative factors, Definition 4 only considers the main effects and two-factor interactions. Consider the case of a three-level factorial design with quantitative factors. Each factor has three orthogonal polynomial contrasts: P_0^i, P_1^i, P_2^i, $i = 1, \ldots, n$, where P_0^i represents a constant term, denoted as "0"; P_1^i is the linear contrast, denoted as "l"; and P_2^i is the quadratic one, denoted as "q". A main effect or two-factor interaction can be denoted by two contrasts. Then the order of effect importance according to the γ WLP is

$$0l == l0 \gg 0q == q0 == ll \gg lq == ql \gg qq,$$

where $\gg$ means "more important than" while $==$ means "as important as"; and $0l$ and $l0$ indicate linear main effects, $0q$ and $q0$ indicate quadratic main effects, lq linear-by-quadratic interaction, etc. An important feature of SSD is its balance property. For a balanced design, it can be shown that $b_{\mathbf{t}} = 0$ for all t with only one nonzero element. For the three-level case, this implies that the linear main effects $0l$ and $l0$, and the quadratic main effects $0q$ and $q0$, have zero correlations with the constant term. So $\gamma_1(D) = 0$, and thus $\gamma_2(D)$ can be easily computed. The γ WLP now reduces to

$(0,\gamma_2(D),\gamma_3(D),\gamma_4(D))$, and the order of effect importance needed to be considered is simplified to

$$ll \gg lq = = ql \gg qq.$$

From (2) and (6), it is obvious that

$$\gamma_i(D) = \beta_i(D) \quad \text{for } i = 1,2$$

for any $D(N,s_1 s_2 \cdots s_n)$ design D with quantitative factors in design space $\mathcal{D}$. Note that $\sum_{i=1}^{K'} \gamma_i(D) = \alpha_1(D) + \alpha_2(D)$ and $\alpha_1(D) = 0$ for a balanced design. We thus have the following theorems regarding the properties of the γ WLP.

Theorem 1. *Let D be a balanced design in design space $\mathcal{D}$, then the sum of $\gamma_i(D)$'s in the γ WLP equals the $\alpha_2(D)$ defined in* (3), *i.e.*

$$\sum_{i=1}^{K'} \gamma_i(D) = \alpha_2(D).$$

Theorem 2. *Let D_1 and D_2 be two geometrically isomorphic designs in design space $\mathcal{D}$. Then their γ WLPs are identical.*

Theorem 1 shows that balanced designs with the same $\alpha_2(D)$ value take the same sum of $\gamma(D)$'s. For any given design with quantitative factors, level permutation may generate designs with different geometric structures, but with the same $\alpha_2(D)$ value (see Remark 1), and hence these resulting designs have the unique sum of $\gamma_i(D)$'s. While Theorem 2 shows that two designs with different γ WLPs must be geometrically nonisomorphic, thus one can differentiate geometrically nonisomorphic designs by comparing their γ WLPs. The proof of Theorem 2 can be straightforwardly obtained, by applying Theorem 3.1 of Cheng and Ye (2004).

Remark 2. For conventional factorial designs (where the number of experimental runs exceeds the number of parameters in the model), the β WLP can be used for quantitative factors to differentiate their geometrical isomorphism. For SSDs, however, all existing criteria are only good for designs with nominal factors. The proposed γ WLP appears to be the first criterion to consider both—it is useful for SSDs with quantitative factors. Note that the β WLP is lengthy and much more complicated to evaluate than the γ WLP. This can be seen by, when $n>2$, $K = \sum_{i=1}^{n}(s_i - 1) > K' = \max\{s_i + s_j - 2 : i \neq j,\ i,j = 1,\dots,n\}$, where K and K' are the total number of elements of β and γ WLP, respectively. Moreover, β WLP involved with many high-order interactions which are normally irrelevant in SSDs.

The next section contains some comparison and analysis results for applying the γ and β WLPs to discriminate geometrically nonisomorphic SSDs.

4. Comparisons and analysis

The basic strategy for applying the γ WLP is as follows:

Step 1. Select a good SSD according to a traditional criterion. As we can see from (4) and (5), an SSD having a smaller value of $\chi^2(D)$ or $E(f_{NOD})$ also has a smaller value of $\alpha_2(D)$, which implies that the design has a smaller sum of $\gamma_i(D)$'s. Thus $\chi^2(D)$ or $E(f_{NOD})$ optimal SSDs are preferred in this stage.

Step 2. For each SSD selected in the first stage, apply level permutations to each factor, and then compute the γ WLPs of the resulting designs. Based on Theorem 2, the resulting designs with different γ WLPs are geometrically nonisomorphic.

Step 3. From the resulting designs, find the optimal ones under the new GMA criterion.

In the following, three examples of multi-level SSDs (Examples 2–4) and one example of mixed-level SSD (Example 5) will be demonstrated for selecting and comparing the geometrically nonisomorphic designs. The β WLPs will also be computed for comparison.

Example 2. Consider the design in Table 4 of Fang et al. (2004) as an illustration. It is an $E(f_{NOD})$- and $\chi^2(D)$-optimal $D(6,3^5)$ design. The design is given in Table 2, where the five factors are headed by A, B, C, D and E, respectively.

Note that there are a total of six permutations among three levels. The six permutations can be divided into three pairs as shown in Table 3. In each pair of the three kinds of permutations, level 0 and level 2 exchange their positions while level 1 stays at its position, i.e., $0,1,2 \to 2,1,0$, $1,2,0 \to 1,0,2$ and $2,0,1 \to 0,2,1$. Therefore, within each pair, one permutation is the reverse of the other, hence, only one is needed in generating geometrically nonisomorphic designs. These three pairs of permutations are denoted as a, b and c in the first row of Table 3. For this design, permutations are applied to each factor to search for all geometrically nonisomorphic designs. Then following the steps given above, we have the results presented in Table 4. Note that in Table 4, "*baaaa*" represents the design obtained by applying permutations b,a,a,a and a (as illustrated in Table 3), respectively to the five factors A, B, C, D and E, and so on. It can be seen from Table 4 that both the γ and β WLPs agree upon the identical optimal designs.

Table 2
$D(6,3^5)$ from Fang et al. (2004).

A	B	C	D	E
0	0	0	0	0
0	1	1	1	1
1	0	2	2	1
1	2	0	1	2
2	1	2	0	2
2	2	1	2	0

Table 3
Six permutations of three levels.

a	b	c
0	1	2
1	2	0
2	0	1
↷	↷	↷
2	1	0
1	0	2
0	2	1

Table 4
Example 2—optimal designs according to γ and β WLPs for the design in Table 2.

Subject	γ WLP	β WLP
Optimal WLP	(0, 0.625, 3.75, 0.625)	(0, 0.625, 7.5, 8.8281, 4.6875, 10.625, 4.6875, 1.0156, 0, 1.5313)
Optimal designs	*baaaa, caaaa, bbbca, cbbca, bcbca, ccbca, bbcca, cbcca, bccca, cccca*	*baaaa, caaaa, bbbca, cbbca, bcbca, ccbca, bbcca, cbcca, bccca, cccca*

Table 5
Example 3—$D(8,4^4)$ from Xu and Wu (2005).

A	B	C	D
0	0	0	0
1	1	1	1
2	2	2	2
3	3	3	3
0	1	2	3
1	2	3	0
2	3	0	1
3	0	1	2

Note that, since $\gamma_1(D)=\beta_1(D)=0$, we only need to compute three elements $\gamma_2(D)$, $\gamma_3(D)$ and $\gamma_4(D)$ for each γ WLP, but have to compute nine elements for each β WLP. Moreover, the results show that the γ WLP performs efficiently in finding the optimal SSDs.

Example 3. Next we consider a four-level $D(8,4^4)$ design, given in Table 5. This design is optimal under the GMA criterion defined in Remark 1, hence it is also optimal under the $E(f_{NOD})$ and $\chi^2(D)$ criteria.

For the four-level case, there are a total of 24 permutations which can be divided into 12 different pairs as shown in Table 6. The numbers $a,b,\ldots,l$ in the first row of the table represent these 12 pairs. As shown in Table 6, with level exchanges $0\to3$, $1\to2$, $2\to1$ and $3\to0$, we could get one permutation from the other in each pair. Take the two permutations in column f as an example, with the level exchanges, 0, 3, 2, 1 becomes 3, 0, 1, 2, accordingly. Similar to Example 2, Table 7 is obtained.

From Table 7, we see that both the γ and β WLPs find the identical optimal designs. However, the γ WLP can save much more computational efforts than the β WLP.

There are often more than one optimal multi-level SSDs under the $E(f_{NOD})$ or $\chi^2(D)$ criteria, these designs have the same $\alpha_2(D)$ value (cf. Eq. (5)). Then if all factors are quantitative, they will have the same sum of $\gamma_i(D)$'s. Thus we can further

Table 6
Example 3—12 pairs of permutations among four levels.

a	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*	*l*
0	0	0	0	0	0	1	1	1	1	1	1
1	1	2	2	3	3	0	0	2	2	3	3
2	3	1	3	1	2	2	3	0	3	0	2
3	2	3	1	2	1	3	2	3	0	2	0
↷	↷	↷	↷	↷	↷	↷	↷	↷	↷	↷	↷
3	3	3	3	3	3	2	2	2	2	2	2
2	2	1	1	0	0	3	3	1	1	0	0
1	0	2	0	2	1	1	0	3	0	3	1
0	1	0	2	1	2	0	1	0	3	1	3

Table 7
Example 3—optimal designs according to γ and β WLPs for the design in Table 5.

Subject	γ WLP	β WLP
Optimal WLP	(0, 0.04, 0, 5.92, 0, 0.04)	(0, 0.04, 0, 9.36, 0, 11.12, 0, 8.52, 0, 1.96, 0, 0)
Optimal designs	*dlgb, lgbd, bdlg, gbdl*	*dlgb, lgbd, bdlg, gbdl*

Table 8
Example 4—$D(9,3^{4\,s})$ $(1 \le s \le 7)$.

1				2				3				4				5				6				7			
0	2	1	0	2	0	0	0	1	1	2	0	1	0	1	2	0	1	0	2	1	2	0	1	0	0	2	1
0	0	2	1	0	2	1	0	2	0	0	0	1	1	2	0	1	0	1	2	0	1	0	2	1	2	0	1
1	2	0	1	0	0	2	1	0	2	1	0	2	0	0	0	1	1	2	0	1	0	1	2	0	1	0	2
0	1	0	2	1	2	0	1	0	0	2	1	0	2	1	0	2	0	0	0	1	1	2	0	1	0	1	2
1	0	1	2	0	1	0	2	1	2	0	1	0	0	2	1	0	2	1	0	2	0	0	0	1	1	2	0
1	1	2	0	1	0	1	2	0	1	0	2	1	2	0	1	0	0	2	1	0	2	1	0	2	0	0	0
2	0	0	0	1	1	2	0	1	0	1	2	0	1	0	2	1	2	0	1	0	0	2	1	0	2	1	0
2	1	1	1	2	1	1	1	2	1	1	1	2	1	1	1	2	1	1	1	2	1	1	1	2	1	1	1
2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2

Table 9
Example 4—optimal designs according to γ WLP based on the designs in Table 8.

γ WLP	Optimal design
(0, 1.25, 5.5, 1.25)	*1 2* (*aabb baba*) *2 3* (*aabb baba*) *3 4* (*aabb aabb*) *4 5* (*aabb baba*) *5 6* (*aabb aabb*) *6 7* (*aabb baba*) *1 4* (*baab baba*) *2 5* (*baab baba*) *3 6* (*abaa abcb*) *4 7* (*baab baba*) *1 6* (*aaab abcb*) *2 7* (*aaab abcb*) *1 7* (*baba aaba*)
(0, 1.5, 5, 1.5)	*1 3* (*baaa bbbb*) *2 4* (*baab bbcb*) *3 5* (*baab bbcb*) *4 6* (*baab bbcb*) *5 7* (*baab bbcb*) *1 5* (*abba abab*) *2 6* (*abbb abab*) *3 7* (*abba abab*)

discriminate their resulting designs from level permutations, and select the optimal ones under the new GMA criterion, as demonstrated in the next example.

Example 4. A class of $E(f_{NOD})$-optimal $D(9,3^{4s})$ designs for $s=1,\ldots,7$ obtained in Fang et al. (2004) are listed in Table 8. There are seven designs in the table, each design is an $OA(9,3^4)$, and every two designs form an $E(f_{NOD})$-optimal $D(9,3^8)$ design. There are altogether $\binom{7}{2}$ such $D(9,3^8)$ designs. For each design, permutations given in Table 3 are applied to each factor, and the optimal design under the new GMA criterion is shown in Table 9. Note that in this table, "*1 2* (*aabb baba*)" represents the SSD obtained by applying permutations *a*,*a*,*b*,*b*,*b*,*a*,*b* and *a* to the respective eight factors of the first two designs in Table 8. From Table 9, we can see that there are only two different kinds of optimal designs among the $\binom{7}{2}$ designs, the better ones are those with the γ WLP of (0, 1.25, 5.5, 1.25), we can select any of these, e.g. *1 2* (*aabb baba*), as an optimal $D(9,3^8)$ design with quantitative factors for further study.

Table 10
Example 5—$D(6,3^5 2^{10})$ from Yamada et al. (2006).

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	1	2	2	0	0	0	0	1	1	1	1	1	1
2	1	2	2	0	0	1	1	1	0	0	0	1	1	1
0	1	1	1	1	1	0	1	1	0	1	1	0	0	1
1	2	2	0	1	1	1	0	1	1	0	1	0	1	0
2	2	0	1	2	1	1	1	0	1	1	0	1	0	0

Table 11
Example 5—optimal designs according to γ and β WLPs for the design in Table 10.

Subject	γ WLP	β WLP
Optimal WLP	(0, 40.625, 23.750, 0.625)	$(0,40,440,1940,\ldots)$
Optimal designs (total of 31)	*baaaa*, *caaaa*, *bbbbb*, *bbbbb*, ...	*baaaa*, *caaaa*, *bbbbb*, *bbbbb*, ...

Example 5. Consider a mixed-level $\chi^2(D)$-optimal SSD $D(6,3^5 2^{10})$ obtained in Yamada et al. (2006). This design has 6 runs and 15 factors, 5 with 3 levels and 10 with 2 levels. For two-level factors, there are only two permutations, 0, 1 and 1, 0, which are geometrically identical to each other, so the geometrical nonisomorphism only depends on the permutations of the three-level factors. The design is listed in Table 10 and the selected optimal designs are listed in Table 11. In Table 11, the optimal designs are represented by the five permutations on the five three-level factors. For example, "*baaaa*" represents the design obtained by applying permutations *b*,*a*,*a*,*a* and *a* to the five three-level factors, *A*, *B*, *C*, *D* and *E*, accordingly. Totally 31 optimal geometrically nonisomorphic designs were selected under the γ and β WLPs, respectively, while only four of them are listed in Table 11 for saving space. Thus, in this mixed-level SSD case, the γ and β WLPs agree on the same optimal geometrically nonisomorphic designs again.

5. Concluding remarks

SSD is a special kind of factorial design, all existing criteria for assessing SSDs are invariant to level permutation within the factors and thus only applicable to the case of nominal factors. Design criteria for quantitative factors are not as well-developed as those for nominal ones, however.

In this paper, we propose the γ WLP for SSDs with quantitative factors. The properties of this new WLP are explored, and it is applied to discriminating geometrically nonisomorphic SSDs and finding the optimal ones. Several examples have been provided for illustration, some comparisons are also made with the β WLP. It is shown that the γ WLP is able to efficiently identify the optimal SSDs. Although the β WLP can also classify geometrically nonisomorphic SSDs and find the optimal ones, the computation of the β WLP is much more complicated. Specifically, given an SSD $D(N,s^n)$, the computation intensity of the γ WLP is $C_n^2 s^2$ since this WLP considers any 2 of n factors and each factor has "s" orthogonal polynomial contrasts, while the computation intensity of the β WLP is s^n since it needs to consider all the factors with "s" orthogonal polynomial contrasts. As for an SSD, the number of factors n is large, the computation could be dramatically reduced by using the γ WLP.

The γ WLP can be further extended in the following way. For two interaction contrasts $P_{\mathbf{t}_1}(\mathbf{x})$ and $P_{\mathbf{t}_2}(\mathbf{x})$ with $\|\mathbf{t}_1\|_0 = \|\mathbf{t}_2\|_0 = 2$ and $\|\mathbf{t}_1\|_1 = \|\mathbf{t}_2\|_1$, $P_{\mathbf{t}_1}(x)$ is considered to be more important than $P_{\mathbf{t}_2}(x)$ if $|t_{j_1} - t_{i_1}| < |t_{j_2} - t_{i_2}|$, where $\mathbf{t}_1 = (0,\ldots,0,t_{i_1},0,\ldots,0,t_{j_1},0,\ldots,0)$ and $\mathbf{t}_2 = (0,\ldots,0,t_{i_2},0,\ldots,0,t_{j_2},0,\ldots,0)$. Namely, for interaction effects with the same order, those of two medium-order effects are more important than those of one high-order and one low-order effects. Take the quantitative four-level factorial design as an example, we have the original order of effect importance according to the γ WLP:

$$0l == l0 \gg ll == 0q == q0 \gg lq == ql == 0c == c0 \gg qq == lc == cl \gg qc == cq \gg cc,$$

where "c" denotes the cubic polynomial contrast. While the improved order of effect importance changes to

$$0l == l0 \gg ll == 0q == q0 \gg lq == ql == 0c == c0 \gg qq \gg lc = cl \gg qc == cq \gg cc,$$

which has one more order than the original one. Because this extension only increases the number of different orders, not of the $b_{\mathbf{t}}$'s, so it also holds the advantage of computation convenience.

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