(M,S)-optimality in selecting factorial designs

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Abstract

Use of the (M,S) criterion to select and classify factorial designs is proposed and studied. The criterion is easy to deal with computationally and it is independent of the choice of treatment contrasts. It can be applied to two-level designs as well as multi-level symmetrical and asymmetrical designs. An important connection between the (M,S) and minimum aberration criteria is derived for regular fractional factorial designs. Relations between the (M,S) criterion and generalized minimum aberration criteria on nonregular designs are also discussed. The (M,S) criterion is then applied to study the projective properties of some nonregular designs.

Keywords: Fractional factorial designs, orthogonal arrays, minimum aberration, (M,S)-optimality.

1. Introduction

Screening designs are popularly used in practice to identify a few significant factors among many potential candidate factors. A fundamental question in physical experimentation as well as scientific research is how to select the best design. A lot of research has been done and many criteria have been proposed. Box and Hunter (1961) proposed the maximum resolution criterion for regular fractional factorial designs. Fries and Hunter (1980) extended Box and Hunter's criterion and suggested the minimum aberration (MA) criterion. The MA criterion is the most popular criterion in design selection and it has many good properties such as model robustness. For details, see Cheng, Steinberg and Sun (1999) and references therein. In this paper, (M,S)-optimality will be used to select two-level factorial designs. The (M,S) procedure (Eccleston and Hedayat, 1974) has been

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widely used and advocated in optimal design literature. Shah and Sinha (1989) has many examples of theory and applications of (M,S)-optimality.

For a two-level design d with N runs of n factors, consider the following linear model

$$E[y(x_1, x_2, \ldots, x_n)] = \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} x_i x_j, \tag{1}$$

where $y(x_1, x_2, \ldots,\ x_n)$ is the observed response of treatment $(x_1, x_2, \ldots,\ x_n)$, x_i is the level of factor i and takes the value -1 or 1 $(i = 1, \ldots, n)$. β_0 is the grand mean, β_i is the main effect of factor i, β_{ij} is the interaction between factors i and j, and so on. All the three-factor or higher-order interactions are omitted in model (1). Model (1) can also be written in matrix form, i.e.,

$$\mathbf{Y} = X_1 \beta_{\mathbf{1}} + X_2 \beta_{\mathbf{2}} + \epsilon, \tag{2}$$

where $\mathbf{Y}$ is an $N \times 1$ vector of observations, $X_1 = (\mathbf{1_N}, \mathbf{x_1}, \cdots, \mathbf{x_n})$, $\mathbf{1_N}$ denotes an $N \times 1$ vector of 1's, $\beta_{\mathbf{1}}' = (\beta_0, \beta_1, \cdots, \beta_n)$ represents the grand mean and the n main effects. $\beta_{\mathbf{2}}$ is the vector of $\binom{n}{2}$ two-factor interaction (2fi's) parameters, X_2 is the corresponding coefficient matrix of 2fi's and ϵ is a vector of independent random errors with mean 0 and constant variance σ^2. In general $\beta_{\mathbf{1}}$ can be any parameter subset that is of primary interest, with $\beta_{\mathbf{2}}$ representing "secondary" parameters. For example, for a design of resolution V $\beta_{\mathbf{1}}$ could contain all main effects and 2fi's and $\beta_{\mathbf{2}}$ could contain three-factor (and even higher-order) interactions. Under the assumption of normality of errors, the Fisher information matrix of $\beta_{\mathbf{2}}$ adjusted for β_1 is

$$C_d = X_2' X_2 - (X_1' X_2)'(X_1' X_1)^{-1}(X_1' X_2).$$

Since C_d is symmetric, we denote $C_d' C_d$ as C_d^2 in the following discussion. The (M,S) criterion first identifies a subclass of designs that maximize trace(C_d) and then finds designs within this subclass that minimize trace(C_d^2). If a design has the maximum trace(C_d) and minimum trace(C_d^2) within a class of designs, $\mathcal{D}$, it is called an (M,S)-optimal design in $\mathcal{D}$. For a 2^{n-p} regular design with one replicate,

$$X_1' X_1 = 2^{n-p} I_{n+1},$$

where I_{n+1} is the $(n+1)$-dimensional identity matrix. Thus,

$$C_d = X_2' X_2 - 2^{-(n-p)}(X_1' X_2)'(X_1' X_2).$$

It is important to note that, even though the (M,S) criterion defined here is based on model (2) and only for two-level designs, trace(C_d) and trace(C_d^2) are actually independent of the choice of orthonormal contrasts [see Remark 2.3.1 of Dey and Mukerjee (1999)]. Therefore, the (M,S) criterion can be applied to multi-level symmetrical and asymmetrical designs as well. Cheng, Deng, and Tang (2002) and Mandal and Mukerjee (2004) studied (M,S)-optimality in factorial designs. They considered the joint information on $\beta_\mathbf{1}$ and $\beta_\mathbf{2}$ while our focus is the conditional information on $\beta_\mathbf{2}$ given $\beta_\mathbf{1}$. The (M,S) criterion proposed in this paper is especially useful in the scenario in which main effects are of primary interest but the experimenter would like to have as much information on 2fi's as possible under the assumption that three-factor and higher-order interactions are negligible. As is shown in the following, trace(C_d) and trace(C_d^2) contain not only the contamination information of 2fi's on main effects but information on 2fi's themselves as well.

2. (M,S)-Optimality in Selecting Regular Designs

Minimum aberration has been a popular criterion in choosing regular fractional factorial designs. The purpose of this section is to explore the detailed relationship between (M,S) and MA criteria when selecting regular designs of two-level factors. Jacroux (2004) briefly discussed the connection between the two criteria for regular designs of resolution III or higher, but his formulation only holds for designs of resolution IV or resolution III designs in which each main effect is aliased with exactly one 2fi.

For a 2^{n-p} regular fractional factorial design, say d, let $W_i(d)$ be the number of words of length i in the defining relation. Then $W(d) = (W_1(d), \cdots, W_n(d))$ is the wordlength pattern of design d. For any two designs d_1 and d_2, let l be the smallest integer such that $W_l(d_1) \neq W_l(d_2)$, then d_1 is said to have less aberration than d_2 if $W_l(d_1) < W_l(d_2)$. If no design has less aberration than d_1, then d_1 is called the MA design.

In a 2^{n-p} design d of resolution III or higher, following Cheng, Steinberg, and Sun (1999), $2^p - 1$ of the $2^n - 1$ factorial effects appear in the defining relation. The remaining $2^n - 2^p$ effects are partitioned into $g = 2^{n-p} - 1$ alias sets each of size 2^p, where n of the g alias sets contain main effects (one each). Let $f = g - n$ and the f alias sets not containing main effects be M_1, $\cdots$, M_f. Also let the n alias sets containing main effects be M_{f+1}, $\cdots$,

M_g. For $1 \le i \le g$, let $m_i(d)$ be the number of 2fi's in M_i. Then

$$\sum_{i=f+1}^{g} m_i(d) = 3W_3(d)$$

because each three-letter word in the defining relation generates three 2fi's that are aliased with (the corresponding) main effects. Note that the diagonal element of $(X_1'X_2)'(X_1'X_2)$ is 4^{n-p} if the 2fi is aliased with a main effect, and zero otherwise (since the design resolution is at least III, there cannot be two main effects aliased with the same 2fi). The off-diagonal element is zero if the two 2fi's are not aliased with a main effect and 4^{n-p} if they are both aliased with the same main effect. Similarly, the (i,i)th diagonal element of $X_2'X_2$ is 2^{n-p}, and the (i,j)th off-diagonal element is zero if the ith and jth 2fi's are not aliased with each other and 2^{n-p} if they are. Hence, trace(C_d) is equal to the number of 2fi's that are not aliased with main effects (i.e., 2fi's in $M_1, \cdots, M_f$) multiplied by 2^{n-p}, and

$$\text{trace}(C_d^2) = \left[\sum_{i=1}^{f} m_i(d) + 2 \times \sum_{i=1}^{f} \binom{m_i(d)}{2}\right] 4^{n-p} = 4^{n-p} \sum_{i=1}^{f} m_i(d)^2.$$

Recall that (equation (2.2) in Cheng, Steinberg, and Sun, 1999)

$$6W_4(d) = \sum_{i=1}^{g} m_i(d)^2 - \binom{n}{2}.$$

Thus

$$\text{trace}(C_d^2) = \left[\binom{n}{2} - \sum_{i=f+1}^{g} m_i(d)^2 + 6W_4(d)\right] 4^{n-p}. \quad (3)$$

Therefore, we have the following theorem.

Theorem 1. *For any regular two-level design d of resolution III or higher,*

1. *trace*$(C_d) = 2^{n-p} \sum_{i=1}^{f} m_i(d) = 2^{n-p} \left[\binom{n}{2} - 3W_3(d)\right]$.
2. *trace*$(C_d^2) = 4^{n-p} \sum_{i=1}^{f} m_i(d)^2 = 4^{n-p} \left[\binom{n}{2} - \sum_{i=f+1}^{g} m_i(d)^2 + 6W_4(d)\right]$.

Theorem 1 shows that the (M,S) criterion selects the design that maximizes $\sum_{i=1}^{f} m_i(d)$ (or, equivalently, minimizes $W_3(d)$) first and then minimizes $\sum_{i=1}^{f} m_i(d)^2$, while the MA criterion minimizes $W_3(d)$ first and then minimizes $W_4(d)$ (or, equivalently, minimizes $\sum_{i=1}^{g} m_i(d)^2$). The following example shows that these two criteria are not equivalent when used in design selection.

Example 1. Consider the following two 2^{11-6}_{III} designs.

$d_1 : F = AB,\, G = AC,\, H = AD,\, J = BE,\, K = CDE,\, L = ABCDE$

$d_2 : F = AB,\, G = AC,\, H = AD,\, J = AE,\, K = BCDE,\, L = ABCDE$

It can be shown that $W(d_1) = (0, 0, 5, 9, 17, 19, 7, 2, 3, 1)$ and $W(d_2) = (0, 0, 5, 10, 16, 16, 10, 5, 1)$. Let $\mathbf{m}(d) = (m_1(d), \cdots, m_{31}(d))$. Then

$\mathbf{m}(d_1) = (3, 3, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 1; 3, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1)$,

$\mathbf{m}(d_2) = (2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2; 5, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$,

$\text{trace}(C_{d_1}) = \sum_{i=1}^{20} m_i(d_1) = 40 \times 2^{11-6} = \text{trace}(C_{d_2}) = \sum_{i=1}^{20} m_i(d_2)$,

$\text{trace}(C^2_{d_1}) = \sum_{i=1}^{20} m_i(d_1)^2 = 84 \times 4^{11-6}$, $\text{trace}(C^2_{d_2}) = \sum_{i=1}^{20} m_i(d_2)^2 = 80 \times 4^{11-6}$,

$\sum_{i=1}^{31} m_i(d_1)^2 = 109$, and $\sum_{i=1}^{31} m_i(d_2)^2 = 115$.

Therefore, the MA criterion will choose d_1 over d_2 while the (M,S) criterion selects d_2 over d_1. Neither of these designs is optimal by either criterion, but the difference between them illustrates the nature of the MA and (M,S) criteria. The MA criterion favors designs that treat all factors equally by making the alias chains of low order effects roughly equal in length. In contrast, the (M,S) criterion seems to put some 2fi's into longer alias chains with main effects in order to keep the uniformity of 2fi's distribution across the alias chains that don't contain main effects. Note that, in this example, both d_1 and d_2 have maximized Jacroux's E (the number of estimable contrasts that contain at least one main effect or 2fi) at 31.

One interesting question is whether (M,S)-optimal designs are also MA designs and vice versa. For designs of resolution IV or higher, it is easy to see that maximizing trace(C_d) and then minimizing trace(C_d^2) is equivalent to minimizing $W_3(d)$ and then minimizing $W_4(d)$. Therefore, MA designs must be (M,S)-optimal. However, an (M,S)-optimal design is not necessarily an MA design. For example, designs 2^{6-1}_{VI} and 2^{6-1}_{V} with defining relations $6 = 12345$ and $6 = 1234$ have word-length patterns $(0, 0, 0, 0, 0, 1)$ and $(0, 0, 0, 0, 1, 0)$ respectively. Both designs have minimum $W_3(d)$ and $W_4(d)$, so they are (M,S)-optimal. However, it is obvious that 2^{6-1}_{V} is not an MA design. Actually, 2^{6-1}_{V} is the smallest (M,S)-optimal design that doesn't have minimum aberration. The major reason is that the current setting of (M,S)-optimality doesn't cover information on three-factor or higher-order interactions while the MA criterion considers interactions of any order. As is pointed out above, three-factor or higher-order interactions could be included in β_2 if all main effects and 2fi's are parameters of primary interest, β_1.

Recall that a 2^{n-k} design has resolution III if $2^{n-k-1}+1 \leq n \leq 2^{n-k}-1$. For designs of 8, 16, and 32 runs with more than 4, 8, and 16 factors, respectively, a complete computer search using the algorithm in Xu (2002) shows that the (M,S)-optimal design is unique up to isomorphism (two designs are *isomorphic* if one can be obtained from the other by relabeling factors, reordering runs or switching the levels of factors), and it is the MA design. For designs of 64 runs with more than 32 factors, it is not easy to identify all the nonisomorphic designs. The concept of complementary designs proposed by Tang and Wu (1996) could be used to reduce the complexity of the computation.

Let H_{n-k} be the collection of all $2^{n-k}-1$ combinations generated by $n-k$ independent columns, then for any design d, the complementary design, say $\bar{d}$, consists of the remaining $2^{n-k}-1-n$ columns in H_{n-k}. Tang and Wu show that $W_3(d)$ = constant $- W_3(\bar{d})$ and $W_4(d)$ = constant $+ W_3(\bar{d}) + W_4(\bar{d})$. Therefore, to find all nonisomorphic resolution III designs of 64 runs with minimum $W_3(d)$, we only need to find their complementary designs $\bar{d}$ with the maximum $W_3(\bar{d})$. Since these complementary designs contain 1 to 31 factors, we only need to find nonisomorphic designs with the maximum $W_3(\bar{d})$ in H_5 (Chen and Hedayat, 1996). These complementary designs (only generators are given and the five independent columns are 1, 2, 3, 4, and 5) are listed in Table 1.

Chen and Hedayat (1996) listed nonisomorphic complementary designs of 1 to 15 factors with the maximum $W_3(\bar{d})$ and Table 1 has complementary designs of 16 to 31 factors and their wordlength pattern up to five-letter words (M_{10}, M_{10}^*, M_{11}, and M_{11}^* are from Chen and Hedayat, 1996 and are included for demonstration later). For example, M_{25} stands for the complementary design with 25 factors and the maximum $W_3(\bar{d}) = 80$, the minimum $W_4(\bar{d}) = 435$ and the minimum $W_5(\bar{d}) = 1622$ (if two designs have the same $W_3(\bar{d})$ and $W_4(\bar{d})$). M_{25}^{*1} to M_{25}^{*3} are other nonisomorphic designs with the maximum $W_3(\bar{d}) = 80$. It is clear from the list of nonisomorphic complementary designs that there is only one design up to isomorphism with maximum $W_3(\bar{d})$ for 1 to 9, 12 to 18, 28 to 31 factors. Hence, there is only one design up to isomorphism having minimum $W_3(d)$ with 62 to 54, 51 to 45, and 35 to 32 factors. Therefore, (M,S)-optimal and MA designs are the same in these cases. For other cases where there are more than one nonisomorphic design, trace(C_d) and trace(C_d^2) are given in Table 2. Table 2 shows that (M,S)-optimal design is unique up to isomorphism except for designs with 37 and 38 factors. There are two (M,S)-optimal designs with 37 factors and they are the complementary designs of M_{26} and M_{26}^{*1} (denoted by $H_6 \setminus M_{26}$ and $H_6 \setminus M_{26}^{*1}$). By checking wordlength patterns of M_{26} and M_{26}^{*1}, we know that $H_6 \setminus M_{26}$ is MA and $H_6 \setminus M_{26}^{*1}$ is not. Similarly, there are two (M,S)-optimal designs with 38 factors and they are the complementary designs of M_{25} and M_{25}^{*1}, where $H_6 \setminus M_{25}$ is MA and $H_6 \setminus M_{25}^{*1}$ is not. Therefore, (M,S)-optimal designs are not unique and not necessarily MA. However, all MA designs with 64 runs are (M,S)-optimal. For resolution III designs with more than 64 runs, whether an MA design is (M,S)-optimal is still under investigation.

In general, the (M,S) and MA criteria are different. The former compares designs based on the aliasing of 2fi's with main effects as well as among 2fi's themselves, while the latter also factors in higher-order interactions. The MA criterion distributes the 2fi's uniformly across alias sets including main effects as well as those containing only 2fi's, while the (M,S) criterion distributes 2fi's evenly across only the alias sets that do not contain any main effects. It is important to notice that the (M,S) criterion is equivalent to maximizing the first two components of the maximum estimation capacity, i.e., $E_1(d)$ and $E_2(d)$, in Cheng, Steinberg, and Sun (1999). An (M,S)-optimal design usually has large estimation capacity, i.e., it accommodates large numbers of models containing all the main effects and a certain number of 2fi's.

In addition to the ease of computation, the (M,S) criterion can be naturally carried over from regular designs to nonregular designs. In contrast, the MA criterion has to be modified. Next, the (M,S) criterion will be used to study nonregular designs, and relations between the (M,S) and minimum G_2-aberration criteria are also discussed.

3. (M,S)-Optimality for Nonregular Designs

In this section some properties of trace(C_d) and trace(C_d^2) when used in selecting nonregular designs are studied. For a design d of N runs with n factors, where each row of the design matrix corresponds to a run and each column to a factor, let $s = \{c_1, \ldots, c_k\}$ be any k-subset with $1 \le k \le n$, define

$$j_k(s) = \sum_{i=1}^{N} c_{i1} \cdots c_{ik},\ J_k(s) = |j_k(s)|$$

where c_{ij} is the ith component of column c_j. The $J_k(s)$ values are called the J-characteristics of a design in Tang and Deng (1999). For an orthogonal design, $J_1(s) = J_2(s) = 0$. A design is regular if and only if $J_k(s) = 0$ or N for all k. If $J_k(s) = N$, the k columns

Table 1: Nonisomorphic designs with the maximum $W_3(\bar{d})$

Design	Design Generators	(W_3, W_4, W_5)
M_{16}	12, 13, 14, 23, 24, 34, 123, 124, 134, 234, 1234	(35, 105, 168)
M_{17}	12, 13, 14, 23, 24, 34, 123, 124, 134, 234, 1234, 12345	(36, 112, 196)
M_{18}	12, 13, 14, 23, 24, 34, 123, 124, 134, 135, 234, 1234, 12345	(38, 126, 252)
M_{19}	12, 13, 14, 23, 24, 34, 123, 124, 134, 135, 234, 245, 1234, 12345	(41, 148, 336)
M_{19}^*	12, 13, 14, 23, 24, 34, 123, 124, 134, 135, 145, 234, 245, 1234, 12345	(41, 147, 337)
M_{20}	12, 13, 14, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234, 1234, 2345	(45, 175, 453)
M_{20}^*	12, 13, 14, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234, 1234, 12345	(45, 176, 452)
M_{21}	12, 13, 15, 23, 24, 25, 35, 123, 124, 134, 135, 234, 245, 1234, 12345	(50, 205, 592)
M_{21}^{*1}	12, 13, 14, 15, 23, 24, 25, 34, 123, 124, 134, 135, 145, 234, 1234, 12345	(50, 210, 603)
M_{21}^{*2}	12, 13, 14, 15, 23, 25, 35, 123, 125, 135, 145, 235, 1234, 1235, 1245, 2345	(50, 211, 602)
M_{21}^{*3}	12, 13, 14, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234, 235, 1234, 12345	(50, 213, 600)
M_{22}	12, 13, 14, 15, 24, 25, 45, 123, 124, 134, 135, 234, 245, 1234, 1235, 12345	(56, 251, 784)
M_{22}^{*1}	12, 14, 15, 23, 24, 25, 45, 123, 124, 125, 134, 135, 145, 234, 235, 1234, 12345	(56, 252, 784)
M_{22}^{*2}	12, 13, 14, 15, 23, 24, 34, 125, 135, 145, 234, 1234, 1235, 1245, 1345, 2345, 12345	(56, 254, 789)
M_{22}^{*3}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234, 235, 1234, 12345	(56, 255, 788)
M_{22}^{*4}	12, 13, 14, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234, 235, 245, 1234, 12345	(56, 259, 784)

Table 1: Nonisomophic designs with the maximum $W_3(\bar{d})$ (continued)

Design	Design Generators	(W_3, W_4, W_5)
M_{23}	12, 13, 14, 15, 23, 34, 35, 45, 123, 124, 125, 134, 135,	
	145, 234, 235, 1345, 12345	(63, 304, 1015)
M_{23}^{*1}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135,	
	145, 234, 235, 1234, 1345, 12345	(63, 306, 1017)
M_{23}^{*2}	12, 13, 14, 15, 23, 24, 34, 123, 124, 134, 135, 234, 245,	
	1234, 1235, 1245, 1345, 12345	(63, 307, 1016)
M_{23}^{*3}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 145,	
	234, 235, 245, 1234, 12345	(63, 308, 1015)
M_{23}^{*4}	12, 13, 14, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234,	
	235, 245, 345, 1234, 12345	(63, 315, 1008)
M_{24}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 234,	
	235, 245, 1235, 1245, 1345, 12345	(71, 365, 1292)
M_{24}^{*1}	12, 13, 14, 15, 23, 25, 35, 123, 124, 125, 134, 135, 234	
	, 235, 245, 1235, 1245, 1345, 12345	(71, 366, 1293)
M_{24}^{*2}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 145,	
	234, 235, 245, 1234, 1235, 12345	(71, 367, 1292)
M_{24}^{*3}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 145,	
	234, 235, 245, 345, 1234, 12345	(71, 371, 1288)
M_{25}	12, 13, 14, 15, 23, 24, 25, 34, 123, 124, 125, 134, 135, 234,	
	235, 245, 1235, 1245, 1345, 12345	(80, 435, 1622)
M_{25}^{*1}	12, 13, 14, 15, 23, 24, 25, 35, 123, 124, 125, 134, 135,	
	234, 235, 245, 1235, 1245, 1345, 12345	(80, 435, 1623)
M_{25}^{*2}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135,	
	234, 245, 345, 1235, 1245, 1345, 12345	(80, 436, 1622)
M_{25}^{*3}	12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 145,	
	234, 235, 245, 345, 1234, 1235, 12345	(80, 438, 1620)

Table 1: Nonisomorphic designs with the maximum $W_3(\bar{d})$ (continued)

Design	Design Generators	(W_3, W_4, W_5)
M_{26}	$12, 13, 14, 15, 23, 24, 25, 45, 123, 124, 125, 134, 135, 145,$	
	$234, 235, 245, 345, 1234, 1235, 12345$	$(90, 515, 2012)$
M_{26}^{*1}	$12, 13, 14, 15, 23, 24, 25, 34, 123, 124, 125, 134, 135, 234,$	
	$245, 345, 1234, 1235, 1245, 1345, 12345$	$(90, 515, 2013)$
M_{26}^{*2}	$12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234,$	
	$235, 245, 345, 1234, 1235, 1245, 12345$	$(90, 516, 2012)$
M_{27}	$12, 13, 14, 15, 23, 24, 25, 34, 123, 124, 125, 134, 135, 145, 234,$	
	$235, 245, 345, 1234, 1235, 2345, 12345$	$(101, 605, 2473)$
M_{27}^{*}	$12, 13, 14, 15, 23, 24, 34, 123, 124, 125, 134, 135, 145, 234,$	
	$235, 245, 345, 1234, 1235, 1245, 1345, 12345$	$(101, 606, 2472)$
M_{28}	$12, 13, 14, 15, 23, 24, 25, 34, 123, 124, 125, 134, 135, 145, 234,$	
	$235, 245, 345, 1234, 1235, 1245, 1345, 12345$	$(113, 706, 3012)$
M_{29}	$12, 13, 14, 15, 23, 24, 25, 34, 123, 124, 125, 134, 135, 145,$	
	$234, 235, 245, 345, 1234, 1235, 1245, 1345, 2345, 12345$	$(126, 819, 3640)$
M_{30}	$12, 13, 14, 15, 23, 24, 25, 34, 35, 123, 124, 125, 134, 135,$	
	$145, 234, 235, 245, 345, 1234, 1235, 1245, 1345, 2345, 12345$	$(140, 945, 4368)$
M_{31}	$12, 13, 14, 15, 23, 24, 25, 34, 35, 45, 123, 124, 125, 134, 135,$	
	$145, 234, 235, 245, 345, 1234, 1235, 1245, 1345, 2345, 12345$	$(155, 1085, 5028)$
M_{10}	$1, 2, 3, 4, 1234, 12, 23, 34, 123, 234$	$(10, 15, 12)$
M_{10}^{*}	$1, 2, 3, 4, 1234, 12, 23, 13, 14, 123$	$(10, 16, 12)$
M_{11}	$1, 2, 3, 4, 1234, 12, 13, 14, 23, 24, 34$	$(13, 25, 25)$
M_{11}^{*}	$1, 2, 3, 4, 1234, 14, 23, 24, 34, 234, 123$	$(13, 26, 24)$

Table 2: Trace(C_d) and trace(C_d^2) of 64-run designs

No. of Factors	Nonisomorphic Design	trace(C_d)	trace(C_d^2)
36	$H_6 \setminus M_{27}$	438×64	7110×64^2
36	$H_6 \setminus M_{27}^*$	438×64	7116×64^2
37	$H_6 \setminus M_{26}$	426×64	6986×64^2
37	$H_6 \setminus M_{26}^{*1}$	426×64	6986×64^2
37	$H_6 \setminus M_{26}^{*2}$	426×64	6992×64^2
38	$H_6 \setminus M_{25}$	415×64	6895×64^2
38	$H_6 \setminus M_{25}^{*1}$	415×64	6895×64^2
38	$H_6 \setminus M_{25}^{*2}$	415×64	6901×64^2
38	$H_6 \setminus M_{25}^{*3}$	415×64	6913×64^2
39	$H_6 \setminus M_{24}$	405×64	6843×64^2
39	$H_6 \setminus M_{24}^{*1}$	405×64	6849×64^2
39	$H_6 \setminus M_{24}^{*2}$	405×64	6855×64^2
39	$H_6 \setminus M_{24}^{*3}$	405×64	6879×64^2
40	$H_6 \setminus M_{23}$	396×64	6830×64^2
40	$H_6 \setminus M_{23}^{*1}$	396×64	6842×64^2
40	$H_6 \setminus M_{23}^{*2}$	396×64	6848×64^2
40	$H_6 \setminus M_{23}^{*3}$	396×64	6854×64^2
40	$H_6 \setminus M_{23}^{*4}$	396×64	6896×64^2
41	$H_6 \setminus M_{22}$	388×64	6856×64^2
41	$H_6 \setminus M_{22}^{*1}$	388×64	6862×64^2
41	$H_6 \setminus M_{22}^{*2}$	388×64	6874×64^2
41	$H_6 \setminus M_{22}^{*3}$	388×64	6880×64^2
41	$H_6 \setminus M_{22}^{*1}$	388×64	6904×64^2
42	$H_6 \setminus M_{21}$	381×64	6921×64^2
42	$H_6 \setminus M_{21}^{*1}$	381×64	6951×64^2
42	$H_6 \setminus M_{21}^{*2}$	381×64	6957×64^2
42	$H_6 \setminus M_{21}^{*3}$	381×64	6969×64^2
52	$H_6 \setminus M_{11}$	270×64	6630×64^2
52	$H_6 \setminus M_{11}^*$	270×64	6636×64^2
53	$H_6 \setminus M_{10}$	250×64	6250×64^2
53	$H_6 \setminus M_{10}^*$	250×64	6256×64^2

in s form a word of length k in the defining relation of regular designs. For nonregular designs, $0 \leq J_k(s) \leq N$. Deng and Tang (1999) introduced a generalized minimum aberration (GMA) criterion based on the confounding frequency vector (CFV) that consists of the frequencies of $J_k(s)$. Let f_{kj} be the frequency of k column combinations that give $J_k(s) = 4(t+1-j)$ for $j = 1, \ldots, t$ in a Hadamard matrix with $N = 4t$ runs. Then the CFV is

$$CFV = [(f_{31}, \ldots, f_{3t}), (f_{41}, \ldots, f_{4t}), \ldots, (f_{n1}, \ldots, f_{nt})].$$

The GMA criterion minimizes the components of CFV sequentially, i.e, a GMA design has the lowest frequency of the largest $J_k(s)$ values. They proved that $J_k(s)$ must be a multiple of 4 for orthogonal first-order designs. The quantity $J_k(s)/N$ could be interpreted as the extent of aliasing among k columns. In particular, $J_3(s)/N = 0$ (or $J_3(s)/N = 1$) suggests that there is no (or complete) aliasing between the main effect of one factor in s and the 2fi of two other factors; $J_4(s)/N = 0$ (or $J_4(s)/N = 1$) indicates that there is no (or complete) aliasing between two 2fi's of the four factors in s. The values of $J_3(s)$ and $J_4(s)$ are closely related to N. For example, Deng and Tang (2002) pointed out that if N is a multiple of 8, so are $J_3(s)$ and $J_4(s)$. As with regular designs where trace(C_d) and trace(C_d^2) depend on $W_3(d)$ and $W_4(d)$, Theorem 2 shows that trace(C_d) and trace(C_d^2) are determined by $j_3(s)$ and $j_4(s)$.

Theorem 2. *For any two-level orthogonal design d with N runs and n factors,*

1. *trace*$(C_d) = N\binom{n}{2} - \frac{3}{N}\sum_{1\leq i<k<l\leq n} j_3^2(c_ic_kc_l)$.
2. *trace*$(C_d^2) = \sum_{1\leq i<k\leq n}\left[N - \frac{1}{N}\sum_{1\leq i<k\leq n, h\neq i,k} j_3^2(c_ic_kc_h)\right]^2$

$$+ \sum_{1\leq i<k\leq n, 1\leq l<m\leq n; (i,k)\neq(l,m)} \left[j_4(c_ic_kc_lc_m) - \frac{1}{N}\sum_{h\neq i,k,l,m} j_3(c_ic_kc_h)j_3(c_lc_mc_h)\right]^2.$$

Proof. Note that the diagonal elements of $X_2'X_2$ are N's, the nonzero off-diagonal elements of $X_1'X_2$ are $j_3(s)$'s with each one appearing three times, and trace($(X_1'X_2)'X_1'X_2$) is the sum of squares of the elements in $X_1'X_2$. For example, the element corresponding to main effect 1 and 2fi 23 in $X_1'X_2$ is $j_3(c_1c_2c_3)$. It is straightforward to show that

$$\text{trace}(C_d) = N\binom{n}{2} - \frac{3}{N}\sum_{1\leq i<k<l\leq n} j_3^2(c_ic_kc_l).$$

For trace(C_d^2), note that the off-diagonal elements of $X_2'X_2$ are either zero ($j_2(s) = 0$) or $j_4(s)$. The diagonal element of $(X_1'X_2)'X_1'X_2$ is the sums of squares of $j_3(s)$ containing two factors in the corresponding 2fi. For instance, the diagonal element at the position of 2fi 23 is $\frac{1}{N}\sum_{h\neq 2,3} j_3^2(c_2c_3c_h)$. The off-diagonal element is the sum of all products of $j_3(s_1)$ and $j_3(s_2)$ where s_1 and s_2 contain two factors from each 2fi and a main effect that doesn't appear in both 2fi's. For example, the off-diagonal element at the position of 2fi's 12 and 34 is $\sum_{h=5}^{n} j_3(c_1c_2c_h)j_3(c_3c_4c_h)$. $\diamondsuit$

Tang and Deng (1999) proposed the minimum G_2-aberration criterion as follows. Let $B_k(d) = \frac{1}{N^2}\sum_{|s|=k} J_k^2(s)$. For two designs d_1 and d_2, let r be the smallest integer such that $B_r(d_1) \neq B_r(d_2)$. Design d_1 has less G_2-aberration than d_2 if $B_r(d_1) < B_r(d_2)$. If no design has less G_2-aberration than d_1, then d_1 is said to have minimum G_2-aberration. Theorem 2 shows that maximizing trace(C_d) is equivalent to minimizing $B_3(d)$. However, minimizing trace(C_d^2) is more complicated than simply minimizing $B_4(d)$. If all $j_3(s)$'s are zero (for example, d is an orthogonal array of strength three), then minimizing trace(C_d^2) is equivalent to minimizing $B_4(d)$. Direct calculation shows that all minimum G_2-aberration designs in Table 2 of Tang and Deng (1999) are (M,S)-optimal and all (M,S)-optimal designs from H16.III have minimum G_2-aberration. It is not known in general whether the (M,S) criterion is equivalent to the minimum G_2-aberration criterion for nonregular designs. Moreover, for regular designs, trace(C_d) and trace(C_d^2) are multiples of N and N^2, but this is not generally true for nonregular designs (examples are given in Table 6). If d is a saturated orthogonal design, $X_1(d)X_1'(d) = X_1'(d)X_1(d) = NI_N$, thus $C_d = 0$ and trace(C_d)=trace(C_d^2)=0. Therefore, all saturated orthogonal designs are (M,S) equivalent. However, saturated orthogonal designs of N runs are not GMA equivalent (Xu and Deng, 2002). Theorem 3 links trace(C_d) with J-characteristics for projections of saturated orthogonal arrays.

Theorem 3. *Let d_1 be an m-dimensional projection from a saturated orthogonal array d of N runs by deleting columns $a_1, \cdots, a_g$, where $g = N - m - 1 \geq 1$. Then*

$$\begin{aligned} \textit{trace}(C_{d_1}) &= \frac{1}{N}[\sum_{1\leq i<k\leq m} j_3^2(c_ic_ka_1) + \cdots + \sum_{1\leq i<k\leq m} j_3^2(c_ic_ka_g)] \quad (4)\\ &= \frac{g}{2N}[mN^2 - \sum_{i=1}^{m} j_3^2(a_1a_2c_i) - \cdots - \sum_{i=1}^{m} j_3^2(a_1a_gc_i)] \quad (5) \end{aligned}$$

Proof. Let $X_1(d)$ be the main effect matrix of design d in the model, then $X_1(d)X_1'(d) = X_1'(d)X_1(d) = NI_N$. Without loss of generality, assume the first m factors are in projection d_1, then $X_1(d) = [X_1(d_1), a_1, \ldots, a_g]$, where $a_1, a_2, \ldots, a_g$ stands for main effects of the g factors. Note that

$$I_N = \frac{1}{N}[X_1(d_1), a_1, \ldots, a_l][X_1(d_1), a_1, \ldots, a_g]' = \frac{1}{N}X_1(d_1)X_1'(d_1) + \frac{1}{N}a_1a_1' + \cdots + \frac{1}{N}a_ga_g'.$$

Recall that

$$\begin{aligned} C_{d_1} &= X_2'(d_1)X_2(d_1) - \frac{1}{N}(X_1'(d_1)X_2(d_1))'(X_1'(d_1)X_2(d_1)) \\ &= X_2'(d_1)[I_N - \frac{1}{N}X_1(d_1)X_1'(d_1)]X_2(d_1) \\ &= \frac{1}{N}X_2'(d_1)[a_1a_1' + \cdots + a_ga_g']X_2'(d_1), \end{aligned}$$

where $X_2(d_1)$ is the coefficient matrix of 2fi's in projection d_1. Therefore

$$\begin{aligned} \text{trace}(C_d) &= \frac{1}{N}[\text{trace}([X_2'(d_1)a_1][a_1'X_2(d_1)]) + \cdots + \text{trace}([X_2'(d_1)a_g][a_g'X_2(d_1)]) \\ &= \frac{1}{N}\{[a_1'X_2(d_1)][X_2'(d_1)a_1] + \cdots + [a_g'X_2(d_1)][X_2'(d_1)a_g]\} \\ &= \frac{1}{N}[\sum_{1\le i<k\le m} j_3^2(c_ic_ka_1) + \cdots + \sum_{1\le i<k\le m} j_3^2(c_ic_ka_g)]. \end{aligned}$$

To show equation (5), consider $W_i = X_1'(d_1)D(a_i)X_1(d_1)$ for $i = 1, 2, \ldots, g$, where $D(a_i)$ is the diagonal matrix with diagonal elements equal to the elements of a_i. Then it is easy to see that the diagonal elements of W_i are zeros and its off-diagonal element $w_{kl} = j_3(c_kc_la_i)$ for $1 \le k < l \le m$. Therefore, $\sum_{1\le k<l\le m} j_3^2(c_kc_la_i)$ is the half of the sum of squares of all off-diagonal elements in W_i. Note that the sum of squares of all off-diagonal elements in W_i is trace(W_iW_i'). Let's calculate trace(W_1W_1') first.

$$\begin{aligned} \text{trace}(W_1W_1') &= \text{trace}(X_1'(d_1)D(a_1)X_1(d_1)X_1'(d_1)D(a_1)X_1(d_1)) \\ &= \text{trace}(X_1'(d_1)D(a_1)[NI_N - a_1a_1' - \cdots - a_ga_g']D(a_1)X_1(d_1)) \\ &= \text{trace}(NX_1'(d_1)D(a_1)D(a_1)X_1(d_1)) \\ &- \text{trace}(X_1'(d_1)D(a_1)a_1a_1'D(a)X_1(d_1)) \\ &- \cdots - \text{trace}(X_1'(d_1)D(a_g)a_ga_g'D(a)X_1(d_1)) \\ &= \text{trace}(NX_1'(d_1)X_1(d_1)) - \text{trace}(X_1'(d_1)\mathbf{1_N}\mathbf{1_N'}X_1(d_1)) \end{aligned}$$

$$
\begin{aligned}
&- \ \operatorname{trace}(X_1'(d_1)D(a_1)a_2a_2'D(a_1)X_1(d_1)) - \cdots \\
&- \ \operatorname{trace}(X_1'(d_1)D(a_1)a_ga_g'D(a_1)X_1(d_1)) \\
&= \ N^2m - \sum_{i=1}^{m} j_3^2(a_1a_2c_i) - \cdots - \sum_{i=1}^{m} j_3^2(a_1a_gc_i)
\end{aligned}
$$

where $\mathbf{1_N}$ is the $N \times 1$ vector with elements 1, $D(a_1)a_1 = \mathbf{1_N}$ and $D(a_1)a_i$ is the Hadamard product of a_1 and a_i for $i = 2, 3, \ldots, g$.

Similarly, for $h = 2, 3, \ldots, g$,

$$
\begin{aligned}
\operatorname{trace}(W_hW_h') &= N^2m - \sum_{i=1}^{m} j_3^2(a_1a_2c_i) - \cdots - \sum_{i=1}^{m} j_3^2(a_1a_{h-1}c_i) \\
&- \sum_{i=1}^{m} j_3^2(a_1a_{h+1}c_i) - \cdots - \sum_{i=1}^{m} j_3^2(a_1a_gc_i).
\end{aligned}
$$

Therefore,

$$
\operatorname{trace}(C_d^2) = \frac{g}{2N}[mN^2 - \sum_{i=1}^{m} j_3^2(a_1a_2c_i) - \cdots - \sum_{i=1}^{m} j_3^2(a_1a_gc_i)].
$$

$\diamondsuit$

Equation (4) in theorem 3 should be applied when $m \leq (N-1)/2$ and equation (5) is applied when $m \geq (N-1)/2$. In particular,

Corollary 1. Let d_1 be an $(N-2)$-dimensional projection from a saturated orthogonal array d and $X_1(d_1)$ and $X_2(d_1)$ be its main effect and 2fi model matrices. Then

1. $\operatorname{trace}(C_{d_1}) = \frac{1}{N}\sum_{1\leq i<k\leq n-2} j_3^2(c_ic_ka) = \frac{N(N-2)}{2}$, where a is the factor that is not in the projection.
2. $\operatorname{trace}(C_{d_1}^2) = [\operatorname{trace}(C_{d_1})]^2$
3. If d is the 12-run Plackett-Burman design, then for any m-dimensional projection d_1 $\operatorname{trace}(C_{d_1}) = 12\binom{m}{2} - 4\binom{m}{3}$.

Proof. Let $X_1(d)$ be the main effect matrix of design d in the model. Without loss of generality, assume the first $n-2$ factors are in projection d_1, then $X_1(d) = [X_1(d_1), a]$, where a is the main effect of the $(n-1)$th factor. Here, $g = 1$ and $m = N - 2$. Therefore, $\text{trace}(C_d) = \frac{N(N-2)}{2}$ and (1) holds. To obtain (2), note that

$$\begin{aligned}
\text{trace}(C_d^2) &= \frac{1}{N^2}\text{trace}([X_2'(d_1)a][a'X_2(d_1)][X_2'(d_1)a][a'X_2(d_1)]) \\
&= \frac{1}{N^2}[a'X_2(d_1)X_2'(d_1)a]\text{trace}([X_2'(d_1)a][a'X_2(d_1)]) \\
&= \frac{1}{N^2}[a'X_2(d_1)][X_2'(d_1)a]^2 = [\text{trace}(C_d)]^2.
\end{aligned}$$

As for (3), Lin and Draper (1992) showed that any 3-dimensional projection has one copy of 2^3 and one copy of 2^{3-1}. Hence, $j_3(s) = \pm 4$ for any three columns and the result is obtained by directly plugging $j_3(s)$ in (1) of Theorem 2. $\diamondsuit$

4. Projective Properties of Nonregular Designs

In this section, the (M,S) criterion is used to study the projective properties of nonregular designs of 12, 16, and 20 runs. Since all these designs are saturated, they are indistinguishable by the (M,S) criterion, their $\text{trace}(C_d)$'s and $\text{trace}(C_d^2)$'s are zero. Instead, the (M,S) criterion is applied to projections onto different dimensions. Projections will be classified by their $\text{trace}(C_d)$'s and $\text{trace}(C_d^2)$'s (called (M,S) classifier, hereafter) and (M,S)-optimal projections are selected from each dimension. There has been a lot of research on projections using the generalized minimum aberration (GMA) criteria (Deng and Tang, 1999 and Xu and Wu, 2001). The (M,S)-optimal projections will be compared with the GMA projections to show the difference between the two criteria in projections of nonregular designs.

4.1. Plackett-Burman Design of 12 Runs

As is well known, there is only one projection up to isomorphism for 3 to 11 factors (except for 5 and 6 factors) in the 12-run Plackett-Burman design generated by $\{1, 1, -1, 1, 1, 1, -1, -1, -1, 1, -1\}$. For projections onto 5 factors, the (M,S)-optimal projections (396 of the total 462) have $\text{trace}(C_d) = 80.00$ and $\text{trace}(C_d^2) = 1208.89$. The projection consisting of columns 1, 2, 3, 4, and 5 is an example. It has two mirror runs, 7 and 10 and it is also the GMA projection. The other 66 projections have $\text{trace}(C_d) = 80.00$ and $\text{trace}(C_d^2) = 1280$. The projection consisting of columns 1, 2, 3, 4, and 10 is one and it has two identical runs, 3 and 11. For projections onto 6 factors, the (M,S)-optimal projections (again 396 out of 462) have trace(C_d) = 100.00 and trace(C_d^2) = 2035.56. The projection consisting of columns 1, 2, 3, 4, 5, and 6 is (M,S)-optimal. The other 66 projections have trace(C_d) = 100.00 and trace(C_d^2) = 2320.00. The projection consisting of columns 1, 2, 3, 4, 5, and 7, which is the GMA projection, is an example and has two mirror runs, 7 and 11. Hence, a GMA projection is not necessarily (M,S)-optimal. Li and Wang (2004) showed that both (M,S)-optimal projections onto five and six factors have maximum estimation capacity among all five and six dimensional projections respectively, while the GMA projection onto six factors doesn't have maximum estimation capacity.

4.2. Hall's Designs of 16 Runs

According to Hall (1961), there are exactly five nonisomorphic Hadamard matrices of order 16, labeled as H16.I, H16.II, H16.III, H16.IV, and H16.V in Deng and Tang (2002), where H16.I is a regular design. For $3 \leq m \leq 14$, a complete computer search of $\binom{15}{m}$ projections was done for each of Hall's designs. Table 3 lists the (M,S)-optimal projections and their frequencies (the numbers in parentheses are the total numbers of projections in each design, $\{\}^c$ stands for the complement). For example, the (M,S)-optimal projections onto six factors have trace(C_d) = 240 and trace(C_d^2) = 8448. The frequencies of 6-dimensional (M,S)-optimal projections among 5005 projections in each of H16.I, H16.II, H16.III, H16.IV and H16.V are 420, 120, 46, 21, and 28, respectively. The projection consisting of columns 1, 2, 3, 4, 6, and 8 in H16.I is (M,S)-optimal. The projection is a regular MA design of resolution IV with defining relations and 6 = 124 and 8 = 123. All columns selected in Table 3 are from H16.I.

According to the frequencies of (M,S)-optimal projection in each dimension, regular design H16.I has the most (M,S)-optimal projections, H16.II ranks second, H16.III third, H16.V fourth, and H16.IV fifth. Design H16.IV doesn't have any (M,S)-optimal projections onto 5, 7, 8, and 9 factors in Table 3. The best (in terms of the (M,S) criterion) projections onto 5, 7, 8, and 9 factors for H16.IV have trace(C_d)'s 160, 288, 352, 336, and trace(C_d^2)'s 4096, 11776, 19456, 19200, respectively. Similarly, H16.V does't have any (M,S)-optimal projections onto 5 factors, and the best projections in H16.V have trace(C_d) = 160 and trace(C_d^2) = 4096. Even though the regular design H16.I has fewer classes than the nonregular designs (Table 4), it has the largest frequencies of (M,S)-optimal projections. Since factorial effects in (M,S)-optimal projections have less aliasing than those in others, it is

Table 3: (M,S)-optimal projections in 16-run Hall's designs

No. of Factors	Trace of C_d	Trace of C_d^2	H16.I	H16.II	H16.III	H16.IV	H16.V	Columns Selected
3(455)	48	768	420	372	348	336	336	$1, 2, 3$
4(1365)	96	1536	840	600	480	420	420	$1, 2, 3, 4$
5(3003)	160	2560	168	72	24	0	0	$1, 2, 3, 4, 7$
6(5005)	240	8448	420	120	46	21	28	$1, 2, 3, 4, 6, 8$
7(6435)	336	16128	120	24	8	0	8	$1, 2, 3, 4, 6, 8, 9$
8(6435)	448	28672	15	3	1	0	1	$1, 2, 3, 4, 6, 8, 9, 12$
9(5005)	384	24576	105	21	7	0	7	$\{7, 10, 11, 13, 14\}^c$
10(3003)	336	22784	315	99	39	21	21	$\{10, 11, 13, 14\}^c$
11(1365)	304	23296	420	228	132	84	84	$\{11, 13, 14\}^c$
12(455)	288	27648	35	19	11	7	7	$\{11, 14\}^c$
13(105)	192	18432	105	105	105	105	105	any 13 columns
14(15)	112	12544	15	15	15	15	15	any 14 columns

not surprising to see that the regular design H16.I has the largest frequencies of (M,S)-optimal projections because regular designs usually have less effect aliasing than nonregular designs.

It is interesting to note that all (M,S)-optimal projections onto 3 to 8 factors in Table 3 are regular factorial designs because their values of J-characteristics are either 0 or 16. Some of the (M,S)-optimal projections onto 9 to 14 factors are nonregular. In terms of (M,S)-optimality, these nonregular designs are as good as their regular counterparts. For example, the projection consisting of columns 4, 5, 6, 7, 8, 9, 10, 11, and 13 of H16.II is a nonregular design because $j_3(c_4c_8c_{13}) = 8$. It has the same trace(C_d) and trace(C_d^2) as the (M,S)-optimal projection consisting of columns 1, 2, 3, 4, 5, 6, 8, 9, and 12 (which is a regular design) in H16.I.

Deng and Tang (2002) used the GMA criterion to select and classify projections in the five Hall's designs. They also listed some GMA projections from Hall's designs (Table 2 in their paper). It is easy to check that all the GMA projections given there are (M,S)-optimal.

However, not all (M,S)-optimal projections are GMA. For example, the 5-dimensional, (M,S)-optimal projection consisting of columns 1, 2, 3, 4, and 7 in 16H.I has $F_3[16, 8] = (1, 0)$ and $F_4[16, 8] = (0, 0)$. The GMA projection consisting of columns 8, 9, 13, 14, and 15 in 16H.I has $F_3[16, 8] = (0, 0)$ and $F_4[16, 8] = (0, 0)$. The difference between (M,S) and GMA criteria lies in the fact that the CFV in GMA only uses $J_k(s)$ to order f_{kj}'s and doesn't take the magnitude of $J_k(s)$ into consideration. On the other hand, the (M,S) criterion considers both the magnitude and frequency of $J_k(s)$. For Hadamard matrices with $N = 4t$, $J_k(s) = 4(t + 1 - j)$ and $\text{trace}(C_d) = 4t\binom{n}{2} - \frac{3}{4t}\sum_{j=1}^{t} f_{3j}[4(t + 1 - j)]^2$.

Table 4 gives the numbers of nonisomorphic projections identified by the (M,S) classifier as well as the total numbers of nonisomorphic projections for each dimension across the five designs. The exact number of nonisomorphic projections (Sun and Wu, 1993) and Deng and Tang's results (where GMA-4 and GMA-5 total are the numbers of nonisomorphic projections using GMA-4 and GMA-5 classifiers) are included for comparisons. It is evident that, for $3 \le m \le 14$, H16.III has more nonisomorphic projections than any other of Hall's designs. For $m = 3, 4, 5$, the (M,S) classifier can identify all the nonisomorphic projections. For $m \ge 6$, the numbers of nonisomorphic projections found by the (M,S) classifier are less than the exact or GMA numbers. This is mainly because, as the number of factors increases, the degrees of freedom used to capture information on main effects and 2fi's are decreased, and the (M,S) classifier becomes less powerful.

4.3. Hall's Designs of 20 Runs

According to Hall (1965), there are three non-isomorphic Hadamard matrices of order 20, commonly called N, P, and Q. In particular, Q is equivalent to the 20-run Plackett-Burman design. Designs N, P and Q are given in appendix C of Deng and Tang (2002). A similar procedure could be applied in selecting and classifying projections of these designs. Table 5 lists the numbers of nonisomorphic projections for $m = 3, 4, \ldots, 18$. The (M,S) classifier finds many more nonisomorphic projections than the GMA classifier in Deng and Tang (2002) for projections onto 3 to 13 factors. For projections onto 14 or more factors, due to insufficient degrees of freedom, the (M,S) classifier becomes less powerful but still identifies as many nonisomorphic projections as the GMA classifier. Note that the number of nonisomorphic projections identified by the (M,S) classifier is less than the total number of nonisomorphic projections. For instance, Wang and Wu (1995) reported 59 projections

Table 4: Numbers of nonisomorphic projections identified by the (M,S) classifier

Type\ m	3	4	5	6	7	8	9	10	11	12	13	14
H16.I	2	3	4	5	6	6	5	3	2	2	1	1
H16.II	3	5	10	15	18	17	13	8	4	3	1	1
H16.III	3	5	11	21	31	30	19	9	4	3	1	1
H16.IV	3	5	10	16	18	17	15	9	4	3	1	1
H16.V	3	5	10	17	23	22	16	9	4	3	1	1
Total	3	5	11	23	34	33	19	9	4	3	1	1
GMA-4 Total	3	5	11	26	50	69	74	71	52	31	18	10
GMA-5 Total	3	5	11	26	50	69	75	71	52	31	18	10
Sun and Wu (1993)	3	5	11	27	55	80	87	78	58	36	18	10

Table 5: Numbers of nonisomorphic projections identified by the (M,S) classifier

Type\ m	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
N	2	3	10	54	182	319	356	326	244	159	46	9	2	2	1	1
P	2	3	10	51	142	258	313	276	203	129	44	9	2	2	1	1
Q	2	3	9	47	133	215	261	244	169	118	39	8	2	2	1	1
GMA	2	3	10	34	51	81	125	125	80	51	34	10	3	2	1	1

onto six factors and Xu and Deng (2005) identified 2,282 projections onto ten factors.

Table 6 lists the (M,S)-optimal projections and their proportions for each design. For example, the (M,S)-optimal projections among all 3-dimensional projections have trace(C_d) = 57.60 and trace(C_d^2) = 1105.92; 912 out of 969 3-dimensional projections in designs N, P or Q are (M,S)-optimal. Design N doesn't have any (M,S)-optimal projections onto 8, 9, 10, and 11 factors. In terms of the (M,S) criterion, the best projections onto these numbers of factors have trace(C_d) = 425.00, 480.00, 535.20, 588.80, and trace(C_d^2) = 17909.76, 24130.56, 32384.64, 44554.24, respectively. Similarly, design Q doesn't have any (M,S)-optimal projections onto 8, 9, 10, 11, 12, and 13 factors and the best projections onto these numbers of factors have trace(C_d) = 406.40, 480.00, 554.40, 569.00, 580.80, 585.60, and trace(C_d^2) = 16250.88, 24007.68, 35948.16, 40867.84, 48396.8, 57292.80, respectively. It is obvious that design P has the highest proportions of (M,S)-optimal projections onto 8, 9, 10, 11, 12 and 13 factors while it has the lowest proportions of (M,S)-optimal projections onto 5, 6, 7, and 14 factors. It is straightforward to show that the GMA projections of 20 runs in Deng and Tang (2002, Table 4) are not all (M,S)-optimal and the (M,S)-optimal projections are not GMA. For example, the GMA projection consisting of columns 4, 8, 11, 13, 17, and 19 in design N has trace(C_d) = 252 and trace(C_d^2) = 6631.04. It is not (M,S)-optimal because the (M,S)-optimal projections have trace(C_d) = 252 and trace(C_d^2) = 6569.60. The (M,S)-optimal projection consisting of columns 1, 2, 3, 6, 8 and 11 of design N has $F_3[20, 12] = [0, 2]$, while the GMA projection consisting of columns 4, 8, 11, 13, 17 and 19 has $F_3[20, 12] = [0, 0]$. Since not every orthogonal array of 20 runs is a projection of designs N, P, and Q, the (M,S)-optimal projections in Table 6 may not be optimal among all the orthogonal arrays. Our conclusions on the relation between (M,S) and GMA only apply to projections of N, P and Q.

In order to compare the (M,S) criterion and the GMA as well as other model-dependent efficiency criteria in Cheng, Deng and Tang (2002), we consider the ten nonisomorphic projections of N, P, and Q onto five factors given by Deng, Li and Tang (2000). These projections are labeled as 5.1 to 5.10 with the meaning that projection 5.i is the ith best among the ten projections according to the GMA criterion. Table 7 lists the rankings under different criteria where 1 is the best and 10 is the worst. Projection 5.2 is actually the (M,S)-optimal projection onto five factors. Since ranks under D_f vary slightly according to the number of 2fi's (denoted by f), ranks under D_2 are recorded in Table 7. It is evident from Table 7 that the (M,S)-ranking is consistent with rankings based on GMA, minimum G_2, D_f, and S_f^2, while there is only moderate consistency between (M,S) and estimation capacity E_f because E_f doesn't take efficiency into consideration. Nevertheless, the (M,S)-optimal projection performs the best with respect to the estimation capacity criterion. An interesting observation is that the minimum G_2 projection 5.1 is not (M,S)-optimal and the (M,S)-optimal projection 5.2 is not minimum G_2. Since there are additional orthogonal arrays with 20 runs and 5 factors that are not projections from N, P, and Q, it is not clear whether projection 5.1 is minimum G_2 and projection 5.2 is (M,S)-optimal among all orthogonal arrays of this size. This issue is currently under investigation.

Table 6: (M,S)-optimal projections in 20-run Hall's designs

No. of Factors	Trace of C_d	Trace of C_d^2	N	P	Q	Columns Selected
3	57.60	1105.92	$\frac{912}{969}$	$\frac{912}{969}$	$\frac{912}{969}$	$\{1,2,3\}$
4	110.40	2142.72	$\frac{2736}{3876}$	$\frac{2736}{3876}$	$\frac{2736}{3876}$	$\{1,2,3,6\}$
5	176.00	3655.68	$\frac{1488}{11628}$	$\frac{1728}{11628}$	$\frac{1368}{11628}$	$\{1,2,3,6,8\}$
6	252.00	6569.60	$\frac{1248}{27132}$	$\frac{1008}{27132}$	$\frac{1368}{27132}$	$\{1,2,3,6,8,11\}$
7	336.00	11120.64	$\frac{144}{50388}$	$\frac{72}{50388}$	$\frac{171}{50388}$	$\{1,2,3,4,6,11,19\}$
8	425.60	17786.88	$\frac{0}{75582}$	$\frac{36}{75582}$	$\frac{0}{75582}$	$\{1,2,6,8,10,11,13,15\}$
9	518.40	29757.44	$\frac{0}{92378}$	$\frac{9}{92378}$	$\frac{0}{92378}$	$\{1,2,3,4,8,9,13,14,18\}$
10	612.00	43873.92	$\frac{0}{92378}$	$\frac{1}{92378}$	$\frac{0}{92378}$	$\{1,2,3,4,8,9,13,14,18,19\}$
11	608.00	47349.76	$\frac{0}{75582}$	$\frac{9}{75582}$	$\frac{0}{75582}$	$\{6,7,10,11,12,15,16,17\}^c$
12	638.40	58882.56	$\frac{4}{50388}$	$\frac{12}{50388}$	$\frac{0}{50388}$	$\{4,7,9,12,14,17,18\}^c$
13	604.80	61178.88	$\frac{16}{27132}$	$\frac{48}{27132}$	$\frac{0}{27132}$	$\{7,9,12,14,17,18\}^c$
14	562.40	63345.28	$\frac{432}{11628}$	$\frac{288}{11628}$	$\frac{513}{11628}$	$\{9,13,15,18,19\}^c$
15	508.80	64788.48	$\frac{912}{3876}$	$\frac{912}{3876}$	$\frac{912}{3876}$	$\{15,17,18,19\}^c$
16	441.60	65003.52	$\frac{57}{969}$	$\frac{57}{969}$	$\frac{57}{969}$	$\{15,18,19\}^c$
17	320	51200	$\frac{171}{171}$	$\frac{171}{171}$	$\frac{171}{171}$	any 17 columns
18	180	32400	$\frac{19}{19}$	$\frac{19}{19}$	$\frac{19}{19}$	any 18 columns

Table 7: (M,S) Rankings versus others

GMA	$(\text{trace}(C_d), \text{trace}(C_d^2))$	(M,S)	D_f	S_f^2	E_f	G_2	(B_3, B_4, B_5)
5.1	$(176, 3712)$	2	2	1	1	1	$(0.40, 0.20, 0.00)$
5.2	$(176, 3655.68)$	1	1	1	1	2	$(0.40, 0.20, 0.16)$
5.3	$(176, 4367.36)$	4	4	3	1	3	$(0.40, 0.52, 0.00)$
5.4	$(176, 4270.08)$	3	3	3	8	4	$(0.40, 0.52, 0.16)$
5.5	$(156.80, 3159.04)$	6	6	5	1	5	$(0.72, 0.20, 0.00)$
5.6	$(156.80, 3143.68)$	5	5	5	7	6	$(0.72, 0.20, 0.16)$
5.7	$(156.80, 3814.40)$	7	7	7	5	7	$(0.72, 0.52, 0.00)$
5.8	$(137.60, 2606.08)$	8	8	8	5	8	$(1.04, 0.20, 0.00)$
5.9	$(137.60, 3261.44)$	10	10	9	9	9	$(1.04, 0.52, 0.00)$
5.10	$(137.60, 3246.08)$	9	9	9	10	10	$(1.04, 0.52, 0.16)$

5. Concluding Remarks

In this paper, the use of (M,S)-optimality in selecting and classifying regular designs as well as nonregular designs is studied. Compared to the MA or GMA criterion, the (M,S) criterion proposed is easier to compute and it is also independent of the choice of orthonormal contrasts. Although main effects and 2fi's are the focus in this paper, the (M,S) criterion can easily be applied when higher-order interactions are also of interest.

For regular designs, the two components of the (M,S) criterion, i.e., $\text{trace}(C_d)$ and $\text{trace}(C_d^2)$, are derived as explicit functions of the numbers of three- and four-letter words. Generally, (M,S)-optimal designs are not MA designs. All MA designs up to 64 runs are (M,S)-optimal.

For nonregular designs, $\text{trace}(C_d)$ and $\text{trace}(C_d^2)$ are written as functions of $j_3(s)$ and $j_4(s)$. When applied to nonregular designs, the (M,S) criterion takes both the magnitude and the frequencies of J-characteristics into consideration, while the GMA criterion uses only ordinal information on the magnitude. The (M,S) criterion is different from the minimum G_2-aberration criterion. Minimum G_2 projections of Hadamard matrices are not necessarily (M,S)-optimal, and vice versa. Among projections from Hadamard matrices of 12, 16, and 20 runs, (M,S)-optimal projections are generally not MA, and MA projections are not (M,S)-optimal.

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