Two-Level Augmented Definitive Screening Designs

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Definitive screening designs (DSDs) constitute a well-known class of screening designs for three-level factors. DSDs are comprised of orthogonal main effects plans for which main effects estimates are statistically independent of estimates of two-factor interactions. Jones and Nachtsheim (2013) proposed two methods for augmenting DSDs with two-level categorical factors, namely the DSD-augment and the ORTH-augment approaches. However, these two versions produce distinct features that are not sufficiently flexible to accommodate versatile performance preferences in practice. In this paper, we provide a comprehensive overview of the augmented designs with DSD structures and show how to construct compromise designs that share the desirable traits of both DSD-augment and ORTH-augment designs. In addition to the DSD-augment and ORTH-augment designs, we suggest routine consideration of nondominated compromise designs as described in the paper. Additionally, we provide some theoretical properties of randomly assigned augmented DSDs.

Key Words: Conference Matrix; Correlation Cell Plot; D_s-Optimality; Fold-Over Design; Pareto Front.

1. Introduction

JONES AND NACHTSHEIM (2011) introduced a class of screening designs called definitive screening designs (DSDs). Originally presented as three-level screening designs, DSDs require $2m + 1$ runs for a design with m factors. The structure of a DSD consists of m fold-over pairs. Each factor is set to zero in one fold-over pair, which leads to two center values in each column. Finally, at least one overall center run is included to ensure that all linear and quadratic main effects are estimable. The addition of the row of zeros allows for all quadratic effects to be estimated, while the presence of the fold-over pairs ensures that estimates of main effects are statistically independent of the estimates of two-factor interactions. The designs were originally constructed using an algorithm that maximized the determinant of the information matrix subject to the structural constraints described (one center value per run and m fold-over runs). As Jones and Nachtsheim (2011) note, the structure of these designs provides several advantages over other screening designs. These benefits include the small number of runs required (only one more than twice the number of factors); the independence of main effects and two-factor interactions, which provides the ability to estimate main effects separately from two-factor interactions; the absence of complete confounding among two-factor interactions; the ability to estimate all quadratic effects; and the orthogonality of main effects for 4, 6, 8, and 10 factors.

Xiao et al. (2012) noted that the design matrix could be determined using conference matrices rather than relying on the algorithmic approach outlined in Jones and Nachtsheim (2011). For most values of even m, the design matrix may be constructed using a conference matrix, its fold-over, and one row of

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zeros. For odd m, the same method can be used but the design matrix is constructed for $m' = m + 1$ factors rather than for m factors and one column can be dropped from the design, giving an m-factor DSD in $2m+3$ runs. This conference matrix approach maintains all of the positive traits of DSDs and has the added advantage of always producing orthogonal designs. Conference matrix type designs with odd m are investigated in Phoa and Lin (2015).

Jones and Nachtsheim (2013) presented a modification of DSDs that accommodates two-level categorical factors as well as three-level factors. These mixed-level designs preserve the original structure of a DSD but replace the zeros in the columns corresponding to categorical factors with ± 1's. Jones and Nachtsheim (2013) provide two methods for adding two-level categorical factors to their designs, each method taking a different approach to the assignment of the ± 1's in place of the zeros, and each resulting in a different set of advantages and disadvantages. The first method, referred to as DSD-augment, assigns $+1$ and -1 in place of the two zeros in the columns corresponding to the categorical factors, where the order is determined by optimization. DSD-augment is highly D-efficient and, by preserving the fold-over structure of DSDs, it retains independence between the main effects and the second-order effects. However, it is not orthogonal for main effects and it results in partial aliasing between the intercept and the two-factor interactions. The second approach, called ORTH-augment, substitutes two $+1$'s (or two -1's) and then augments the design with additional runs to balance the design in a way that leads to orthogonality of the main effects. The disadvantage of ORTH-augment is that main effects and two-factor interactions are correlated.

These two approaches currently represent the only methods for including two-level categorical factors in DSDs. In this paper, however, we comprehensively examine more general classes of augmented DSDs that accommodate the presence of two-level categorical factors. Instead of the alternating ± 1 pairs (DSD-augment) or identical $+1$ or -1 pairs (ORTH-augment) by which Jones and Nachtsheim (2013) replace the zeros in the columns corresponding to the categorical factors, we assign ± 1 in a probabilistic fashion to the zero entries. As we will show, the scheme leads to a series of alternative designs that possess a mixture of the traits of both the DSD-augment and the ORTH-augment designs. Key traits include (1) the D_s efficiency of the design for estimating the augmented categorical main effects, (2) the average absolute correlation among main effects columns, (3) the average absolute correlation between main effects columns and two-factor interaction columns, and (4) the average absolute correlation among two-factor interaction columns.

Because there are multiple measures of goodness of a given design, we will identify "compromise" designs that do well along multiple criteria. In particular, we will identify sets of "nondominated" designs. A solution design is called nondominated, or Pareto optimal, if none of its characteristics of interest can be improved without degrading some other characteristic of interest. For example, consider Figure 1. The two design characteristics of interest are the average absolute correlation among main effects columns and the average absolute correlation between main effects columns and two-factor interaction columns. For these two criteria, for which smaller is better, there are six nondominated designs, and the plot symbols for these designs are connected by a solid line. This solid line is often referred to as the *Pareto front.* The Pareto front always contains the designs that minimize each of the individual criteria. These fall at the two ends of the Pareto front as shown in Figure 1. Figure 1 also identifies the minimax design, another compromise design that will be of interest in the sequel. To see that any of the designs not on the Pareto front are dominated, consider the design denoted by "A" in the figure. This design is clearly dominated by the minimax design. Similarly, the design denoted "B" is dominated by the two right-most designs along the Pareto front. If any design is dominated by some other design, there is no reason to give it further consideration. As a result, the sets of nondominated designs can provide experimenters a richer library of designs and an enhanced ability to augment a DSD with two-level factors in ways that meet the practical needs of the experimenter. In short, the proposed approach provides a series of compromise designs that more flexibly accommodate practical use.

The remainder of this article is organized as follows. In Section 2, we present our design structure and scheme to study a more general class of two-level augmented DSDs. In Section 3, we explore potential performance measures of compromise designs and propose the nondominated compromise designs. In Section 4, we investigate empirically the key population properties of the produced design class and compromise designs. In Section 5, we discuss the the-

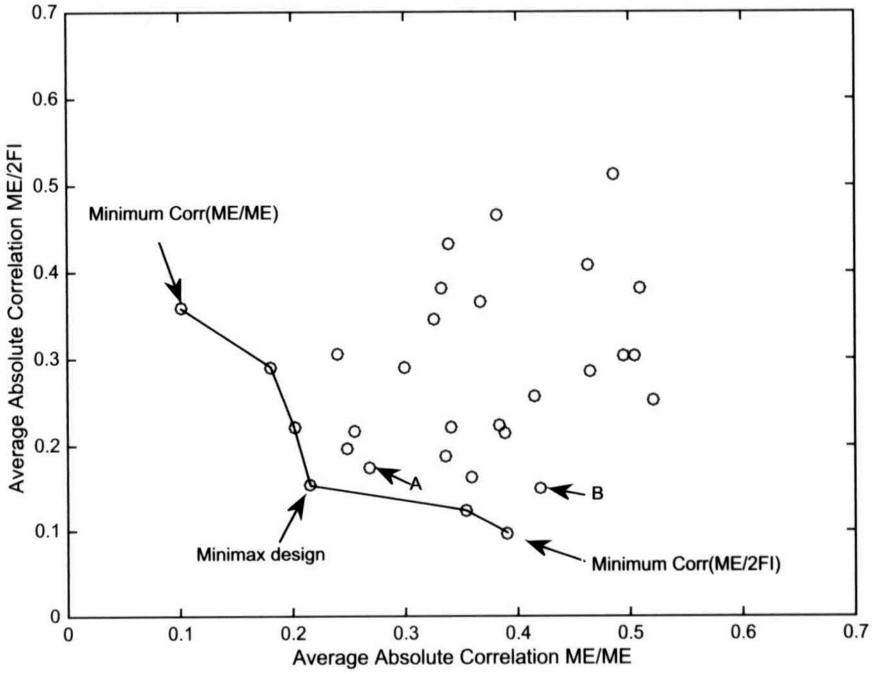


FIGURE 1. A Simple Example Showing the Nonndominated and Minimax Designs in a Set of 30 Designs.

oretical properties inherent to our method. In Section 6, a discussion of benefits and limitations of our method is provided.

2. Proposed Design Structure

In this section, we introduce our design structure for augmenting a DSD with two-level categorical factors. Following Jones and Nachtsheim (2013), it is useful to add an even number of $k \geq 2$ center value runs (in the continuous factors) when augmenting a DSD with two-level categorical factors. Given m continuous factors, c categorical factors, and k center value runs, we propose the following steps to randomly generate a DSD with added two-level factors:

1. Create a DSD for $m' = m + c$ factors if $m + c$ is even or for $m' = m + c + 1$ if $m + c$ is odd.
2. Eliminate the center-point run so that the design matrix consists of $2m'$ rows.
3. Replace the two zeros in the column corresponding to the jth categorical factor with the variables $z_{1,j}$ and $z_{2,j}$ for $j = 1, \ldots, c$.
4. For even k, add k rows, rows $2(m + c) + 1, \ldots, 2(m + c) + k$, to the design matrix. For these rows, assign zeros to each column that corresponds to the m continuous factors. For rows $2(m+c)+1, \ldots, 2(m+c)+k$, assign variables $z_{3,j}, \ldots, z_{2+k,j}$, respectively, to the column corresponding to the jth categorical factor, for $j = 1, \ldots, c$.
5. Independently assign each $z_{h,j}$ to $+1$ or -1 at random (i.e., $P(z_{h,j} = -1) = P(z_{h,j} = 1) = 0.5$) for $h = 1, \ldots, 2 + k$ and $j = 1, \ldots, c$.

Based on the partitioning of the design matrix in Table 1, we extract the set of $\{z_{h,j}\}$ variables from the table to form the following matrix:

$$\mathbf{Z} = \begin{pmatrix} z_{1,1} & z_{1,2} & \cdots & z_{1,c} \\ \vdots & \vdots & \ddots & \vdots \\ z_{2+k,1} & z_{2+k,2} & \cdots & z_{2+k,c} \end{pmatrix},$$

where row h of $\mathbf{Z}$ is denoted by $\mathbf{Z}'_h$, for $h = 1, \ldots, 2+k$.

We note that, given m, c, and k, the method samples with replacement from a population class of designs. We will use "DSD(m, c, k)" to denote the class of designs. This class covers DSD-augment and ORTH-augment designs as special cases. For instance, the DSD-augment design can be thought of as a member of the DSD(m, c, k) class of designs, where (1) $k = 2$ (so that the $\mathbf{Z}$ matrix has four rows and c columns), (2) the first two entries and the last two entries in each column of $\mathbf{Z}$ are comprised of a $+1$ and a -1, (3) the order of the ± 1's within each of the two pairs in each column are chosen to maximize the determinant of the resulting design (for the linear main effects model). Likewise, the ORTH-augment

TABLE 1. Design Matrix Structure for Augmented Design with $m + 1$ Through $m + c$ Factors

Run (i)	Continuous factors						Categorical factors			
	$\mathbf{1}$	$\mathbf{d}_1$	$\mathbf{d}_2$	$\mathbf{d}_3$	$\cdots$	$\mathbf{d}_m$	$\mathbf{a}_1$	$\mathbf{a}_2$	$\cdots$	$\mathbf{a}_c$
1	1	0	± 1	± 1	$\cdots$	± 1	± 1	± 1	$\cdots$	± 1
2	1	± 1	0	± 1	$\cdots$	± 1	± 1	± 1	$\cdots$	± 1
3	1	± 1	± 1	0	$\cdots$	± 1	± 1	± 1	$\cdots$	± 1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
m	1	± 1	± 1	± 1	$\cdots$	0	± 1	± 1	$\cdots$	± 1
$m + 1$	1	± 1	± 1	± 1	$\cdots$	± 1	$z_{1,1}$	± 1	$\cdots$	± 1
$m + 2$	1	± 1	± 1	± 1	$\cdots$	± 1	± 1	$z_{1,2}$	$\cdots$	± 1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$m + c$	1	± 1	± 1	± 1	$\cdots$	± 1	± 1	± 1	$\cdots$	$z_{1,c}$
$m + c + 1$	1	0	∓ 1	∓ 1	$\cdots$	∓ 1	∓ 1	∓ 1	$\cdots$	∓ 1
$m + c + 2$	1	∓ 1	0	∓ 1	$\cdots$	∓ 1	∓ 1	∓ 1	$\cdots$	∓ 1
$m + c + 3$	1	∓ 1	∓ 1	0	$\cdots$	∓ 1	∓ 1	∓ 1	$\cdots$	∓ 1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$2m + c$	1	∓ 1	∓ 1	∓ 1	$\cdots$	0	∓ 1	∓ 1	$\cdots$	∓ 1
$2m + c + 1$	1	∓ 1	∓ 1	∓ 1	$\cdots$	∓ 1	$z_{2,1}$	∓ 1	$\cdots$	∓ 1
$2m + c + 2$	1	∓ 1	∓ 1	∓ 1	$\cdots$	∓ 1	∓ 1	$z_{2,2}$	$\cdots$	∓ 1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$2(m + c)$	1	∓ 1	∓ 1	∓ 1	$\cdots$	∓ 1	∓ 1	∓ 1	$\cdots$	$z_{2,c}$
$2(m + c) + 1$	1	0	0	0	0	0	$z_{3,1}$	$z_{3,2}$	$\cdots$	$z_{3,c}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$2(m + c) + k$	1	0	0	0	0	0	$z_{2+k,1}$	$z_{2+k,2}$	$\cdots$	$z_{2+k,c}$

design is a member of the DSD(m, c, k) class of designs in which (1) $k = 4$ (so that the $\mathbf{Z}$ matrix has six rows and c columns), (2) the first two entries in each column are $+1$'s, (3) the order of the ± 1's in the remaining rows of $\mathbf{Z}$ leads to orthogonality of the main effects.

As noted above, our purpose here is to explore these classes of designs and search for possible alternatives to the DSD-augment and ORTH-augment designs. When the number of designs in a class is small, it is easy to enumerate all of the possible alternatives. We note that, because $\mathbf{Z}$ has $c(2 + k)$ entries, there are $n_d = 2^{c(2+k)}$ candidate designs for a given (c, k) pair. Many of these designs will be isomorphic to other designs in the class. Two designs are isomorphic if one can be obtained from the other by permutation of rows or columns, in which case they will have the same statistical properties. The population of designs is easily constructed as long as $2^{c(2+k)}$ is not prohibitively large. In general, for given c and k, we evaluate the entire collection of designs as long as $n_d \leq 10{,}000$. For $n_d > 10{,}000$, we use the simulation algorithm above (i.e., sampling with replacement) to generate a sample of 10,000 designs. We next consider criteria used to identify particularly advantageous designs from within this set of compromise designs.

3. Assessing Compromise Designs

In this section, we explore the entire set of candidate designs that result from our method. This set consists of the designs generated by considering every possible combination of the values of $z_{h,j}$ in $\mathbf{Z}$. We refer to this set of designs as the population of designs that constitute the DSD(m, c, k) class. As noted, however, this set contains different values of $\mathbf{Z}$

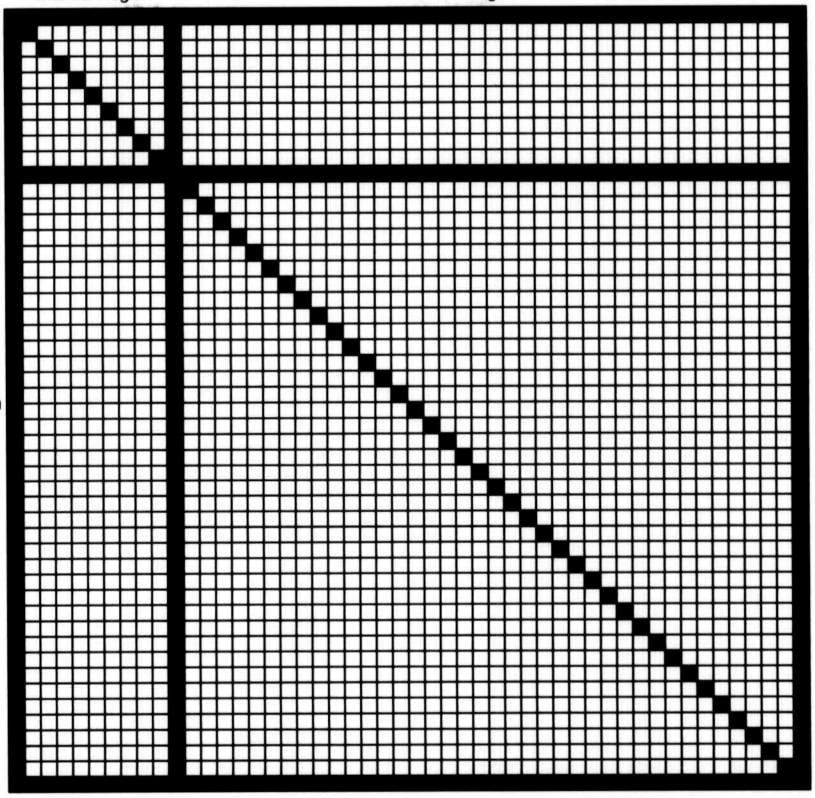


FIGURE 2. Regions in a Correlation Cell Plot.

only and does not also encompass different settings of the continuous factors. We have two objectives. First, we wish to characterize the population of designs that obtain from the method. Second, we seek a method by which we might identify designs from within this population that may be particularly advantageous in the compromise that they strike between the traits inherent to the DSD-augment and those inherent to the ORTH-augment designs.

Depending on the design, nonzero correlation may exist (1) among the main effects, (2) between main effects and two-factor interactions, and (3) among two-factor interactions. The correlation cell plot serves as a tool by which an experimenter may assess the presence of each in any particular design (Errore et al. (2017)). Let $p_{\mathrm{ME}} = m + c$ denote the number of main effects, let $p_{\mathrm{2FI}} = p_{\mathrm{ME}}(p_{\mathrm{ME}} - 1)/2$ denote the number of two-factor interactions, and let $p = p_{\mathrm{ME}} + p_{\mathrm{2FI}}$. A correlation cell plot is a $p \times p$ symmetric matrix of square cells shaded in gray-scale ranging from white to black. Cell (i, j) of a correlation cell plot represents the magnitude of the correlation between column i and column j of the design settings matrix. Cell (i, j) will be shaded black if the magnitude of the correlation between factors i and j equals one; it will be shaded white if the magnitude of the correlation equals zero; and it will be shaded a gray tone for magnitudes between zero and one, with darker grays corresponding to magnitudes that are closer to one. A correlation cell plot contains four key regions as shown in Figure 2: (1) the $p_{\mathrm{ME}} \times p_{\mathrm{ME}}$ square in the upper left corner corresponds to correlation among the main effects and is referred to as the "ME/ME region". (2) The upper right $p_{\mathrm{ME}} \times p_{\mathrm{2FI}}$ rectangle, referred to as the "ME/2FI region", corresponds to the correlation between main effects and two-factor interactions. (3) The transpose of the upper right rectangle appears in the lower right rectangle, also referred to as the "ME/2FI region". (4) The lower left $p_{\mathrm{2FI}} \times p_{\mathrm{2FI}}$ square corresponds to the correlations between pairs of two-factor interactions and is referred to as the "2FI/2FI region". Therefore, by considering depth of shading of the cells in each region, an experimenter can use a correlation cell plot to determine the level of pairwise correlation that is present in a particular design.

While attaining zero correlation in each cell across all three regions is ideal, a design of resolution V or higher is required, which is often impractical from a budgetary view. Thus, experimenters must determine what type of correlation pattern will best support the goals of their experiment and choose a design accordingly. For instance, when considering DSDs with added two-level factors, an experimenter may choose a DSD-augment design if avoiding correlation between main effects and two-factor interactions is of particular importance. On the other hand, if correlation among main effects is of more concern, then an experimenter may decide to use an ORTH-augment design.

However, other correlation patterns could instead be of particular consequence. For instance, an experimenter may wish to obtain minimum correlation among two-factor interactions. Similarly, achieving minimum average overall correlation could be of particular importance. Finally, an experimenter may prefer obtaining low correlation among main effects and low correlation between two-factor interactions and main effects to achieving zero correlation either among main effects or between main effects and two-factor interactions. In such cases, when the primary concern involves correlation patterns other than those solely among main effects or those solely between main effects and two-factor interactions, an experimenter may wish to consider using a compromise design from the DSD(m, c, k) class of designs as an alternative to either an ORTH-augment or a DSD-augment design. Therefore, examining the properties of the proposed design class provides a comprehensive overview of the design structure and is important to experimenters who have different practical needs.

In the following, we will explore some of these alternatives. We plot design characteristics for designs in a given class in order to observe the corresponding range of performances. As mentioned, the preferences of the experimenter will determine which design from within this set is most useful. As noted in the introduction, in the presence of multiple performance measures for evaluating designs, we suggest consideration of *nondominated* designs— those designs that are not inferior in all performance measures of interest to any other design within the class and that (equivalently) fall on the Pareto front. More precise definitions of dominated and nondominated designs can be given as follows.

Definition

Suppose there are Q design performance measures, for which smaller is better. For a given design $d^{(i)}$, these performance measures are denoted $d_1^{(i)}, \ldots, d_Q^{(i)}$. Let $\mathcal{D}$ denote the set (or class) of designs of interest. A design $d^{(1)} \in \mathcal{D}$ dominates a design $d^{(2)} \in \mathcal{D}$ if $d^{(1)}$ is "better" than $d^{(2)}$ with respect to at least one performance measure and at least as good with respect to all other performance measures. That is,

1. $d_i^{(1)} \le d_i^{(2)}$, for $i = 1, \ldots, Q$, and
2. There exists at least one value of i, $1 \le i \le Q$ for which $d_i^{(1)} < d_i^{(2)}$.

Finally, a design d is a *nondominated* design if it is not dominated by any other design $d' \in \mathcal{D}$. The set of nondominated designs comprises the *Pareto front.*

One design on the Pareto front that will have particular interest to us is the *minimax compromise design.* For each design $d^{(i)} \in \mathcal{D}$, let $d_{\max}^{(i)} = \max\{d_1^{(i)}, \ldots, d_Q^{(i)}\}$. Let $i^* = \text{argmin}_i\{d_{\max}^{(i)}\}$. Then d_{i^*} is a minimax compromise design.

4. Exploring the Class of Designs DSD(m, c, k)

In this section, we explore empirically the population of potential designs that result from our method. A useful measure of the efficacy with which we have augmented the design is the D_s efficiency of the resulting design. D_s efficiency is relevant when precise prediction of a subset of the factor effects is of primary interest. Aside from adding center-value runs to the continuous factors, the augmentation procedure modifies entries only in the columns of the design matrix that correspond to categorical factors. Therefore, the accuracy with which we estimate the subset of parameters corresponding to the categorical factor effects is of considerable interest. Partition the columns of $\mathbf{X}$ as $\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_2]$, where the columns of $\mathbf{X}_1$ correspond to the intercept column and the continuous factor columns only. $\mathbf{X}_2$ is made up of the columns for the categorical factors. The information matrix and its inverse can be written

$$\mathbf{X}'\mathbf{X} = \begin{pmatrix} \mathbf{X}_1'\mathbf{X}_1 & \mathbf{X}_1'\mathbf{X}_2 \\ \mathbf{X}_2'\mathbf{X}_1 & \mathbf{X}_2'\mathbf{X}_2 \end{pmatrix}$$

$$(\mathbf{X}'\mathbf{X})^{-1} = \mathbf{V}(\mathbf{X}) = \begin{pmatrix} \mathbf{V}(\mathbf{X})_{11} & \mathbf{V}(\mathbf{X})_{12} \\ \mathbf{V}(\mathbf{X})_{21} & \mathbf{V}(\mathbf{X})_{22} \end{pmatrix},$$

where the partitioning of the normalized variance–covariance matrix of the parameters $(\mathbf{V}(\mathbf{X}))$ is consistent with the partitioning of the information matrix. $\mathbf{V}(\mathbf{X})_{22}$ is the normalized variance–covariance matrix of the effects of interest. Then the relative D_s efficiency of any design having design matrix $\mathbf{X}_A$, relative to a design having design matrix $\mathbf{X}_B$, is

$$\mathrm{D_s}(\mathbf{X}_A, \mathbf{X}_B) = \left[\frac{|\mathbf{V}(\mathbf{X}_B)_{22}|}{|\mathbf{V}(\mathbf{X}_A)_{22}|}\right]^{1/c}.$$

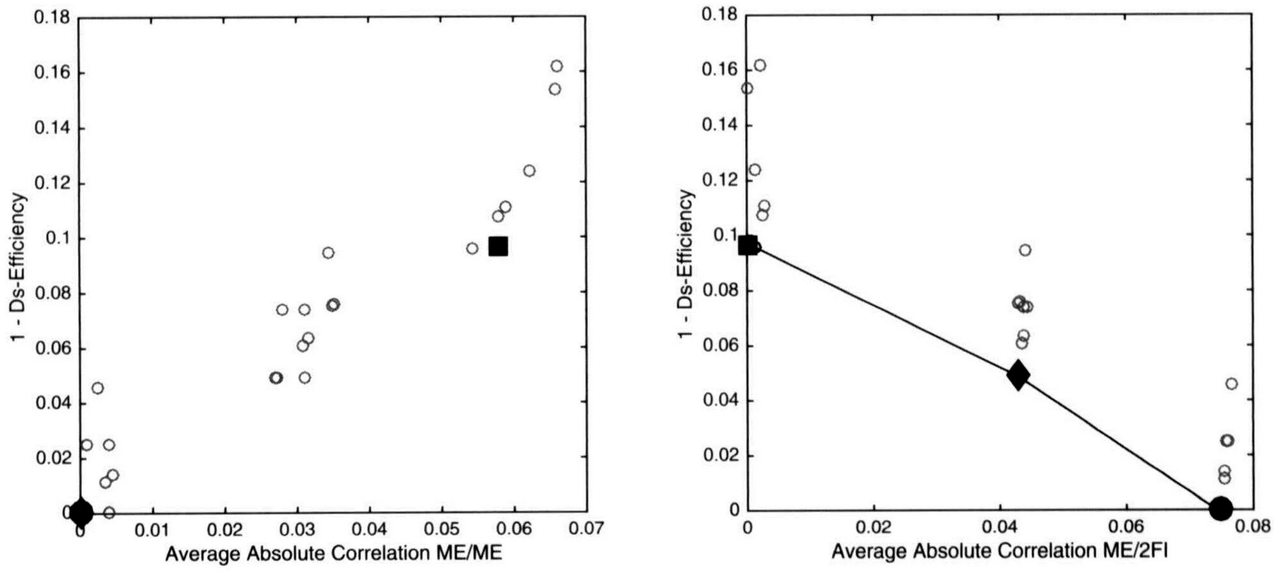
For plotting purposes, we define the *D_s inefficiency* of any design to be one minus the design's $\mathrm{D_s}$ efficiency relative to a D-optimal design, so that we have a smaller-is-better measure.

We will use both $k = 2$ to examine alternative designs that are similar in structure to DSD-augment designs and $k = 4$ to consider designs that can serve as alternatives to ORTH-augment designs. Finally, we will compare the performances of the DSD-augment, the ORTH-augment, and other designs along various Pareto fronts.

4.1. Class DSD(6, 2, 2)

First, we consider the case with $m = 6$, $c = 2$, and $k = 2$. There are $n_d = 2^{2(2+2)} = 256$ candidate designs. Therefore, we evaluate the entire collection of designs.

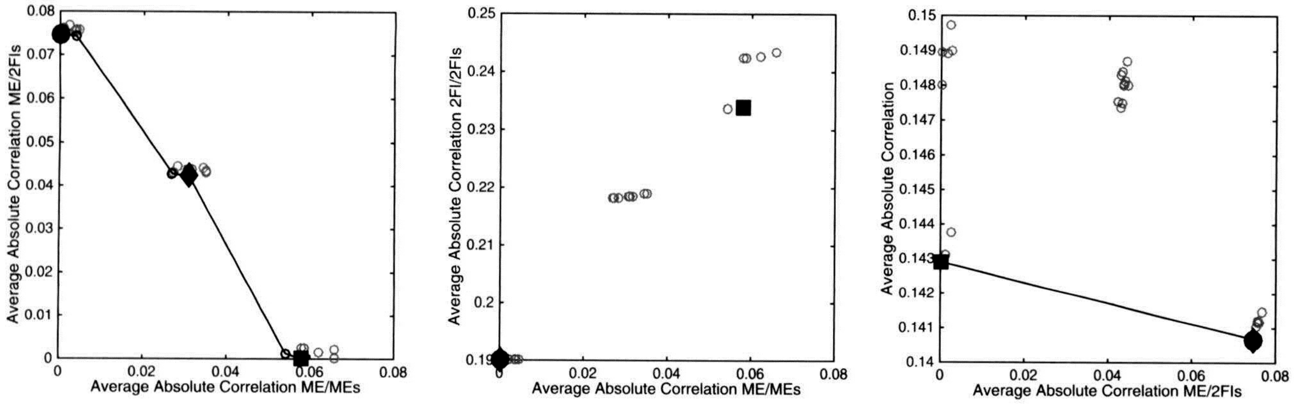
Figure 3 provides a plot of the relative $\mathrm{D_s}$ inefficiencies of the designs against both the average absolute correlation among main effects, denoted $\bar{r}_{\mathrm{MEME}}$, and the average absolute correlation between main effects and two-factor interactions, denoted $\bar{r}_{\mathrm{ME2FI}}$, for each resulting design. Because we focus on $\mathrm{D_s}$ inefficiencies, smaller is better for all of our criteria. Hence, best designs tend to be nearest to the origin. From Figure 3(a) we see that the $\mathrm{D_s}$-optimal design (solid circle) has zero average absolute correlation among main effects and, from Figure 3(b), we observe that the design indicated by the solid square the DSD-augment design is one of several that have zero average absolute correlation between main effects and two-factor interactions. Therefore, our method has produced both the DSD-augment and another design that can be thought of as an alternative to the ORTH-augment design. Jones and Nachtsheim (2013) noted that $k = 4$ is required to produce ORTH-augment designs (unless $c = 1$, in which case only $k = 2$ center-value runs are required). Here we find that, with $k = 2$, it is possible to produce a design that is orthogonal for main effects; however, the estimated intercept term for this design has a nonzero covariance with one or more of the estimated main effects. In this sense, our method has produced an alternative to ORTH-augment for $k = 2$, saving two runs. We will refer to designs that provide zero correlations among main effects as *ORTH-augment(ME)* designs. In some cases, neither an ORTH-augment nor an ORTH-augment(ME) design will exist. In these cases, we will identify the design that minimizes the average absolute correlation of all pairs of main effects columns. We call this



(a) $\mathrm{D_s}$ inefficiency vs. $\bar{r}_{\mathrm{MEME}}$

(b) $\mathrm{D_s}$ inefficiency vs. $\bar{r}_{\mathrm{ME2FI}}$

FIGURE 3. One Minus $\mathrm{D_s}$ Efficiency Versus $\bar{r}_{\mathrm{MEME}}$ and $\bar{r}_{\mathrm{ME2FI}}$ for DSD(6, 2, 2). The solid circle identifies the ORTH-augment(ME) design; the solid square identifies the DSD-augment design; the solid diamond identifies the minimax design. In panel (a) the ORTH-augment(ME) design is the minimax design.



(a) $\bar{r}_{\text{MEME}}$ vs. $\bar{r}_{\text{ME2FI}}$ (b) $\bar{r}_{\text{MEME}}$ vs. $\bar{r}_{\text{2FI2FI}}$ (c) $\bar{r}_{\text{ME2FI}}$ vs. $\bar{r}_{\text{All}}$

FIGURE 4. Average Absolute Correlation Plots for Designs in DSD(6, 2, 2). The solid circle identifies the ORTH-augment(ME) design; the solid square identifies the DSD-augment design; the solid diamond indicates the minimax compromise design. In panels (b) and (c), the ORTH-augment(ME) design is the minimax design.

design the *MINCORR-augment* design. If the number of designs in the class under consideration is less than 10,000, we identify the MINCORR-augment design by exhaustive search; otherwise, we use the coordinate exchange algorithm (Meyer and Nachtsheim (1995)), with the determinant criterion replaced by the absolute average correlation.

From Figure 3, we can also see that each plot contains three clusters of designs. One cluster contains designs that are relatively similar to the ORTH-augment(ME) design, one cluster contains those designs that are relatively similar to the DSD-augment design, and the final cluster is located between the first two. The center cluster is comprised of designs that provide compromises between the ORTH-augment(ME) design and the DSD-augment design. The minimax compromise design of Figure 3(b) (black diamond) provides one possible compromise between the DSD-augment and ORTH-augment(ME) designs.

In Figure 4, we have displayed three comparisons of average absolute correlations for the various portions of the correlation matrix for the DSD(6,2,2) design class. Figure 4(a) provides a plot of $\bar{r}_{\text{MEME}}$ versus $\bar{r}_{\text{ME2FI}}$. This plot clearly identifies the ORTH-augment(ME) design, the DSD-augment design, and the cluster of compromise designs in the middle. Figure 4(b) compares the average absolute correlations among main effects to those among two-factor interactions. From the plot, we see that the ORTH-augment(ME) design minimizes the correlations among two-factor interactions—one reason an experimenter might favor this design. Similarly, Figure 4(c) plots the average absolute correlation between main effects and two-factor interactions against the overall average correlation among model effects. This plot seems to favor the DSD-augment design. Although the overall average correlation is nearly identical for the DSD-augment and the ORTH-augment(ME) designs (0.1429 vs. 0.1407), the DSD-augment fares substantially better in terms of the average absolute correlation between main effects and two-factor interactions. In a related point, note that, in Figures 4(b) and 4(c) (and in analogous plots to follow for other examples), the origin has not been included in the plot. Although including the origin is generally good statistical practice, we have omitted it so that the differences among the clusters can be easily seen.

Table 2 provides a statistical summary of the D_s inefficiencies (when the subset of interest is made up of the categorical factor effects) and the average absolute correlations in the various areas of the correlation cell plot for designs in DSD(6, 2, 2). We note that, within DSD(6, 2, 2), the worst-case design is about 16% D_s inefficient. Also, the range of average absolute correlations, which varies from 0.0090 (for all correlations) to 0.0767 (for the correlation between main effects and two-factor interactions), is not particularly large. We note that D_s inefficiencies less than a few percent matter little. However, inefficiencies in excess of about 5% or 10% are material. Recall that, if a design d_1 is 90% efficient relative to another design d_2, then d_1 needs to be replicated $1/0.90 \approx 1.11$ times to achieve the same precision as

TABLE 2. Statistical Summary of Performance of Designs in DSD(6, 2, 2)

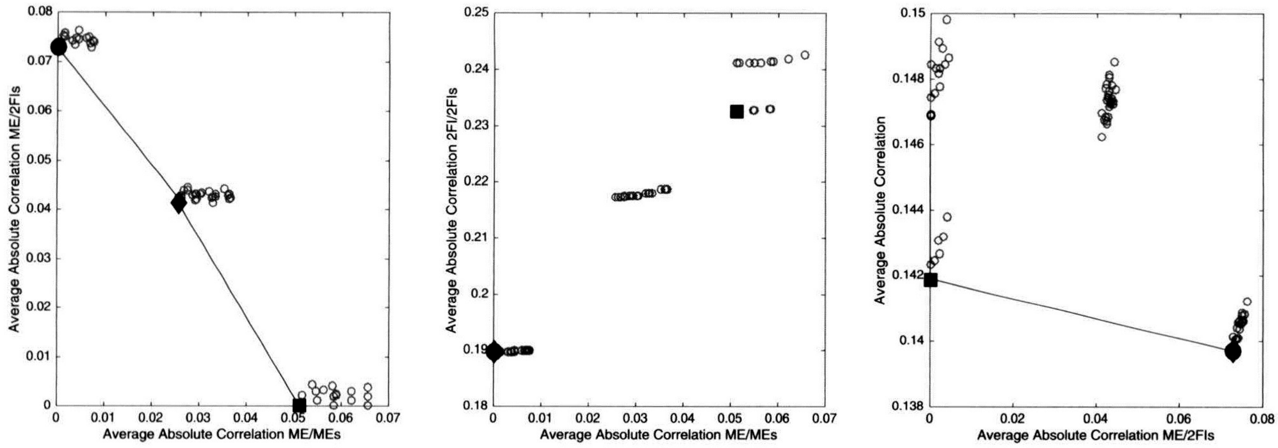
	D_s inefficiency	$\bar{r}_{MEME}$	$\bar{r}_{ME2FI}$	$\bar{r}_{2FI2FI}$	$\bar{r}_{ALL}$
Minimum	0.0000	0.0000	0.0000	0.1901	0.1407
Average	0.0644	0.0310	0.0407	0.2165	0.1457
Maximum	0.1621	0.0659	0.0767	0.2433	0.1497
Range	0.1621	0.0659	0.0767	0.0532	0.0090

d_2. In other words, the design must be 11% larger to achieve the same level of precision. In terms of absolute correlations, our view is that differences in excess of about 0.05 can matter. For example, our ability to identify a few active two-factor interactions correctly degrades with the level of column correlation between main effects and two-factor interactions and among two-factor interactions (Errore et al. (2016)). Here and in the examples that follow, we have found that the impact of design differences on the *overall* correlation is generally quite small and not of concern. For this reason, we give greater focus in what follows to the correlations (1) among main effects, (2) between main effects and two-factor interactions, and (3) among two-factor interactions.

In Figure 5, we compare the correlation cell plots for the DSD-augment design, the ORTH-augment(ME) design, and the minimax design identified in Figure 4(a). From Figure 5(a), we see that the correlation cell plot corresponding to the DSD-augment design has all white cells in the ME/2FI region, while the ME/ME region has mostly white cells but it also includes some light gray cells. This is expected because the characteristics of DSD-augment designs include independence between main effects and two-factor interactions and the absence of orthogonality among main effects. Likewise, Figure 5(c) shows all white cells corresponding to the ME/ME region of the correlation cell plot for the ORTH-augment(ME) design, but some light gray in addition to white in the ME/2FI region. Again, this is not surprising because ORTH-augment and ORTH-augment(ME) designs are orthogonal among main effects but do not guarantee independence between main effects and two-factor interactions. Figure 5(b) shows mostly white cells with some light gray cells in both the ME/ME region and the ME/2FI region of the correlation cell plot. From Figure 5, we note that the compromise design contains fewer gray cells in the ME/ME region than the DSD-augment design but more gray cells than the ORTH-augment(ME) design. In the ME/2FI region, the compromise design shows more gray cells than the ME/2FI region of the DSD-augment design but fewer gray cells than the ME/2FI region of the ORTH-

(a) DSD-Augment Design (b) Minimax Compromise Design (c) ORTH-Augment(ME) Design

FIGURE 5. Correlation Cell Plots for DSD-Augment, Minimax Compromise, and ORTH-Augment(ME) Designs from Class DSD(6, 2, 2).



(a) $\bar{r}_{\text{MEME}}$ vs. $\bar{r}_{\text{ME2FI}}$ (b) $\bar{r}_{\text{MEME}}$ vs. $\bar{r}_{\text{2FI2FI}}$ (c) $\bar{r}_{\text{ME2FI}}$ vs. $\bar{r}_{\text{All}}$

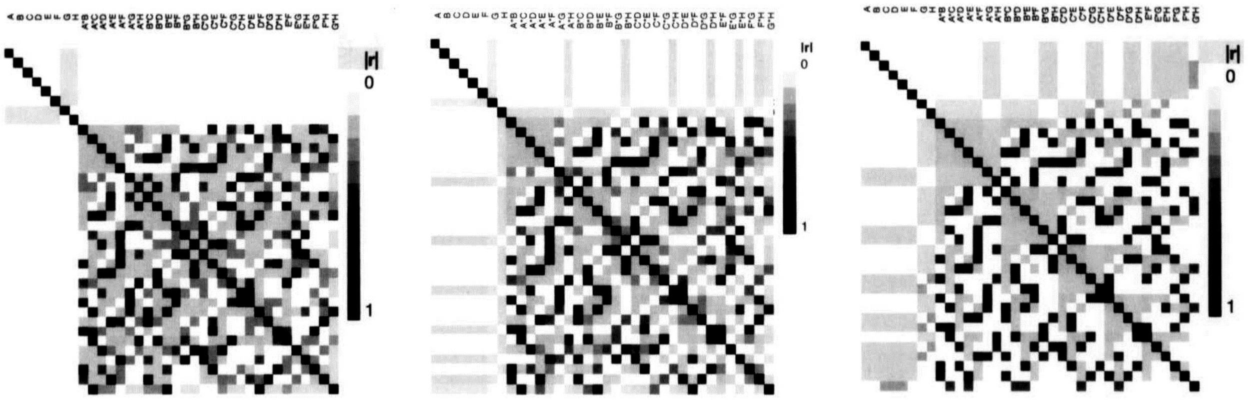
FIGURE 6. Average Absolute Correlation Plots for Designs in DSD(6, 2, 4). The solid circle identifies the ORTH-augment design; the solid square identifies the DSD-augment design; the solid diamond indicates the minimax compromise design. In panels (b) and (c), the ORTH-augment design is the minimax design.

augment(ME) design. The 2FI/2FI region of the correlation cell plots of all three designs include cells that vary in shading from white to dark gray. Here the shading of the ORTH-augment(ME) is noticeably lighter than the shading of the DSD-augment, while the shading of the compromise design again falls between DSD-augment and ORTH-augment(ME). We note in particular that the correlation cell plot for the DSD-augment design reveals some absolute correlations as high as 0.887, where the shading is nearly black. When pairs of interactions are this highly correlated, standard model-selection procedures will have difficulty in distinguishing their effects. Such pairs are nearly fully confounded. In contrast, the largest absolute correlation between interaction pairs for the ORTH-augment(ME) design is 0.667, as reflected by the medium-dark cells. Here the level of confounding is not so extreme and we have some hope for distinguishing the two-factor interaction effects. The average absolute correlations among two-factor interactions are 0.2338, 0.2182, and 0.1901 for the DSD-augment design, the compromise design, and the ORTH-augment(ME) design, respectively. This example suggests that the DSD-augment design pays a price in higher correlation among *both* 2FIs and MEs in order to obtain zero correlations between MEs and 2FIs.

4.2. Class DSD(6, 2, 4)

Next we consider the DSD(6, 2, 4) class. There are $n_d = 2^{2(4+2)} = 4{,}096$ candidate designs, so we again evaluate the entire population of designs. Because $k = 4$, the class contains the ORTH-augment design but not the DSD-augment design as recommended by Jones and Nachtsheim (2013). However, for even k, there always exists a fold-over design, and therefore a design with average absolute correlation equal to zero in the ME/2FI region of the correlation cell plot. We will refer to any design that has $\bar{r}_{\text{ME2FI}} = 0$ and that maximizes the determinant (of $\mathbf{X}'\mathbf{X}$) among all designs having $\bar{r}_{\text{ME2FI}} = 0$ as the DSD-augment design.

Plots of average absolute correlations for the various regions of the correlation matrix for designs in the DSD$(6, 2, 4)$ class are shown in Figure 6 in a form analogous to Figure 4 for the DSD$(6, 2, 2)$ class. This plot again identifies the ORTH-augment design, the DSD-augment design, and the minimax compromise design. These plots are remarkably similar to those for the DSD$(6, 2, 2)$ case, as are the correlation cell plots shown in Figure 7. Again the ORTH-augment design minimizes the average absolute correlation among 2FIs, while there is very little difference between the ORTH-augment design and the DSD-augment design in terms of overall correlation among the model effects. Table 3 provides a summary of the performance measures for the population of designs in DSD$(6, 2, 4)$. We note the very small difference (0.0101) between the smallest overall average absolute correlation and the largest. This provides support to the idea that the overall level of correlation does not change appreciably from design to



(a) DSD-Augment Design (b) Minimax Compromise Design (c) ORTH-Augment(ME) Design

FIGURE 7. Correlation Cell Plots for DSD-Augment, Minimax Compromise, and ORTH-Augment Designs from DSD(6, 2, 4).

design. Rather, a relatively fixed level of correlation gets reapportioned from one area of the correlation matrix to another as the designs change.

4.3. Classes DSD(6, 4, 2) and DSD(6, 4, 4)

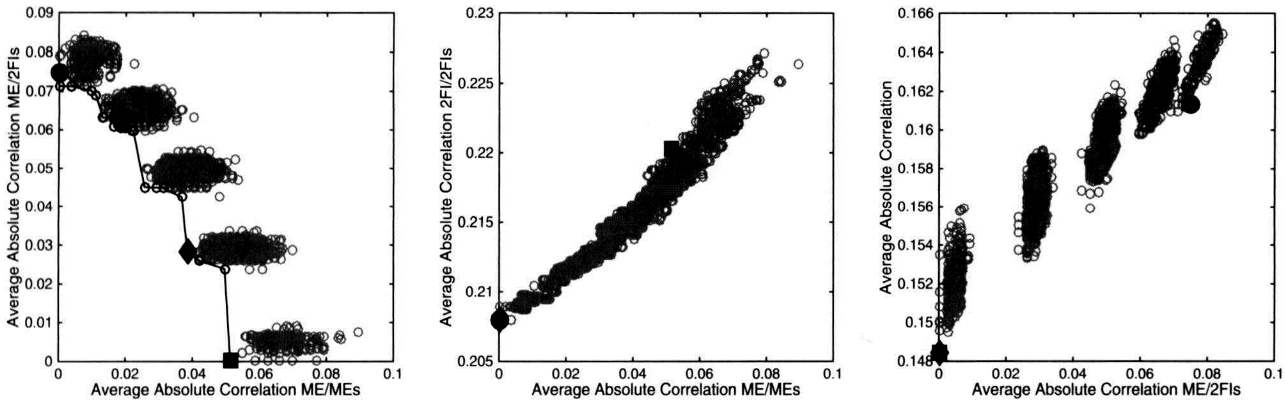
In this section, we consider the case having six continuous factors, four categorical factors, and either $k = 2$ or $k = 4$ center runs. As was the case for two categorical factors, the results for two and four center runs are very similar. For that reason, we will provide graphical results only for the four-center-run case.

For the DSD(6,4,4) class, there are $n_d = 2^{4(4+2)} =$ 16,777,216 designs. For this reason, we generate a random sample of 10,000 designs (with replacement) and consider the characteristics of the sample. Average absolute correlation plots are provided in Figure 8. The first thing we notice (besides the large number of points plotted), in Figure 8(a), is that the number of clusters of points has increased to five and we now identify 22 nondominated designs. As previously, the ORTH-augment design and the DSD-augment design are clearly indicated. We note that, for $k = 2$, the form of the plot is similar and we again found the ORTH-augment(ME) design. The design having $r_{\text{MEME}} \approx 0.04$ and $r_{\text{ME2FI}} \approx 0.03$ has been identified via the solid diamond as the minimax compromise design. From Figure 8(b), we observe that the ORTH-augment design, the only nondominated design in Figure 8(b), has again minimized the average absolute correlation among two-factor interactions, while from Figure 8(c), we see that the DSD-augment design has minimized the overall average absolute correlation among all model effects, and is one of only two nondominated designs. These observations also held true for the DSD(6,4,2) class (not shown). The statistical summary for class DSD(6,4,4) is provided in Table 4.

The correlation cell plots for the DSD-augment, the ORTH-augment, and the compromise design are displayed in Figure 9. The patterns that we observed in the previous cases hold up. The DSD-augment design clearly pays a price in terms of the average absolute correlation among two-factor interactions and among main effects, in order to keep main effects independent of two-factor interactions.

TABLE 3. Statistical Summary of Performance of Designs in DSD(6, 2, 4)

	D_s inefficiency	$\bar{r}_{\text{MEME}}$	$\bar{r}_{\text{ME2FI}}$	$\bar{r}_{\text{2FI2FI}}$	$\bar{r}_{\text{ALL}}$
Minimum	0.0000	0.0000	0.0000	0.1897	0.1397
Average	0.0688	0.0297	0.0402	0.2156	0.1450
Maximum	0.2033	0.0657	0.0763	0.2426	0.1498
Range	0.2033	0.0657	0.0763	0.0529	0.0101



(a) $\bar{r}_{\text{MEME}}$ vs. $\bar{r}_{\text{ME2FI}}$ (b) $\bar{r}_{\text{MEME}}$ vs. $\bar{r}_{\text{2FI2FI}}$ (c) $\bar{r}_{\text{ME2FI}}$ vs. $\bar{r}_{\text{All}}$

FIGURE 8. Average Absolute Correlation Plots for Designs in DSD(6, 4, 4). The solid circle identifies the ORTH-augment design; the solid square identifies the DSD-augment design; the solid diamond indicates the minimax compromise design. In panels (b) and (c), the ORTH-augment design is the minimax design.

4.4. Observations on Other DSD(m, c, k) Classes

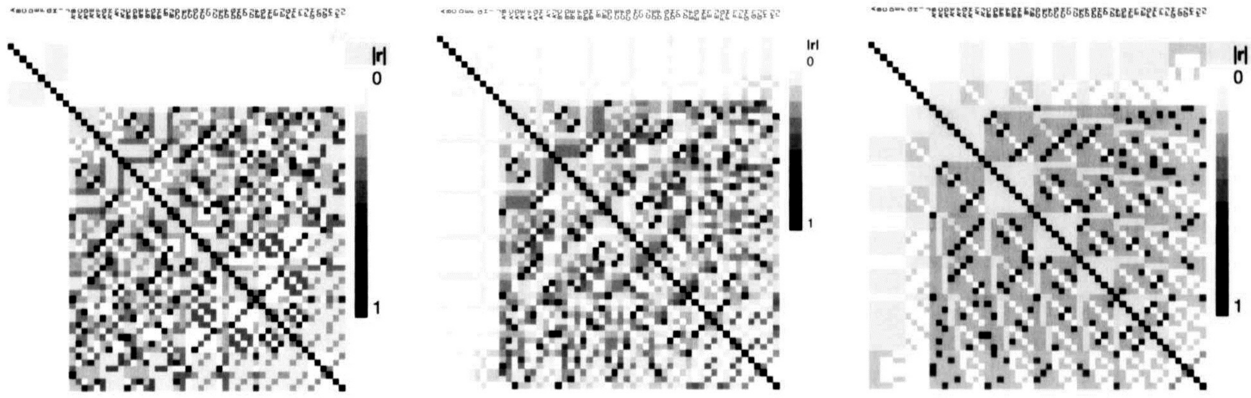
We examined many different combinations of m, c, and k and found that the patterns observed here generally held up, but we also gained some new insights into these classes. In particular, we examined the 24 DSD(m, c, k) that arose from (1) varying m from 6 to 10 in steps of size two, (2) varying c from one to four, and (3) varying k from two to four in a step of size two. Table 5 provides key performance measures for the DSD-augment design, the ORTH- or MINCORR-augment design, and the design that minimizes the maximum of $\bar{r}_{\text{MEME}}$ and $\bar{r}_{\text{ME2FI}}$. We summarize our findings as follows:

1. The ORTH-augment or MINCORR-augment designs always minimized the average correlation among two-factor interactions.
2. The minimax($\bar{r}_{\text{MEME}}$,$\bar{r}_{\text{ME2FI}}$) design for 8 and 10 factors with $c = 1$ and $k = 2$ or $k = 4$ is the DSD-augment design.
3. Jones and Nachtsheim (2013) only provided an ORTH-augment scheme for $k = 4$. In every case that we examined except six, we were able to produce an ORTH-augment or ORTH-augment(ME) design. The six cases in which ORTH-augment and ORTH-augment(ME) designs do not exist correspond to $k = 2$ and either $c = 3$ or $c = 4$. In these cases, $\bar{r}_{\text{MEME}} = 0.001$, $\bar{r}_{\text{MEME}} = 0.002$, or $\bar{r}_{\text{MEME}} = 0.004$. Clearly these designs are nearly orthogonal.
4. These results show, quite convincingly, that it is almost never necessary to use $k = 4$ (as suggested by Jones and Nachtsheim (2013)) to obtain designs for which main effects columns are orthogonal. Of course, full orthogonality for the main effects columns and the intercept column does require $k = 4$.
5. If the experimenter is interested in trying to make all interactions as independent as possible, then the minimax design may reflect this goal better than either the DSD- or the ORTH-augment designs.

The **Z** matrices for all designs in Table 5 will be made available at http://www.asq.org/pub/jqt.

TABLE 4. Statistical Summary of Performance of Designs in DSD(6, 4, 4)

	D_s inefficiency	$\bar{r}_{\text{MEME}}$	$\bar{r}_{\text{ME2FI}}$	$\bar{r}_{\text{2FI2FI}}$	$\bar{r}_{\text{ALL}}$
Minimum	0	0	0.0000	0.2079	0.1484
Average	0.0596	0.0379	0.0474	0.2151	0.1589
Maximum	0.1785	0.0896	0.0843	0.2272	0.1655
Range	0.1785	0.0896	0.0843	0.0193	0.0171



(a) DSD-Augment Design (b) Minimax Compromise Design (c) ORTH-Augment(ME) Design

FIGURE 9. Correlation Cell Plots for DSD-Augment, Minimax Compromise, and ORTH-Augment Designs from DSD(6, 4, 4).

5. Theoretical Properties of Randomly Augmented DSDs

After designating performance measures, nondominated compromise designs can be found numerically. However, if ± 1 are assigned to z_{ij} entries in an independent probabilistic manner, some statistical properties of DSD(m, c, k) designs can be shown straightforwardly. Below we show that randomly augmented DSDs with $P(z_{ij} = 1) = P(z_{ij} = -1) = 0.5$ have orthogonal main effects and are balanced in expectation. We also derive a bound on the expected logarithm of the determinant of the information matrix.

Lemma 1

Denote $\mathbf{R}$ as the design matrix shown in Table 1. z_{ij} are independent and $P(z_{ij} = 1) = P(z_{ij} = -1) = 0.5$. Then $\mathrm{E}(\mathbf{R}^{\mathrm{T}}\mathbf{R})$ is diagonal and $\mathrm{E}(\mathbf{1}^{\mathrm{T}}\mathbf{R}) = \mathbf{0}$. Furthermore, $\mathrm{E}[\log\det(\mathbf{R}^{\mathrm{T}}\mathbf{R})] \leq m\log(2p-1) + c\log(n)$, where m, c are as in Section 2, $p = m + c$ is the number of factors, $n = 2(m+c)+k$ is the number of runs.

Proof

In addition to matrix $\mathbf{Z}$, we define the following matrix based on the partitioning of the design matrix in Table 1:

$$\mathbf{B} = \begin{pmatrix} z_{3,1} & z_{3,2} & \cdots & z_{3,c} \\ \vdots & \vdots & \ddots & \vdots \\ z_{2+k,1} & z_{2+k,2} & \cdots & z_{2+k,c} \end{pmatrix}'.$$

$\mathbf{A}_1 = \mathrm{diag}(\mathbf{Z}_1)$ and $\mathbf{A}_2 = \mathrm{diag}(\mathbf{Z}_2)$ are diagonal matrices with $\mathbf{Z}_1$ and $\mathbf{Z}_2$ for diagonal entries, respectively. Then, without the intercept column, the design matrix can be written as

$$\mathbf{R} = \begin{pmatrix} \mathbf{C} \\ -\mathbf{C} \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{P}_1 \\ \mathbf{P}_2 \\ \mathbf{P}_3 \end{pmatrix},$$

where

$$\mathbf{P}_1 = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_1 \end{pmatrix},\ \mathbf{P}_2 = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 \end{pmatrix},\ \mathbf{P}_3 = (\mathbf{0} \quad \mathbf{B}),$$

and $\mathbf{C}$ is the conference matrix. Partitioning the rows of $\mathbf{C}$ and $-\mathbf{C}$ in conformance with $\mathbf{P}_1$ and $\mathbf{P}_2$, we have

$$\mathbf{C} = \begin{pmatrix} \mathbf{C}_u \\ \mathbf{C}_l \end{pmatrix} \text{ and } \mathbf{R} = \begin{pmatrix} \mathbf{C}_u \\ \mathbf{C}_l \\ -\mathbf{C}_u \\ -\mathbf{C}_l \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_1 \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 \\ \mathbf{0} & \mathbf{B} \end{pmatrix},$$

from which it follows that

$$\begin{aligned} \mathbf{R}^{\mathrm{T}}\mathbf{R} = &\begin{pmatrix} 2(m+c-1)\mathbf{T}_m & \\ & 2(m+c)\mathbf{T}_c \end{pmatrix} \\ &+ \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{B}^{\mathrm{T}}\mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ \mathbf{A}_1\mathbf{C}_l \end{pmatrix} + (\mathbf{0} \quad \mathbf{C}_l^{\mathrm{T}}\mathbf{A}_1^{\mathrm{T}}) \\ &- \begin{pmatrix} \mathbf{0} \\ \mathbf{A}_2\mathbf{C}_l \end{pmatrix} - (\mathbf{0} \quad \mathbf{C}_l^{\mathrm{T}}\mathbf{A}_2^{\mathrm{T}}). \end{aligned}$$

Because when $P(z_{ij} = 1) = P(z_{ij} = -1) = 0.5$, the entries are balanced in probability, $\mathrm{E}(\mathbf{A}_1) = \mathrm{E}(\mathbf{A}_2) = \mathbf{0}$, and $\mathrm{E}(\mathbf{B}^{\mathrm{T}}\mathbf{B}) = \mathrm{diag}(k, \cdots, k)$. Therefore,

$$\begin{aligned} \mathrm{E}(\mathbf{R}^{\mathrm{T}}\mathbf{R}) &= \begin{pmatrix} 2(m+c-1)\mathbf{T}_m & \\ & [2(m+c)+k]\mathbf{T}_c \end{pmatrix} \\ &= \begin{pmatrix} 2(p-1)\mathbf{T}_m & \\ & n\mathbf{T}_c \end{pmatrix}. \end{aligned}$$

TABLE 5. Comparisons of DSD-Augment, ORTH-Augment (or MINCORR-Augment), and Minimax Designs for Selected DSD Classes

DSD Class			DSD-Augment				ORTH- or MINCORR-Augment				Minimax($\bar{r}_{\text{MEME}}, \bar{r}_{\text{ME2FI}}$)			
m	c	k	D_s ineff	$\bar{r}_{\text{MEME}}$	$\bar{r}_{\text{ME2FI}}$	$\bar{r}_{\text{2FI2FI}}$	D_s ineff	$\bar{r}_{\text{MEME}}$	$\bar{r}_{\text{ME2FI}}$	$\bar{r}_{\text{2FI2FI}}$	D_s ineff	$\bar{r}_{\text{MEME}}$	$\bar{r}_{\text{ME2FI}}$	$\bar{r}_{\text{2FI2FI}}$
6	1	2	0.048	0.036	0	0.226	0	0.000	0.049	0.197	0.048	0.036	0.000	0.226
6	1	4	0.086	0.034	0	0.226	0	0.000	0.048	0.197	0.086	0.034	0.000	0.226
6	2	2	0.096	0.058	0	0.234	0	0.000	0.075	0.190	0.049	0.031	0.042	0.219
6	2	4	0.086	0.051	0	0.233	0	0.000	0.073	0.190	0.044	0.026	0.041	0.217
6	3	2	0.059	0.058	0	0.223	0	0.002	0.073	0.209	0.041	0.036	0.032	0.215
6	3	4	0.056	0.048	0	0.217	0	0.000	0.069	0.208	0.038	0.032	0.028	0.213
6	4	2	0.062	0.066	0	0.227	0	0.004	0.080	0.211	0.046	0.044	0.030	0.218
6	4	4	0.056	0.051	0	0.220	0	0.000	0.075	0.208	0.049	0.038	0.028	0.216
8	1	2	0.049	0.022	0	0.233	0	0.000	0.031	0.232	0.049	0.022	0.000	0.233
8	1	4	0.074	0.021	0	0.233	0	0.000	0.031	0.232	0.074	0.021	0.000	0.233
8	2	2	0.082	0.038	0	0.234	0	0.000	0.050	0.230	0.042	0.020	0.028	0.232
8	2	4	0.074	0.034	0	0.233	0	0.000	0.049	0.230	0.038	0.017	0.027	0.231
8	3	2	0.055	0.041	0	0.218	0	0.001	0.052	0.192	0.038	0.026	0.021	0.210
8	3	4	0.058	0.038	0	0.217	0	0.000	0.049	0.191	0.042	0.023	0.020	0.208
8	4	2	0.058	0.048	0	0.226	0	0.002	0.059	0.192	0.043	0.033	0.019	0.217
8	4	4	0.061	0.043	0	0.224	0	0.000	0.057	0.191	0.050	0.030	0.020	0.215
10	1	2	0.047	0.015	0	0.213	0	0.000	0.022	0.205	0.047	0.015	0.000	0.213
10	1	4	0.065	0.015	0	0.213	0	0.000	0.021	0.205	0.065	0.015	0.000	0.213
10	2	2	0.070	0.027	0	0.220	0	0.000	0.036	0.204	0.036	0.014	0.020	0.212
10	2	4	0.065	0.024	0	0.220	0	0.000	0.036	0.204	0.033	0.012	0.019	0.212
10	3	2	0.051	0.030	0	0.198	0	0.001	0.040	0.195	0.035	0.019	0.016	0.196
10	3	4	0.048	0.027	0	0.197	0	0.000	0.039	0.195	0.032	0.018	0.015	0.196
10	4	2	0.053	0.036	0	0.200	0	0.001	0.046	0.195	0.039	0.025	0.015	0.198
10	4	4	0.048	0.030	0	0.198	0	0.000	0.045	0.195	0.036	0.023	0.013	0.197

A bound on the expected logarithm of the determinant of the information matrix, from Jensen's inequality, is then

$$\begin{aligned}\mathrm{E}[\log\det(\mathbf{R}^{\mathrm{T}}\mathbf{R})] &\le \log\det(\mathrm{E}[\mathbf{R}^{\mathrm{T}}\mathbf{R}]) \\ &= m\log(2p-1) + c\log(n).\end{aligned}$$

Finally, on average, the design is column balanced, i.e., $\mathrm{E}(\mathbf{1}^{\mathrm{T}}\mathbf{R}) = \mathbf{0}$, because

$$\mathbf{1}^{\mathrm{T}}\mathbf{R} = (\,0 \quad \cdots \quad 0 \quad s_1 \quad \cdots \quad s_c\,),$$

where $s_i = \sum_{j=1}^{2+k} z_{i,j}$. □

The properties of randomly assigned augmented DSDs provide us an overview on the performance range of the entire candidate design set with DSD structure, given the number of runs and variables (n, p, m, c). It helps locate and select good compromise designs with respect to other alternative choices. The lemma indicates that, in terms of balance and orthogonality, the candidate designs center around the ideal unbiased case. The variance can also be derived by the decomposition of $\mathbf{R}^{\mathrm{T}}\mathbf{R}$ but generally depends on the form of the conference matrix $\mathbf{C}$ that is used. Given the conference matrix $\mathbf{C}$, the variance suggests the spread of designs around the orthogonal case. In addition, the derived upper bound of the average log determinant of the information matrix serves as a good benchmark for selecting appropriate compromise designs.

6. Discussion

In this paper, we explored a class of DSDs augmented with additional two-level categorical factors. This class not only covers DSD-augment and ORTH-augment designs as special cases, but also offers a series of alternative designs with traits that are a combination of the traits of the DSD-augment and the ORTH-augment designs. We identified nondominated compromise designs based on design performance measures of importance to practitioners. Minimax compromise designs in particular were given special consideration. Compared with the DSD-augment design, the minimax designs result in lower magnitudes of correlation among main effects but higher levels of correlation between main effects and two-factor interactions. They also provide lower levels of correlation between main effects and two-factor interactions than the ORTH-augment designs.

However, in every case that we considered, the ORTH-augment (or ORTH-augment(ME)) design provided the lowest level of correlations among two-factor interactions. Therefore, an experimenter who is concerned with correlations among two-factor interactions may wish to employ the ORTH-augment design.

In addition, we derived the theoretical properties of randomly assigning ± 1 in place of the zeros in the columns of the design matrix that correspond to the categorical factors. This randomization approach preserves the orthogonality and balance of the main effects probabilistically. An upper bound of the expected logarithm of the determinant of the information matrix was derived.

The cases presented here only involve instances where the number of two-level categorical factors c is less than m. Further investigation on properties of the proposed design class with large c shows that the DSD structure does not have favorable performance when a large proportion of the factors are two levels. In such cases, we recommend the use of an orthogonal array augmented with several three-level factors in order for the design to mainly focus on the two-level factors. When all factors have two levels, the new designs advocated by Errore et al. (2017) should be employed.

References

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