Small Mixed-Level Screening Designs with Orthogonal Quadratic Effects

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This paper discusses an algorithm for constructing mixed-level screening designs (MLSDs) by augmenting some columns of a definitive screening designs (DSDs) with additional two-level columns. The constructed designs have the quadratic effects being orthogonal to main effects. The algorithm is used to construct designs with the number of runs being equal to p (i.e., the number of model parameters) for even p or $p+1$ for odd p. The performance of these small DSD-based MLSDs in terms of the D-efficiency is evaluated against the 60 small MLSDs of Yang et al. (2014).

Key Words: Augmented Designs; Conference Matrix; D-Efficiency; Definitive Screening Designs; Interchange Algorithm.

1. Introduction

Screening designs are designs conducted at the primary stage of the experiment to screen out significant factors from a large number of factors for further studies. Most popular two-level screening designs are fractional factorial designs (FFDs) of resolution III or IV. The type of three-level screening designs that are gaining acceptance and have been incorporated into JMP, R, and Design Expert software is the class of definitive screening designs (DSDs) introduced by Jones and Nachtsheim (2011). For DSDs, the quadratic effects are orthogonal to main effects and are not fully aliased with two-factor interactions. The design matrix for a DSD can be written as

$$\begin{pmatrix} \mathbf{C} \\ -\mathbf{C} \\ \mathbf{0}' \end{pmatrix}, \qquad (1)$$

where $\mathbf{C}_{m\times m}$ is a constituent $(0, \pm 1)$-matrix with zero diagonal and $\mathbf{0}_m$ is a column vector of 0s. Xiao et al. (2012) pointed out that, if we use a *conference* matrix of order m for $\mathbf{C}$, i.e., if $\mathbf{C}'\mathbf{C} = (m-1)\mathbf{I}_m$ where $\mathbf{I}_m$ is the identity matrix of order m, then the DSD is also orthogonal for main effects, i.e., the main effects are orthogonal to one another. Conference matrices for even m and $m \le 50$ are given in Xiao et al. (2012) and Nguyen and Stylianou (2013). For odd m, the $\mathbf{C}$ matrices are given in Jones and Nachtsheim (2011) and Nguyen and Stylianou (2013).

As all factors of a DSD should be quantitative, Jones and Nachtsheim (2013) introduced two types of efficient DSD-based mixed-level screening designs (MLSDs), which they called DSD-augmented designs (ADSDs) and ORTH-augmented designs (OADs). Both ADSDs and OADs can be obtained by converting some columns of a DSD to two-level ones. While the main effects of ADSDs are orthogonal to the quadratic effects, those of the OADs are only orthogonal to one another. In this paper, we will denote the MLSDs of which the quadratic effects are orthogonal to the main effects, such as ADSDs, as MLSD*s.

As ADSDs and OADs require many more runs than the number of parameters, Yang et al. (2014) (hereafter abbreviated as YLL) introduced a new class of minimal-run MLSDs constructed from con-

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ference matrices and maximal determinant matrices (cf. http://indiana.edu/~maxdet/). While YLL's MLSDs are small, they do not have the aforementioned desired property of MLSD*s.

This paper describes an algorithm for constructing small MLSD*s that systematically augments two-level factors to some columns of a DSD. This algorithm is evaluated against the 60 minimal-point MLSDs of YLL.

2. Characterization of a DSD-Based MLSD*

Consider the following linear model for an n-run MLSD where the first m_3 factors are three-level ones and the last m_2 factors are two-level or categorical ones:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \tag{2}$$

where $\mathbf{Y}_n$ is the column vector of responses, $\mathbf{X}_{n\times p}$ is the expanded design matrix of the pure-quadratic model, and $p = 1 + 2m_3 + m_2$ is the number of parameters in Equation (2), $\boldsymbol{\beta}_p$ is the column vector containing p coefficients for fixed effects, $\boldsymbol{\epsilon}_n$ is the column vector of random errors with zero mean and variance–covariance matrix $\sigma_\epsilon^2\mathbf{I}_n$, and $\mathbf{I}_n$ is the identity matrix of order n.

Let the uth row of $\mathbf{X}$ in Equation (2) be written as $(1, x_{u1}^2, \ldots, x_{um_3}^2, x_{u1}, \ldots, x_{um_3}, x_{u(m_3+1)}, \ldots, x_{u(m_3+m_2)})$ and let the information matrix $\mathbf{M} = \mathbf{X}'\mathbf{X}$ be partitioned as

$$\begin{pmatrix} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{M}_{21} & \mathbf{M}_{22} \end{pmatrix}, \tag{3}$$

where $\mathbf{M}_{11}$ and $\mathbf{M}_{12}$ are a $(1+m_3)\times(1+m_3)$ submatrix and a $(m_3+m_2)\times(m_3+m_2)$ submatrix of $\mathbf{M}$, respectively. The entries in $\mathbf{M}_{12}$ are

$$\begin{pmatrix} \sum x_{u1} & \cdots & \sum x_{um_3} & \sum x_{u(m_3+1)} & \cdots & \sum x_{u(m_3+m_2)} \\ \sum x_{u1}^3 & \cdots & \sum x_{u1}^2 x_{um_3} & \sum x_{u1}^2 x_{u(m_3+1)} & \cdots & \sum x_{u1}^2 x_{u(m_3+m_2)} \\ \vdots & & \vdots & \vdots & & \vdots \\ \sum x_{um_3}^2 x_{u1} & \cdots & \sum x_{um_3}^2 x_{um_3} & \sum x_{um_3}^2 x_{u(m_3+1)} & \cdots & \sum x_{um_3}^2 x_{u(m_3+m_2)} \end{pmatrix},$$

where the summations are taken over n design points.

Assuming that (i) the m_3 columns of the MLSD are taken from a DSD of size $n \times m$ ($n = 2m + n_0$, where n_0, the number of center runs for this DSD is either zero or two and (ii) each of the m_2 columns of this MLSD has $(1/2)n$ of ±1's, then all the entries in $\mathbf{M}_{12}$ will be zeros except the sums of cross-products between the quadratic effects of a three-level factor and a two–level main effect. If we can also make these summations be zeros, $\mathbf{M}_{12}$ will be a null matrix and the MLSD will become the MLSD*. In this case, Equation (3) will have the form

$$\begin{pmatrix} \mathbf{M}_{11} & \mathbf{0}' \\ \mathbf{0} & \mathbf{M}_{22} \end{pmatrix} \tag{4}$$

and its inverse will have the form

$$\begin{pmatrix} \mathbf{M}_{11}^{-1} & \mathbf{0}' \\ \mathbf{0} & \mathbf{M}_{22}^{-1} \end{pmatrix}. \tag{5}$$

Because the first m_3 columns of this MLSD* are taken from a DSD, $\mathbf{M}_{11}$ will have the form

$$\begin{pmatrix} n & a\mathbf{1}' \\ a\mathbf{1} & 2\mathbf{I} + (a-2)\mathbf{J} \end{pmatrix} \tag{6}$$

and $\mathbf{M}_{11}^{-1}$ will have the form

$$\begin{pmatrix} b & c\mathbf{1}' \\ c\mathbf{1} & (1/2)\mathbf{I} + d\mathbf{J} \end{pmatrix}. \tag{7}$$

In Equations (6) and (7), $a = n - n_0 - 2,\ b = (2 + m_3(a-2))/e,\ c = -a/e,\ d = (a^2 - n(a-2))/(2e)$, where $e = m_3(n(a-2) - a^2) + 2n$. $\mathbf{1}$ is a column vector of ones of order m_3. $\mathbf{I}$ and $\mathbf{J}$ are the identity matrix and square matrix of ones of order m_3, respectively.

Therefore, it can be seen that, for the pure-quadratic model, $|\mathbf{X}'\mathbf{X}|$ is a function of $|\mathbf{M}_{22}|$ and can be computed as

$$n\ 2^{m_3}\left\{1 + \frac{1}{2}m_3\left(a - 2 - \frac{1}{n}a^2\right)\right\}|\mathbf{M}_{22}|. \tag{8}$$

Assume that $\mathbf{M}_{22}$ is nonsingular and has nonzero eigenvalues $\lambda_1, \ldots, \lambda_{m_3+m_2}$. Because trace$(\mathbf{M}_{22}) = \sum\lambda_i = m_3a + m_2n$ is a constant and trace$((\mathbf{M}_{22})^2) = \sum\lambda_i^2$, minimizing the sum of squares of the entries in $\mathbf{M}_{22}$, which is equivalent to minimizing trace$((\mathbf{M}_{22})^2)$, is the same as making the λ_i's as equal as possible with $\sum\lambda_i$ held to a constant. This is our fast approach of maximizing $\Pi\lambda_i$, which is equivalent to maximizing $|\mathbf{M}_{22}|$ or $|\mathbf{X}'\mathbf{X}|$, which is further equivalent to minimizing $\sum \lambda_i^{-1}$, i.e., trace($(\mathbf{M}_{22})^{-1}$) or the sum of the variances of the three-level and two-level main effects assuming that $\sigma_\epsilon = 1$. This is also the approach used by Booth and Cox (1962) and Nguyen (1996) for the construction of supersaturated designs. Note that minimizing the sum of squares of the entries in $\mathbf{M}_{22}$ is the same as minimizing the sum of squares of the sums of cross-products between a three-level and a two-level main effects and between 2 two-level main effects.

3. The AUGMENT Algorithm

Let $D_{n\times(m_3+m_2)}$ be an n-run MLSD with m_3 three-level columns taken from a DSD and m_2 two-level columns to be augmented to these three-level columns. This DSD was constructed from a conference matrix of order m, where $m = \frac{1}{2}(n - n_0)$, where n_0, the number of center runs for this DSD, is either zero or two. Each of m_2 two-level columns is balanced.

We use the uth row of D to construct the vector $\mathbf{J}_u$ of length $2m_3m_2 + \binom{m_2}{2}$. The first m_3m_2 entries of $\mathbf{J}_u$ are $x_{u1}^2 x_{u(m_3+1)}, \ldots, x_{um_3}^2 x_{u(m_3+m_2)}$. The next m_3m_2 entries of $\mathbf{J}_u$ are $x_{u1}x_{u(m_3+1)}, \ldots, x_{um_3} \times x_{u(m_3+m_2)}$. The last $\binom{m_2}{2}$ entries of $\mathbf{J}_u$ are $x_{u(m_3+1)} \times x_{u(m_3+2)}, \ldots, x_{u(m_3+m_2-1)}x_{u(m_3+m_2)}$. For an MLSD with 4 three-level columns and 3 two-level columns, the 27 terms in $\mathbf{J}_u$ are $x_{u1}^2 x_{u5}, \ldots, x_{u4}^2 x_{u7}, x_{u1}x_{u5}, \ldots, x_{u4}x_{u7}, x_{u5}x_{u6}, \ldots, x_{u6}x_{u7}$. For Figure 1 (2), it can be verified that the 27 values in $\mathbf{J}_1$ are 1, −1, −1, 1, −1, −1, 0, 0, 0, 1 −1, −1, 1, −1, −1, 1, −1, −1, 0, 0, 0, 1, −1, −1, −1, −1, 1.

Let $\mathbf{J} = \sum \mathbf{J}_u$. Let A_1 denote the sum of squares of the first m_3m_2 elements of $\mathbf{J}$ and let A_2 denote the sum of squares of the remaining elements of $\mathbf{J}$. If the value of any element in row u^* and column j ($j > m_3$) of D changes sign, we only have to recalculate $\mathbf{J}_{u^*}$ instead of all the $\mathbf{J}_u$'s. Thus, our approach is less time consuming, as only certain elements of $\mathbf{X}'\mathbf{X}$ are computed (see Ingram and Tang (2005)). This observation prompted us to propose the following interchange algorithm, called AUGMENT, for augmenting m_2 two-level factors to m_3 columns of an n-run DSD:

1. Select at random m_3 columns from m columns of a DSD to form the first m_3 columns of the starting design D_0. Generate the remaining m_2 two-level columns for D_0. Set the value at position i of these m_2 columns to be −1 if i is odd and +1 if i is even.
2. Randomly permute the positions of ±1 in each generated two-level column in step 1. Calculate each $\mathbf{J}_u$, $u = 1, \ldots, n$, and $\mathbf{J} = \sum \mathbf{J}_u$. Evaluate (A_1, A_2) values.
3. Search for a pair of entries in column j ($j = m_3 + 1 \ldots, m_3 + m_2$) such that the sign swap of these two entries in this column will result in the biggest reduction in A_1 (or A_2 if A_1 is already zero). If the search is successful, update A_1 (or A_2), $\mathbf{J}$ and this column. If A_1 (or A_2 if A_1 is already zero), it cannot be reduced further. Repeat this step with the next two-level column. Repeat this step until $A_1 = 0$ and A_2 cannot be reduced further by any further swaps.

(1)	(2)	(3)	(4)	(5)
++0+---	++0++--	++0+---	++0+--+	++0+--+
0-+-+++	0-+----	0-+----	0-+----	0-+---+
-++0---	-++0-++	-++0+++	-++0+++	-++0+++
+++-+++	+++--+-	+++--+-	+++--+-	+++--+-
+-++---	+-+++-+	+-+++-+	+-+++-+	+-+++-+
-0+++++	-0++--+	-0++--+	-0++---	-0++---
0000---	0000-++	0000-++	0000-++	0000-++
--0-+++	--0-++-	--0-++-	--0-++-	--0-++-
0+-+---	0+-++++	0+-++++	0+-++++	0+-+++-
+--0+++	+--0---	+--0---	+--0---	+--0---
---+---	---+-+-	---+-+-	---+-+-	---+-+-
-+--+++	-+--+-+	-+--+-+	-+--+-+	-+--+-+
+0-----	+0--+++	+0--+++	+0--+++	+0--+++
0000+++	0000+--	0000+--	0000+--	0000+--

FIGURE 1. Steps of AUGMENT to Produce a DSD-Based MLSD* for 4 Three-Level Factors and 3 Two-Level Factors in 14 Runs.

Remarks

1. The above steps correspond to one *try* of AUGMENT. For each try that results in an MLSD*, i.e., MLSD with $A_1 = 0$, we calculate $|\mathbf{M}_{22}|$. Among all the MLSD*s obtained from different tries, we select the one with the highest $|\mathbf{M}_{22}|$.
2. When $A_1 = 0$, minimizing A_2 speeds up the maximizing $|\mathbf{M}_{22}|$ or $|\mathbf{X}'\mathbf{X}|$ (see Section 2). However, there is no guarantee that, for two designs with $A_1 = 0$, the one with a smaller A_2 will have a larger $|\mathbf{X}'\mathbf{X}|$.
3. Because AUGMENT attempts to construct optimal MLSD*s for model (2), a reviewer is of the opinion that it might result in designs that have undesirable aliasing structures in the sense that there might be high correlations between certain main effects and two-factor interactions. To rectify this problem, for each try that results in an MLSD*, in addition to the calculation of $|\mathbf{M}_{22}|$, we also calculate $r'_{\max}$, the maximum correlation coefficient between a main effect and a two-factor interaction and eliminate designs for which $r'_{\max}$ exceeds a certain set value.
4. For a given m_3 and m_2, there is no guarantee that a saturated MLSD* with a specified n_0 will always be available, i.e., the condition $A_1 = 0$ is always attainable. It is not possible for AUGMENT, e.g., to construct saturated MLSD*s for $m_3 = 4$ and $m_2 = 3$ or for $m_3 = 4$ and $m_2 = 5$ with $n_0 = 2$.
5. The sign swap or *interchange* of two entries in column j in step 3 is equivalent to two simultaneous *coordinate-exchanges* of these two entries. See Nguyen (1996) for an example of using the interchange algorithm to construct $E(s^2)$-optimal supersaturated designs and Myer and Nachtsheim (1995) for an example of using the coordinate-exchange algorithm to construct D-optimal designs. The main advantage of the interchange algorithm and the coordinate-exchange algorithm is that the candidate sets need not be explicitly constructed.

Figure 1 shows the steps of augmenting 3 two-level columns to four columns of a 14-run DSD of size 14×6. Figure 1 (1) shows a starting design D_0 in step 1 of AUGMENT with the first four columns selected at random from six columns of the DSD. Figure 1 (2) corresponds to step 2 in which columns 5–7 of D_0 are randomized. At this step, (A_1, A_2) =(16, 76). Figure 1 (3) corresponds to the first sign swap in positions 1 and 3 of column 5, after which (A_1, A_2) become (8, 100). Figure 1 (4) corresponds to the second sign swap in positions 1 and 6 of column 7, after which (A_1, A_2) become (0, 124). Figure 1 (5) corresponds to the third sign swap in positions 2 and 9 of column 7, after which (each of the first 12 entries of $\mathbf{J}$ becomes 0 and each of the last 15 entries of $\mathbf{J}$ becomes ± 2) (A_1, A_2) become (0, 60). While a 14-run ADSD with 4 three-level factors and 2 two-level factors has the orthogonality between all main effects and two-factor interactions, the resulting 14-run MLSD* in Figure 1 (5) has $r'_{\max}$=0.41 (24 times). Clearly, this is the price paid for accommodating one more two-level column.

4. Results and Discussion

The D-efficiencies of a design are calculated as

$$|\mathbf{X}'\mathbf{X}|^{1/p}/n, \tag{9}$$

where $\mathbf{X}$ and p are the model matrix and the number of parameters for the model. For the pure-quadratic model, the $\mathbf{X}$ matrix and p in Equation (9) are given in Section 2 and $|\mathbf{X}'\mathbf{X}|$ is computed by Equation (7). For the first-order model, where the m_3 columns in $\mathbf{X}$ that correspond to the squared terms are dropped, p becomes $1 + m_3 + m_2$ and $|\mathbf{X}'\mathbf{X}|$ becomes $n|\mathbf{M}_{22}|$. Let (d_1, d_2) pair be the first-order and pure-quadratic D-efficiency ratios of an MLSD relative to the orthogonal arrays (OAs). They are computed as ratios of the D-efficiencies of this MLSD to the ones of the corresponding OA listed in Appendix A of YLL. These OAs can be found at http://neilsloane.com/oadir/ and http://support.sas.com/techsup/technote/ts723.html.

Table 1 compares 60 small DSD-based MLSD*s constructed by AUGMENT and the designs in Appendix A of YLL for m_3 =4, 6, 8, 10, and 12 and $m_2 = 1, \ldots, m_3 + 4$. This table shows m_3, the number of three-level factors; m_2, the number of two-level factors; p $(= 1 + 2m_3 + m_2)$, the number of parameters; n, the number of runs (and n_0, the number of center runs for the source DSD); $r_{\max}$ and r_{ave}, the maximum and average of the correlation coefficients among the $2m_3 + m_2$ columns of the model matrix $\mathbf{X}$; $r'_{\max}$, the maximum correlation coefficient between a main effect and a two-factor interaction (see remark 3, Section 3); (d_1, d_2), D-efficiency ratios (%) of YLLs MLSDs and our small MLSD*s and the corresponding OA sizes. As an n-runs DSD-based MLSD* can be constructed by using a DSD obtained by a conference matrix (or a $\mathbf{C}$ matrix) of order $m = (1/2)(n - n_0)$, where n_0, the number of

TABLE 1. Comparisons of (d_1, d_1) D-Efficiency Ratios of YLL's MLSD and Ours

#	m_3	m_2	p	n (n_0)	$r_{\max}$	r_{ave}	$r'_{\max}$	YLL's MLSD	New MLSD*
1†	4	1	10	10 (0)	0.45§	0.10	0.00	(98.6, 83.0)	(100.2, 81.7)
2‡	4	2	11	12 (0)	0.20§	0.06§	0.00	(96.5, 80.1)	(109.1, 86.1)
3‡	4	3	12	12 (0)	0.33§	0.07§	0.41	(92.9, 77.1)	(104.7, 85.5)
4‡	4	4	13	14 (2)	0.30§	0.08§	0.41	(93.3, 82.6)	(96.4, 91.9)
5‡	4	5	14	14 (0)	0.31§	0.07§	0.35	(87.7, 83.7)	(99.7, 82.8)
6‡	4	6	15	16 (2)	0.33§	0.06§	0.35	(78.0, 70.9)	(96.3, 89.8)
7‡	4	7	16	16 (2)	0.33§	0.06§	0.60	(77.9, 67.3)	(94.1, 88.6)
8‡	4	8	17	18 (2)	0.38§	0.09§	0.31	(77.7, 69.4)	(86.8, 81.6)
9†	6	1	14	14 (0)	0.31§	0.07§	0.00	(105.3, 81.3)	(111.7, 76.7)
10‡	6	2	15	16 (2)	0.33§	0.11	0.00	(106.9, 77.6)	(88.9, 81.2)
11‡	6	3	16	16 (0)	0.50	0.05§	0.29	(102.7, 74.2)	(111.1, 78.9)
12‡	6	4	17	18 (2)	0.36§	0.08§	0.29	(101.0, 77.1)	(102.4, 86.7)
13‡	6	5	18	18 (0)	0.24§	0.06§	0.26	(97.2, 77.0)	(102.9, 76.1)
14‡	6	6	19	20 (2)	0.40	0.07§	0.26	(94.3, 77.6)	(99.9, 84.2)
15‡	6	7	20	20 (0)	0.32§	0.05§	0.47	(90.9, 78.5)	(103.0, 76.8)
16‡	6	8	21	22 (2)	0.39§	0.07§	0.45	(90.3, 74.0)	(102.8, 85.1)
17‡	6	9	22	22 (0)	0.27§	0.05§	0.41	(82.9, 69.9)	(101.0, 76.2)
18‡	6	10	23	24 (2)	0.40§	0.07§	0.41	(81.7, 68.4)	(97.0, 81.2)
19‡	8	1	18	18 (0)	0.12§	0.05§	0.00	(117.4, 76.5)	(120.4, 72.1)
20‡	8	2	19	20 (2)	0.40§	0.11	0.00	(114.6, 73.1)	(96.9, 77.0)
21‡	8	3	20	20 (0)	0.40§	0.04§	0.23	(109.2, 69.9)	(113.3, 72.2)
22‡	8	4	21	22 (2)	0.45	0.08§	0.22	(110.0, 71.6)	(106.5, 80.6)
23‡	8	5	22	22 (0)	0.27§	0.05§	0.20	(103.8, 71.1)	(106.7, 71.0)
24‡	8	6	23	24 (2)	0.40§	0.09§	0.20	(99.6, 71.2)	(98.7, 76.4)
25‡	8	7	24	24 (0)	0.33§	0.04§	0.38	(98.6, 71.6)	(107.5, 72.3)
26‡	8	8	25	26 (2)	0.41§	0.08	0.38	(102.8, 75.8)	(101.4, 77.5)
27	8	9	26	26 (0)	0.32§	0.05§	0.35	(97.4, 75.6)	(102.9, 70.9)
28	8	10	27	28 (2)	0.42	0.07§	0.35	(91.7, 69.9)	(98.0, 75.6)
29	8	11	28	28 (0)	0.29§	0.04§	0.32	(89.4, 67.5)	(101.7, 71.0)
30	8	12	29	30 (2)	0.42	0.08§	0.33	(89.8, 68.6)	(95.6, 74.2)
31‡	10	1	22	22 (0)	0.19§	0.05§	0.00	(122.3, 71.9)	(123.1, 67.0)
32‡	10	2	23	24 (2)	0.50	0.11	0.00	(119.3, 68.7)	(102.4, 72.3)
33	10	3	24	24 (0)	0.44	0.03§	0.20	(114.3, 65.9)	(117.2, 67.6)
34	10	4	25	26 (2)	0.41	0.09	0.19	(114.3, 66.9)	(106.5, 73.8)
35	10	5	26	26 (0)	0.38	0.04§	0.18	(110.3, 66.2)	(108.6, 66.1)
36	10	6	27	28 (2)	0.43§	0.09§	0.17	(105.4, 66.1)	(102.8, 72.2)
37	10	7	28	28 (0)	0.43§	0.04§	0.32	(103.4, 66.2)	(110.5, 68.0)
38	10	8	29	30 (2)	0.47	0.08§	0.32	(106.0, 69.4)	(105.0, 73.3)
39	10	9	30	30 (0)	0.33§	0.04§	0.30	(101.5, 69.1)	(104.4, 66.4)

(continued on next page)

TABLE 1. *Continued*

#	m_3	m_2	p	n (n_0)	r_{max}	r_{ave}	r'_{max}	YLL's MLSD	New MLSD*
40	10	10	31	32 (2)	0.43	0.08§	0.30	(101.5, 70.5)	(99.7, 71.0)
41	10	11	32	32 (0)	0.50	0.03§	0.29	(98.9, 71.1)	(104.9, 67.4)
42	10	12	33	34 (2)	0.43	0.08§	0.38	(98.1, 68.7)	(97.4, 70.1)
43	10	13	34	34 (0)	0.24§	0.05§	0.39	(94.4, 66.9)	(99.4, 65.6)
44	10	14	35	36 (2)	0.44	0.07§	0.40	(91.2, 65.3)	(95.4, 69.2)
45	12	1	26	26 (0)	0.16§	0.04§	0.00	(126.0, 67.6)	(126.8, 63.1)
46	12	2	27	28 (2)	0.43	0.11	0.00	(123.3, 64.8)	(105.9, 67.8)
47	12	3	28	28 (0)	0.37	0.03§	0.17	(118.2, 62.3)	(120.2, 63.7)
48	12	4	29	30 (2)	0.47	0.09	0.16	(118.6, 62.9)	(110.0, 69.5)
49	12	5	30	30 (0)	0.28§	0.04§	0.15	(113.8, 62.2)	(111.3, 62.4)
50	12	6	31	32 (2)	0.50	0.09	0.15	(111.1, 61.9)	(104.2, 67.6)
51	12	7	32	32 (0)	0.50	0.03§	0.27	(108.2, 61.9)	(113.3, 64.3)
52	12	8	33	34 (2)	0.43	0.08§	0.28	(109.9, 64.4)	(102.6, 67.9)
53	12	9	34	34 (0)	0.29§	0.04§	0.26	(104.9, 64.0)	(104.3, 62.0)
54¶	12	10	35	36 (2)	0.44	0.09	0.27	(104.6, 65.1)	(98.6, 65.8)
55	12	11	36	36 (0)	0.33	0.04§	0.36	(103.8, 65.5)	(104.6, 62.9)
56	12	12	37	38 (2)	0.44	0.08	0.36	(107.3, 68.4)	(99.5, 66.5)
57	12	13	38	38 (0)	0.37	0.04§	0.34	(103.9, 69.1)	(99.6, 61.7)
58	12	14	39	40 (2)	0.44	0.07§	0.35	(98.5, 65.0)	(97.2, 65.8)
59	12	15	40	40 (0)	0.36§	0.04§	0.43	(96.0, 63.6)	(99.8, 62.4)
60	12	16	41	42 (2)	0.45§	0.07§	0.43	(96.0, 64.3)	(97.0, 66.1)

†Corresponding OA size is 18. ‡Corresponding OA size is 36. ¶Corresponding OA size is 54. Corresponding OA size of the remaining MLSD*s is 72. §The r_{max} or r_{ave} value of the new design is smaller than YLL's.

center runs is either zero or two; in most cases, we have two MLSD* solutions for a given m_3 and m_2 and the more satisfactory solution is given in Table 1. In this table, we eliminate all designs with $r_{max} > 0.5$ and $r'_{max} > 0.5$. The only exception is the design #7, for which $r'_{max} = 0.6$. AUGMENT could not find an alternative D-efficient design with lower r'_{max}. It can be seen in this table that, when there are only one or 2 two-level factors, our MLSD*s always achieve orthogonality between all main effects and two-factor interactions (i.e., $r'_{max} = 0$).

Define d_1^* and d_2^* as the first-order and pure-quadratic D-efficiency ratios of the new MLSD*s relative to the YLL's MLSDs. The scatter plot of d_1^* and d_2^* in Figure 2 contains four quadrants: quadrant I, containing 23 points with $d_1^* > 100\%$ and $d_2^* > 100\%$; quadrant II, containing 18 points with $d_1^* \leq 100\%$ and $d_2^* > 100\%$; quadrant III, containing 4 points with $d_1^* \leq 100\%$ and $d_2^* \leq 100\%$; quadrant IV, containing 15 points with $d_1^* > 100\%$ and $d_2^* \leq 100\%$. The points in quadrant I, for example, correspond to MLSD*s that are better than YLL's in terms of both first-order and pure-quadratic D-efficiencies.

Other than the D-efficiencies, our designs possess the following important design properties that make them attractive to experimenters: (i) they are either saturated like the YLL's designs or one run more than the saturated ones; (ii) they are flexible in the sense that they are available for any m_3 values; and (iii) they are MLSD*s designs of which the quadratic effects are orthogonal to the main effects. After all, nearly all popular and well-known designs, such as the Box–Behnken designs (Box and Behnken (1960)), the central-composite designs (Box and Wilson (1951)), the DSDs, and ADSDs, have this design property.

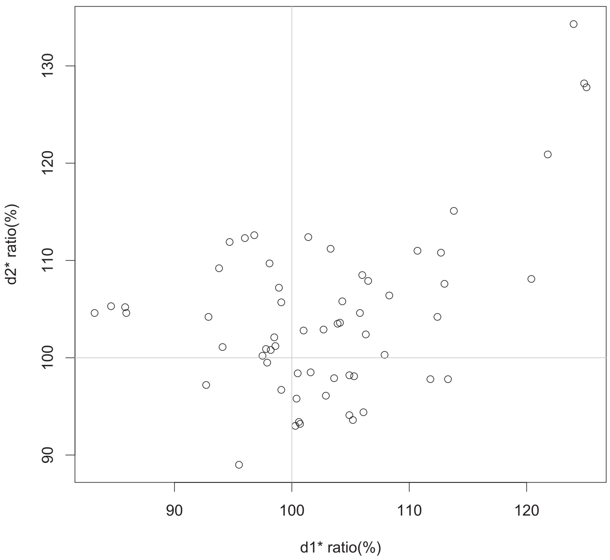

FIGURE 2. Scatter Plot of d_1^* vs d_2^*, the First-Order and Pure-Quadratic D-Efficiency Ratios of the New MLSD*s Relative to YLL's MLSDs.

Bullington et al. (1993) described an experiment with 11 2-level factors in 12 runs conducted to identify the cause of early failures in thermostats manufactured by the Eaton Corporation. This experiment was also summarized in Mee (2009). The 11 factors are (A) diaphragm plating rinse (clean/dirty), (B) current density (minutes @ amps (5 @ 60/10 @ 15), (C) sulfuric acid cleaning in seconds (3/30), (D) diaphragm electro clean in minutes (2/12), (E) beryllium copper grain size (inches (0.008/0.018)), (F) stress orientation to steam weld (perpendicular/parallel), (G) diaphragm condition after brazing (wet/air dried), (H) heat treatment (hours @ 600°F (0.75/4)), (J) brazing machine water and flux (none/extra), (K) power element electro clean time (short/long), and (L) power element plating rinse (clean/dirty). Note that factors B, C, D, and H are quantitative factors but have been treated as two-level factors in the experiment.

There are five candidate MLSDs for this thermostats experiment, all of which allow four quantita-

YLL's MLSD	16-run MLSD*	18-run MLSD*	26-run ADSD
0++++---+++	---++----++	+++0---++++	+0+++++++++
-0-+-+--+++	-+-0-+-+++-	++-+-++-++-	+++++--+--+
-+0---+++-+	+0--++-+---	0+-+++-+-++	0++---+--++
--+0--++-++	0-++-+--+--	-0++--++-+-	-+-++++--++
0000+++++++	-+0--------	---+----+++	+++0-+--++-
0---+---+++	+-----+++-+	+-++-+----+	-+0--++++-+
+0+--+--+++	--+--+++-++	-++++-+-+-+	-+-+---++++
+-0+--+++-+	0000+++-+-+	+-0++--++--	-++-++-+-+-
++-0--++-++	+++-++--+++	0000+----+-	++--++--+-+
0+++-+++---	+-+0+-+----	---0+++----	++--+-++++-
-0-++-++---	-0++--+-++-	--+-++-+++-	++-+-+++---
-+0-++---+-	0+--+-++-+-	0-+---+-+--	-++++-+-+--
--+0++--+--	+-0+++++++-	+0--++--+-+	0000-----+-
0+++---+++-	-++++--++-+	+++-++++---	-0---------
-0-+--+-++-	++-+-++---+	-+-----+---	-----++-++-
-+0-------+	0000---+-++	+---+-++-++	0--+++-++--
		-+0--++--++	+-+----++--
		0000-++++-+	---0+-++--+
			+-0++----+-
			+-+-+++----
			+--+--+-+-+
			--++--++-+-
			--++-+----+
			--+-+---+++
			+----+-+-++
			0000+++++-+

FIGURE 3. Four Candidate MLSDs for the Thermostats Experiment Described in Bullington et al. (1993).

TABLE 2. Comparisons of Five Candidate MLSDs for the Thermostats Experiment Described in Bullington et al. (1993)

MLSDs	n	(d_1, d_2)	$r_{\max}$	$r'_{\max}$	v_Q	v_{M3}	v_{M2}
YLL's MLSD	16	(77.9, 67.3)	0.75	0.76	0.803	$0.167^{\dagger}$	0.247
16-run MLSD*	16	(94.1, 88.6)	0.33	0.60	$0.417^{\dagger}$	0.139	0.083
18-run MLSD*	18	(99.1, 89.9)	0.36	0.29	$0.414^{\dagger}$	0.080	0.066
ADSD	26	(105.7, 86.9)	0.41	$0.00^{\dagger}$	$0.408^{\dagger}$	0.048	0.041
OA	36	(100.0, 100.0)	$0.00^{\dagger}$	0.54	$0.125^{\dagger}$	$0.042^{\dagger}$	$0.028^{\dagger}$

†Maximum value is the same as minimum value.

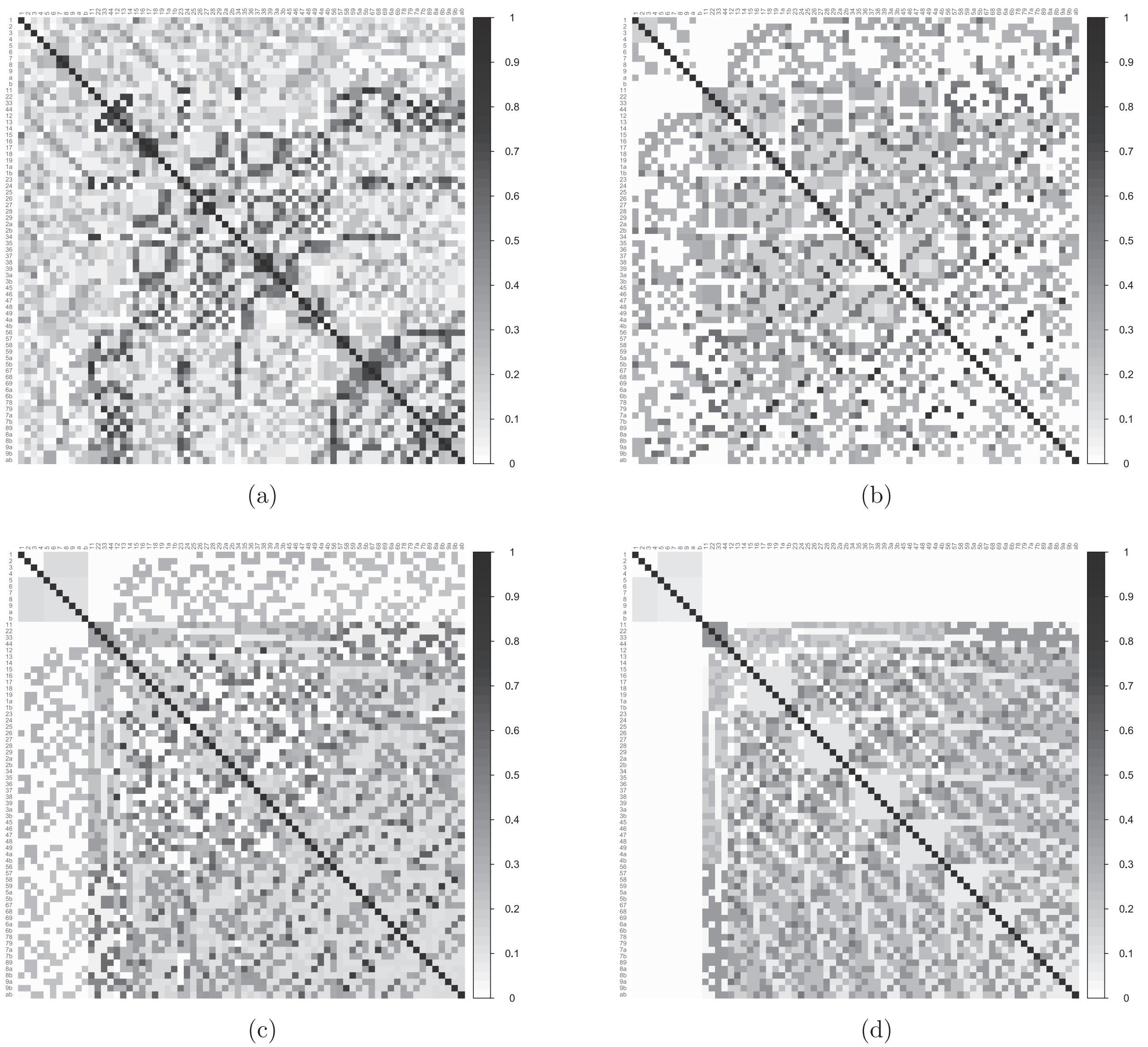

FIGURE 4. Correlation Cell Plots of (a) YLL's 16-Run MLSD, (b) 16-Run MLSD*, (c) 18-Run MLSD*, and (d) 26-Run ADSD for 4 Three-Level and 7 Two-Level Factors.

tive factors B, C, D, and H to be set at three levels: a 16-run MLSD of YLL, a 16-run MLSD*, an 18-run MLSD*, a 26-run ADSD, and a 36-run OA. The first four candidate MLSDs are in Figure 3. The (d_1, d_2) ratios, $r_{\max}$, $r'_{\max}$, v_Q (the maximum variance of the quadratic effect), v_{M3} (the maximum variance of the three-level main effect), and v_{M2} (the maximum variance of the two-level main effect) of these five candidate MLSDs are shown in Table 2.

The correlation cell plots of the first four candidate MLSDs are in Figure 4. These plots were advocated by Jones and Nachtsheim (2011) for studying the aliasing pattern in screening experiments. Each plot shows the pairwise (absolute) correlation between two terms under study as a colored square. Each plot in Figure 4 has 70 rows, 70 columns, and 70^2 $(= 4{,}900)$ colored cells. Here 70 is the number of 11 main effects, four quadratic effects, and $\binom{11}{2}$ $(= 55)$ two-factor interactions. The color of each cell goes from white to dark. The white cells imply no correlation and the dark ones imply a correlation of one, like those in the diagonal, or close to one (see the vertical bar on the right of each graph). It can be seen that, for Figure 4(b), Figure 4(c), and Figure 4(d), the quadratic effects are orthogonal to the main effects and, for Figure 4 (d), the main effects are also orthogonal to two-factor interactions.

Both of our MLSD*s, the ADSD, and the OA have the following properties that are not shared by YLL's MLSD: (i) the quadratic effects are orthogonal to the main effects, (ii) all elements corresponding to the correlations between the intercept estimates and the estimates of the quadratic effects are equal, and (iii) every pair of quadratic-effect estimates has the same correlation (which is zero in the case of the OA). In addition, the main effects of OA are orthogonal to one another. Despite the fact that our MLSD*s are not as D-efficient as the OA in terms of both the first-order as well as pure-quadratic and the OA has more desirable properties than ours, doubling the number of runs would be cost prohibitive to most experimenters. We, therefore highly recommend our 18-run MLSD* with the reasonably high (d_1, d_2) ratios and low $r_{\max}$ and $r'_{\max}$. If the experimenter wishes to get all of the advantages of an MLSD* together with the orthogonality between all linear main effects and two-factor interactions, s/he should opt for the 26-run ADSD in Figure 3. Following is the $\mathbf{X}'\mathbf{X}$ matrix of our 18-run MLSD*:

$$
\begin{pmatrix}
18 & 14 & 14 & 14 & 14 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
14 & 14 & 12 & 12 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
14 & 12 & 14 & 12 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
14 & 12 & 12 & 14 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
14 & 12 & 12 & 12 & 14 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 14 & 0 & 0 & 0 & 2 & 2 & -2 & 2 & 2 & -2 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 14 & 0 & 0 & -2 & 2 & 2 & 2 & -2 & 2 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 14 & 0 & -2 & -2 & 2 & 2 & 2 & -2 & -2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 14 & -2 & -2 & -2 & -2 & 2 & 2 & 2 \\
0 & 0 & 0 & 0 & 0 & 2 & -2 & -2 & -2 & 18 & 2 & -2 & 2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 0 & 2 & 2 & -2 & -2 & 2 & 18 & 2 & -2 & -2 & -2 & 2 \\
0 & 0 & 0 & 0 & 0 & -2 & 2 & 2 & -2 & -2 & 2 & 18 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & -2 & 2 & -2 & -2 & 18 & -2 & 2 & -2 \\
0 & 0 & 0 & 0 & 0 & 2 & -2 & 2 & 2 & -2 & -2 & -2 & -2 & 18 & -2 & 2 \\
0 & 0 & 0 & 0 & 0 & -2 & 2 & -2 & 2 & -2 & -2 & -2 & 2 & -2 & 18 & 2 \\
0 & 0 & 0 & 0 & 0 & 2 & 2 & -2 & 2 & -2 & 2 & -2 & -2 & 2 & 2 & 18
\end{pmatrix}.
$$

5. Conclusion

Most screening experiments in engineering and science have mixed-level factors and should use MLSDs. Mixed-level designs, such as orthogonal arrays, however, have not been popular because they require too many runs. The small DSD-based MLSD*s we discuss in this paper provide more design choices for experimenters and help them to "design for experiments instead of experiment for the design".

The 60 small MLSD*s in Table 1 and the four colored correlation cell plots in Figure 4 of this paper are available in the supplemental materials.

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