A Class of Three-Level Designs for Definitive Screening in the Presence of Second-Order Effects

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Screening designs are attractive for assessing the relative impact of a large number of factors on a response of interest. Experimenters often prefer quantitative factors with three levels over two-level factors because having three levels allows for some assessment of curvature in the factor–response relationship. Yet, the most familiar screening designs limit each factor to only two levels. We propose a new class of designs that have three levels, provide estimates of main effects that are unbiased by any second-order effect, require only one more than twice as many runs as there are factors, and avoid confounding of any pair of second-order effects. Moreover, for designs having six factors or more, our designs allow for the efficient estimation of the full quadratic model in any three factors. In this respect, our designs may render follow-up experiments unnecessary in many situations, thereby increasing the efficiency of the entire experimentation process. We also provide an algorithm for design construction.

Key Words: Alias; Confounding; Coordinate Exchange Algorithm; D-Efficiency; Response Surface Designs; Robust Designs; Screening Designs.

Introduction

Experimenters frequently use screening designs during the early stages of an investigation to identify active effects in the presence of effect sparsity. These designs often target large main (linear) effects, although there is no need to limit the search to first-order terms. As Montgomery (2009) writes, "A major use of fractional factorials is in screening experiments—experiments in which many factors are considered and the objective is to identify those factors (if any) that have large effects." A quantitative factor can be critically important over the experimental range due to its first-order main effect or to potential second-order effects in the form of two-factor interactions and pure-quadratic effects. In this paper, we introduce a new class of designs for screening quantitative factors in the presence of active first- and second-order effects.

Traditionally, resolution III and IV fractional factorial designs have been widely used for early-stage screening experimentation. An undesirable property of resolution III fractional-factorial screening designs (Box and Hunter, 1961) is that they completely confound the main effects of the factors with one or more two-factor interactions. If a confounded effect is active, the experimenter is left with substantial ambiguity. Resolving this ambiguity generally requires the experimenter to perform additional experimental runs. If there is strong reason to suspect the presence of a few active two-factor interactions, a resolution

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IV fractional factorial design is a standard alternative. However, these designs require twice as many runs as the resolution III design and again lead, frequently, to substantial ambiguity. If an interaction contrast is identified as active, the experimenter has no way to definitively identify which of the interactions in the set of confounded two-way interactions are active. Again, follow-up work is required to identify the active effects.

Another limitation of resolution III and IV designs is that they have no capability for capturing curvature due to pure-quadratic effects. Of course, it is traditional to add center runs to two-level screening designs to get a global assessment of curvature. Still, these runs do not allow for separate estimation of the quadratic effects of each factor. So an indication of curvature in the analysis leads to still more ambiguity that can only be resolved with additional runs.

Our new class of three-level screening designs has the structure illustrated in Table 1. We use $x_{i,j}$ to denote the setting of the jth factor for the ith run. For m factors, there are $2m + 1$ runs based on m fold-over pairs and an overall center point. Each run (excluding the centerpoint) has exactly one factor level at its center point and all others at the extremes. As described in the next section, the values of the ± 1 entries in the odd-numbered runs of Table 1 are determined using optimal design; the even-numbered values (∓ 1) result from the fold-over operation. These designs have the following desirable properties:

TABLE 1. General Design Structure for *m* Factors

Foldover pair	Run (i)	Factor levels				
		$x_{i,1}$	$x_{i,2}$	$x_{i,3}$	$\cdots$	$x_{i,m}$
1	1	0	± 1	± 1	$\cdots$	± 1
	2	0	∓ 1	∓ 1	$\cdots$	∓ 1
2	3	± 1	0	± 1	$\cdots$	± 1
	4	∓ 1	0	∓ 1	$\cdots$	∓ 1
3	5	± 1	± 1	0	$\cdots$	± 1
	6	∓ 1	∓ 1	0	$\cdots$	∓ 1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
m	$2m - 1$	± 1	± 1	± 1	$\cdots$	0
	$2m$	∓ 1	∓ 1	∓ 1	$\cdots$	0
Centerpoint	$2m + 1$	0	0	0	$\cdots$	0

1. The number of required runs is only one more than twice the number of factors.
2. Unlike resolution III designs, main effects are completely independent of two-factor interactions. As a result, estimates of main effects are not biased by the presence of active two-factor interactions, regardless of whether the interactions are included in the model.
3. Unlike resolution IV designs, two-factor interactions are not completely confounded with other two-factor interactions, although they may be correlated.
4. Unlike resolution III, IV, and V designs with added center points, all quadratic effects are estimable in models comprised of any number of linear and quadratic main-effects terms.
5. Quadratic effects are orthogonal to main effects and not completely confounded (though correlated) with interaction effects.
6. With 6 through (at least) 12 factors, the designs are capable of estimating all possible full quadratic models involving three or fewer factors with very high levels of statistical efficiency.

We use the term "definitive screening" because of points one through five above. These are small designs that, unlike resolution III and IV factorial designs, permit the unambiguous identification of active main effects, active quadratic effects, and, in the presence of a moderate level of effect sparsity, active two-way interactions.

In our view, another practical advantage of the designs we propose is the explicit use of three levels. It has been our experience that engineers and scientists often feel some discomfort using two-level designs for two reasons. First, statisticians advise them to experiment boldly by choosing a substantial interval between low and high values of each factor. But their scientific training inculcates the notion that the functional relationship between independent and dependent variables is usually nonlinear, particularly over a wide range. This leads to some cognitive dissonance in considering the use of two-level designs. Second, even in the early stages of a study, investigators frequently have an opinion regarding the "best" levels of each factor for optimizing a response. Their experimental region then brackets these levels. If the response values are comparable at either end of the range but different in the middle, the concern is that a two-level design might screen out an important factor. Adding center runs to a two-level design is a very popular procedure because it permits a test for curvature. However, in the event that substantial curvature is present, the investigator cannot determine which factor(s) caused it and will have to do follow-up experimentation to resolve the ambiguity. Our designs avoid this by making it possible to uniquely identify the source of any curvature.

The methodology proposed here is different from, but related to, several prior contributions. For example, Cheng and Wu (2001) develop a novel approach for factor screening and response surface estimation using fractions of 3^m experiments for $n = 27$ and by using fractions of mixed-level orthogonal arrays for $n = 18$ and $n = 36$. Designs produced by Cheng and Wu are related, in that they employ three levels and can provide estimates of first- and second-order effects. The designs proposed here differ in that they (1) generally allow for substantially fewer runs for the same number of factors and (2) do not require orthogonality between main effects.

The approach of Tsai et al. (2000) (TGM) is also related. They consider the design and analysis of three-level designs using a design strategy that considers the efficiencies of low-level projections. We note that this seemingly disparate approach did lead to nearly the same arrangement as ours in one instance. Design 1 of TGM's Table 5 is essentially identical to our design for six factors, discussed below, with the exception that TGM require two center points to our one.

In Jones and Nachtsheim (2011), the authors considered the construction of designs that minimize the squared norm of the alias matrix subject to constraints on the D-efficiency of the design. They found that designs similar to those discussed here were sometimes produced using the proposed constrained optimal-design approach.

The proposed designs, which, as noted, require $2m + 1$ runs, occupy a new center ground between two-level resolution III factorials, which typically require between $m + 1$ and $2m$ runs, and small response surface designs, which require considerably larger numbers of runs. We refer the reader to Hartley (1959), Westlake (1965), Draper (1985), Draper and Lin (1990), and Angelopoulos et al. (2009) for the development of small response surface designs. The book by Box and Draper (1987) provides a nice introduction to small composite designs.

An outline of the paper is as follows. We describe the structure of our designs using a simple illustrative example in the next section. In succeeding sections, we (1) present an algorithm for generating these designs; (2) evaluate the aliasing, efficiency, power, and projection properties of proposed designs; (3) provide a simulated example with suggestions for statistical analysis; and, finally, (4) provide conclusions and suggestions for further work. A pseudo-code description of the algorithm is provided in Appendix 1, and a JMP scripting language (JSL) code for creating any design in this class of designs can be found at http://www.asq.org/pub/jqt/. Let $\mathbf{y} = (y_1, \ldots, y_{2m+1})'$ denote the response vector; let $\mathbf{x}_{jk}$ denote the jkth two-factor interaction column, the ith entry of which is $x_{i,j}x_{i,k}$; and let $\mathbf{x}_{jj}$ denote the jth pure-quadratic effect column, the ith entry of which is $x_{i,j}^2$. Throughout, we assume that the response y_i follows the normal theory linear model,

$$y_i = \beta_0 + \sum_{j=1}^{m} \beta_j x_{i,j} + \sum_{j=1}^{m-1} \sum_{k=j+1}^{m} \beta_{jk} x_{i,j} x_{i,k} + \sum_{j=1}^{m} \beta_{jj} x_{i,j}^2 + \varepsilon_i, \qquad i = 1, \ldots, 2m+1 \quad (1)$$

where the parameters $\beta_0, \ldots, \beta_{mm}$ are unknown constants (of which many are zero by the sparsity of effects assumption), and the $\{\varepsilon_i\}$ are iid $\mathrm{N}(0, \sigma^2)$. In matrix form, we have $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where $\mathbf{X}$ is the $(2m + 1 \times (m + 2)(m + 1)/2)$ design matrix. The least-squares estimate of a parameter β_j is denoted $\hat{\beta}_j$.

Design Structure: An Example

For two-level designs, one way to make two-factor interactions independent of main effects involves mirroring each row in the design by another that reverses the signs of all the entries in that row. Table 2 shows an example design (produced by our design algorithm, as described in the next section) with six factors and 13 runs. Note that each even-numbered row is obtained by multiplying each value of the previous row by -1. The last row is a center run.

Another pattern in Table 2 is apparent by observing the location of the zero entries. The first pair of runs has zeros in the first column and the second pair of runs has zeros in the second column. This pattern

TABLE 2. Three-Level Definitive Screening Design for Six Factors with a Simulated Response Vector

Run (i)	$x_{i,1}$	$x_{i,2}$	$x_{i,3}$	$x_{i,4}$	$x_{i,5}$	$x_{i,6}$	y_i
1	0	1	−1	−1	−1	−1	21.04
2	0	−1	1	1	1	1	10.48
3	1	0	−1	1	1	−1	17.89
4	−1	0	1	−1	−1	1	10.07
5	−1	−1	0	1	−1	−1	7.74
6	1	1	0	−1	1	1	21.01
7	−1	1	1	0	1	−1	16.53
8	1	−1	−1	0	−1	1	20.38
9	1	−1	1	−1	0	−1	8.62
10	−1	1	−1	1	0	1	7.80
11	1	1	1	1	−1	0	23.56
12	−1	−1	−1	−1	1	0	15.24
13	0	0	0	0	0	0	19.91

repeats so that each column has a contiguous pair of zero entries in the first 12 rows. Adding the center run in the last row results in a design that can fit a model including an intercept term, all the main effects, and all the pure-quadratic effects of each factor.

The columns of this design are orthogonal to each other. Because of the mirroring in pairs of runs, the main effects are all independent of any active two-factor interactions. However, the two-factor interactions are correlated among themselves and with the pure-quadratic effects. The section on design properties below considers the correlation structure and the power of tests when both pure-quadratic effects and two-factor interactions are active.

Compared with the 12-run Plackett–Burman design (Plackett and Burman, 1946) with one additional center run, the design in Table 2 has a relative D-efficiency of 85.5% for the model consisting of all first-order main effects. Both designs are orthogonal for the main effects. The relative variance of each main effect in our design ($\mathrm{Var}(\hat{\beta}_i)/\sigma^2$) is 1/10, which compares with 1/12 for the Plackett–Burman design. The ability to estimate pure-quadratic effects and the independence of the main effects and the two-factor interactions compensates for the loss of efficiency in fitting the main effects model. Note that each main effect in the Plackett–Burman design is correlated—or partially aliased—with several two-factor interactions.

Design Construction

The patterns illustrated in the previous section are common to each member of the class of designs. Construction of these designs is accomplished through the use of a numerical algorithm that maximizes the determinant of the information matrix of the main effects model while enforcing this structure. The starting design imposes zeros in all the required places, and these entries are not allowed to change during the course of the algorithm. The other entries in the odd-numbered rows of the starting design are chosen randomly on the interval $[-1, 1]$. The even numbered rows of the starting design are obtained from the odd-numbered rows by multiplying each value by -1. (Because the starting values are chosen from the interval $[-1, 1]$, the endpoints of the interval (± 1) will not appear in the starting design. These interior points are moved to the extremes during the course of the algorithm. One could also choose starting points by restricting all nonzero values to ± 1; however, we have found that choosing starting values from the continuous interval helps in our efforts to avoid local maxima, as described below.)

The starting design is improved using a variant of the coordinate exchange algorithm of Meyer and Nachtsheim (1995). For each nonzero entry in every row of the design matrix, the algorithm evaluates the effect of changing that entry to 1 or -1 while simultaneously changing the corresponding entry in the mirroring row to -1 or 1, respectively. If the determinant of the information matrix improves for either or both of these operations, then the current design is updated for the given row and the mirroring row for the better of the two possible exchanges. After the first pass through each entry in the design matrix, the algorithm makes a second pass through every nonzero value. If any value of the design changes in the second pass, then the algorithm performs another pass. This process continues until there are no changes in any pass through the design or when a maximum iteration limit is reached. The resulting design, having been obtained from one random starting design, may not be globally optimal, so multiple random starting designs are used in an effort to avoid local maxima.

Note that, to create a randomized design, the rows of the design generated by the algorithm should be randomly shuffled.

m = 4

1	0+--
2	0-++
3	-0-+
4	+0+-
5	--0-
6	++0+
7	-++0
8	+--0
9	0000

m = 5

1	0++--
2	0--++
3	+0--+
4	-0++-
5	+-0+-
6	-+0-+
7	+-+0+
8	-+-0-
9	++++0
10	----0
11	00000

m = 6

1	0+----
2	0-++++
3	+0-++-
4	-0+--+
5	--0+--
6	++0-++
7	-++0+-
8	+--0-+
9	+-+-0-
10	-+-+0+
11	++++-0
12	----+0
13	000000

m = 7

1	0+-+-+-
2	0-+-+-+
3	-0+-++-
4	+0-+--+
5	+-0++++
6	-+0----
7	+--0+--
8	-++0-++
9	--++0--
10	++--0++
11	-+-++0+
12	+-+--0-
13	+++++-0
14	-----+0
15	0000000

m = 8

1	0-++-+++
2	0+--+---
3	-0-++++-
4	+0+----+
5	--0++--+
6	++0--++-
7	+-+0++--
8	-+-0--++
9	--+-0-+-
10	++-+0+-+
11	+---+0++
12	-+++-0--
13	-++-++0+
14	+--+--0-
15	+++++-+0
16	-----+-0
17	00000000

m = 9

1	0++++++++
2	0--------
3	+0+-+--+-
4	-0-+-++-+
5	-+0-+-+--
6	+-0+-+-++
7	--+0+---+
8	++-0-+++-
9	+-+-0++--
10	-+-+0--++
11	----+0+++
12	++++-0---
13	++--++0-+
14	--++--0+-
15	---+++-0-
16	+++---+0+
17	-++--+-+0
18	+--++-+-0
19	000000000

m = 10

1	0++-++++-+
2	0--+----+-
3	+0-++-++--
4	-0+--+--++
5	-+0---+---
6	+-0+++-+++
7	-++0+--++-
8	+--0-++--+
9	----0++++-
10	++++0----+
11	-+-++0+-++
12	+-+--0-+--
13	++----0+++
14	--++++0---
15	++++-++0+-
16	----+--0-+
17	++--++--0-
18	--++--++0+
19	+-+-+-+-+0
20	-+-+-+-+-0
21	0000000000

m = 11

1	0-+-----+-+
2	0+-+++++-+-
3	-0--+----++
4	+0++-++++--
5	--0++++---+
6	++0----+++-
7	---0-++-++-
8	+++0+--+--+
9	+--+0+-++++
10	-++-0-+----
11	--++-0-+-+-
12	++--+0+-+-+
13	---++-0++--
14	+++--+0--++
15	-+++--+0+++
16	+---++-0---
17	-+---+-+0-+
18	+-+++-+-0+-
19	+-----++-0+
20	-+++++--+0-
21	++-+------0
22	--+-++++++0
23	00000000000

m = 12

1	0--+-+-+++-+
2	0++-+-+---+-
3	-0+++++++---
4	+0-------+++
5	++0-++-++-++
6	--0+--+--+--
7	+--0+-+-+--+
8	-++0-+-+-++-
9	++++0-++++++
10	----0+------
11	+-+-+0++-+-+
12	-+-+-0--+-+-
13	++++-+0----+
14	----+-0++++-
15	--+++--0--++
16	++---++0++--
17	+-++++--0++-
18	-+----++0--+
19	++-++--+-0--
20	--+--++-+0++
21	-+-++++--+0+
22	+-+----++-0-
23	+--+-+++--+0
24	-++-+---++-0
25	000000000000

FIGURE 1. Designs for $m = 4$ Through $m = 12$ Factors.

Design Properties

Designs for 4 through 12 factors are displayed in Figure 1. These were the best designs found by our algorithm using 10,000 random starting designs. With the exception of $m = 12$, all designs having even numbers of factors are orthogonal for main effects, in the sense that all main-effects estimates are uncorrelated and the levels sum to zero. Despite considerable additional computational search (in the form of 100,000 random starts), we have not been able to find an orthogonal design for $m = 12$. Designs for $m = 4$ through $m = 30$ can be downloaded from http://www.asq.org/pub/jqt/. In this section, we explore the aliasing, efficiency, power, and projective properties of the proposed designs.

Aliasing and Correlation Structure

Assume that the "true" model can be well approximated by full quadratic model (1), and partition this model as follows:

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\epsilon}, \qquad (2)$$

where $\mathbf{X}_1$ is the $(2m + 1 \times m)$ design matrix corresponding to the m linear main-effects terms and $\mathbf{X}_2$ is the $(2m + 1 \times 1 + m(m + 1)/2)$ design matrix corresponding to all other terms in (1). If the analyst

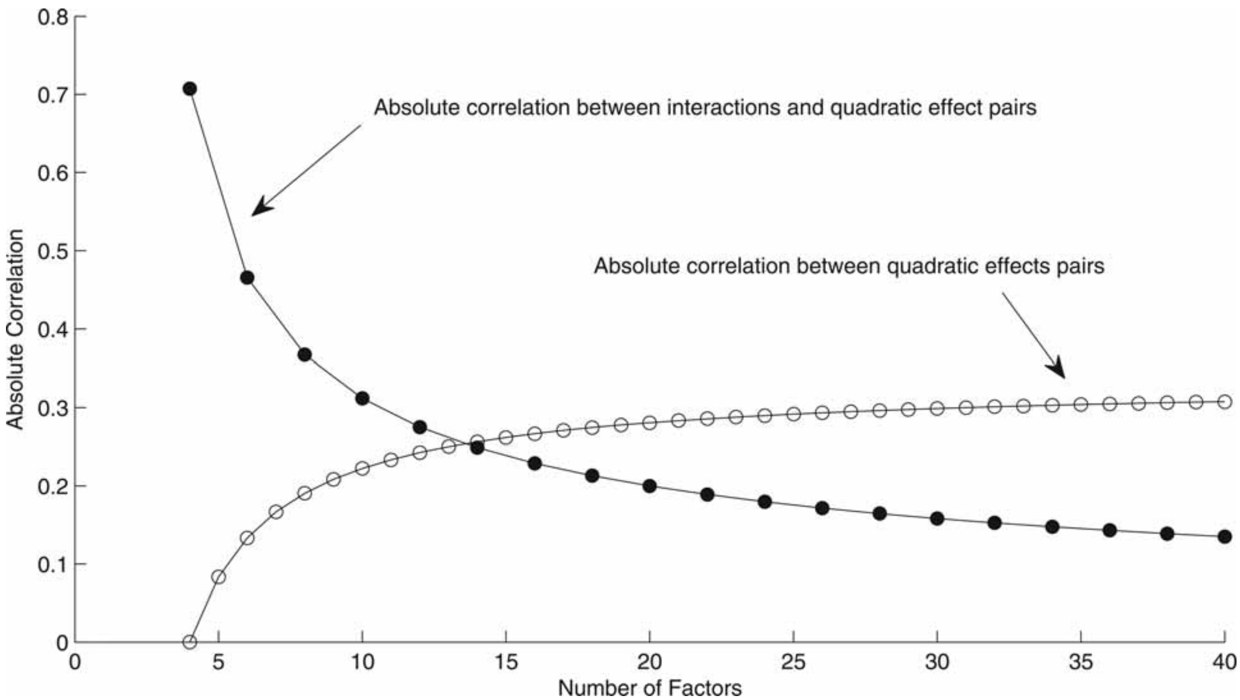

FIGURE 2. Plots of Absolute Correlations Between Quadratic Effect Pairs and Between Interaction and Quadratic Effect Pairs for Four through 40 Factors. Solid dots give $r^c_{qq,st}(m)$ from (6); open dots give $r^c_{qq,ss}(m)$ from (4).

employs the linear main-effects model $\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\epsilon}$ to estimate $\boldsymbol{\beta}_1$ using least squares, it is well known that the expected value of the resulting estimate is

$$\mathrm{E}(\hat{\boldsymbol{\beta}}_1) = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2, \tag{3}$$

where the $(m \times 1 + m(m+1)/2)$ *alias matrix* $\mathbf{A}$ is given by $\mathbf{A} = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}1'\mathbf{X}_2$. It is straightforward to show that $\mathbf{A} = \mathbf{0}$ for all designs defined by Table 1. As a result, for all designs in this class,

1. Main effects are independent of two-factor interactions.
2. Main effects are independent of quadratic effects.

In addition, for all of the designs that we have constructed, no individual two-factor interaction is completely confounded with any other individual two-factor interaction or quadratic effect. Moreover, the designs for $m = 4$, $m = 6$, $m = 8$, and $m = 10$ are orthogonal main-effects plans, in the sense that all main effects are pairwise uncorrelated and the levels sum to zero. Although two-factor interactions are not completely confounded with other two-factor interactions or with quadratic effects, some correlation is present. In this section, we examine the extent of the correlation between (1) pairs of quadratic effects, (2) between quadratic and interaction effect pairs, and (3) between pairs of interactions. There are at least two ways that correlations between pairs of model effects are commonly examined. The first is to consider the correlations between the two columns in the design matrix that correspond to the pair of effects under consideration. This is an omnibus measure that provides a general indication of the extent of confounding between the two effects. The second is to consider the actual correlation between the estimated effects. The latter can only be obtained in the context of a specified model. In this subsection, we consider both types of correlation in turn.

Correlations Between Design Columns

We show in Appendix 2 that, for the proposed class of designs, the correlation between the two columns in the design matrix that correspond to pure-quadratic effects of a factor q and a factor $s \neq q$ for a design involving $m \geq 4$ factors, denoted $r^c_{qq,ss}(m)$, is

$$r^c_{qq,ss}(m) = \frac{1}{3} - \frac{1}{m-1}. \tag{4}$$

This correlation is increasing in m and approaches $+1/3$ as $m \to \infty$. Values for four through 40 factors are shown in Figure 2. We note that, for $m = 4$

factors, the correlation is zero. It turns out that our algorithm produces a graeco-latin square in this case.

Characterizing correlations between quadratic effects columns and interaction columns is more complex. If the number of factors is even and the two-factor interaction columns sum to zero, the correlations between any quadratic effect column and any two-factor interaction column has a simple closed form. Although we have observed that interaction columns frequently do sum to zero for m even (and all do so when our designs are orthogonal for main effects), we cannot guarantee that this condition will be met by all interaction columns in the globally optimal designs for the class. However, when the interaction columns do sum to zero and the number of factors is even, the correlation assumes one of three values, depending on whether or not the two terms have a factor in common. Letting $r^c_{qq,st}(m)$ denote the correlation between a quadratic effect column in factor q and an interaction effect column involving factors s and t, we show in Appendix 2 that, for $q \neq s$, $q \neq t$, $s \neq t$, $m \geq 4$ and even, and $\sum_i x_{i,qs} = \sum_i x_{i,st} = 0$,

$$r^c_{qq,qs}(m) = 0 \tag{5}$$

$$r^c_{qq,st}(m) = \pm\sqrt{\frac{2m+1}{3(m-1)(m-2)}}. \tag{6}$$

The absolute value of this correlation decreases in m, approaching zero as $m \to \infty$. Absolute values of the correlation for even numbers of factors ranging from $m = 4$ through $m = 40$ are shown in Figure 3. We have not been able to develop general closed-form expressions for the correlation if either m is odd or the optimal design does not produce interaction columns that sum to zero. Note that, when the above conditions are met, the quadratic effect column of any factor is uncorrelated with any two-factor interaction column involving that factor. Assuming that models exhibit effect heredity, this is another beneficial property of this design class.

Averages and maximums of absolute column correlations $|r^c_{qq,qs}|$, $|r^c_{qq,st}|$, and $|r^c_{st,uv}|$, for $m = 4$ through $m = 20$, are shown in Table 3. We first note from an examination of columns 2 and 3 that the correlations between quadratic columns and any interaction column involving the quadratic factor are, in general, quite small, and are zero for $m = 4, 6, 8$, and 10. The entries in columns 4 and 5 show that, as expected, the maximum correlation between quadratic

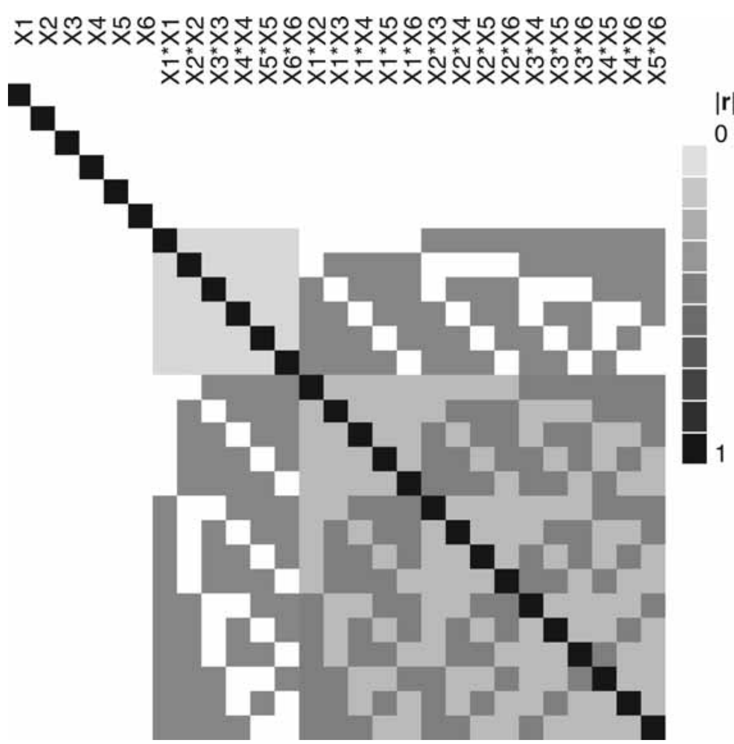

FIGURE 3. Absolute Values of Column Correlations of Terms Through Second Order for the Six-Factor, Three-Level Screening Design in Table 2.

TABLE 3. Average and Maximum Absolute Correlations Between Quadratic Effects Columns and an Interaction Column that Involves the Quadratic Effect Factor ($\overline{|r^c_{qq,qs}|}$ and $|r^c_{qq,qs}|^{\max}$); Between Quadratic Effects Columns and Interaction Columns that Do Not Involve the Quadratic Effect Factor ($\overline{|r^c_{qq,st}|}$ and $|r^c_{qq,st}|^{\max}$); and Between Interaction Columns ($\overline{|r^c_{st,uv}|}$ and $|r^c_{st,uv}|^{\max}$)

m	$\overline{\lvert r^c_{qq,qs}\rvert}$	$\lvert r^c_{qq,qs}\rvert^{\max}$	$\overline{\lvert r^c_{qq,st}\rvert}$	$\lvert r^c_{qq,st}\rvert^{\max}$	$\overline{\lvert r^c_{st,uv}\rvert}$	$\lvert r^c_{st,uv}\rvert^{\max}$
4	0.000	0.000	0.707	0.707	0.400	0.500
5	0.156	0.156	0.518	0.726	0.312	0.774
6	0.000	0.000	0.465	0.465	0.357	0.500
7	0.083	0.083	0.397	0.497	0.276	0.644
8	0.000	0.000	0.367	0.367	0.222	0.667
9	0.054	0.054	0.331	0.392	0.243	0.740
10	0.000	0.000	0.312	0.312	0.250	0.750
11	0.040	0.120	0.289	0.425	0.214	0.848
12	0.010	0.067	0.274	0.347	0.221	0.610
13	0.029	0.029	0.259	0.291	0.206	0.831
14	0.015	0.052	0.247	0.304	0.201	0.706
15	0.025	0.071	0.237	0.315	0.189	0.883
16	0.013	0.042	0.228	0.273	0.170	0.890
17	0.024	0.058	0.219	0.282	0.179	0.874
18	0.016	0.071	0.211	0.290	0.173	0.901
19	0.020	0.082	0.205	0.297	0.173	0.882
20	0.013	0.060	0.199	0.264	0.170	0.797

TABLE 4. Average and Maximum Absolute Correlations for Full Quadratic Models Involving any Three Active Factors, Between Estimated Quadratic Effects and an Estimated Interaction that Involves the Quadratic Effect Factor ($\overline{|r^c_{qq,qs}|}$ and $|r^c_{qq,qs}|^{\max}$); Between Estimated Quadratic Effects and an Estimated Interaction Effect that Do Not Involve the Quadratic Effect Factor ($\overline{|r^c_{qq,st}|}$ and $|r^c_{qq,st}|^{\max}$); and Between Estimated Interaction Effects ($\overline{|r^c_{st,uv}|}$ and $|r^c_{st,uv}|^{\max}$)

m	$\overline{\lvert r^e_{qq,ss}\rvert}$	$\lvert r^e_{qq,ss}\rvert^{\max}$	$\overline{\lvert r^e_{qq,qs}\rvert}$	$\lvert r^e_{qq,qs}\rvert^{\max}$	$\overline{\lvert r^e_{qq,st}\rvert}$	$\lvert r^e_{qq,st}\rvert^{\max}$	$\overline{\lvert r^e_{st,uv}\rvert}$	$\lvert r^e_{st,uv}\rvert^{\max}$
6	0.087	0.087	0.128	0.128	0.483	0.483	0.405	0.405
7	0.091	0.091	0.129	0.129	0.369	0.369	0.038	0.038
8	0.089	0.089	0.121	0.121	0.411	0.411	0.181	0.181
9	0.085	0.085	0.065	0.152	0.334	0.396	0.144	0.298
10	0.080	0.080	0.024	0.024	0.314	0.314	0.134	0.134
11	0.075	0.075	0.087	0.087	0.284	0.284	0.022	0.022
12	0.071	0.071	0.083	0.083	0.304	0.304	0.113	0.113
13	0.067	0.067	0.055	0.096	0.266	0.297	0.080	0.179
14	0.063	0.063	0.042	0.063	0.287	0.295	0.285	0.318
15	0.059	0.059	0.072	0.112	0.275	0.282	0.138	0.189
16	0.056	0.056	0.060	0.076	0.234	0.243	0.063	0.086
17	0.053	0.053	0.064	0.096	0.239	0.247	0.061	0.154
18	0.051	0.051	0.062	0.086	0.226	0.230	0.079	0.088
19	0.049	0.049	0.090	0.151	0.251	0.269	0.242	0.309
20	0.046	0.046	0.058	0.058	0.220	0.220	0.064	0.064

effects and two-factor interaction columns that do not involve the quadratic factor can be large for small m, but tend to zero with increasing m. Note that the entries in columns 4 and 5 for $m = 4$, $m = 6$, $m = 8$, and $m = 10$ correspond to the results shown in Figure 2, as given by (6). As shown in column 6 of Table 3, the average absolute correlation between pairs of interaction columns is generally about 1/3 or less for five or more factors and is decreasing with the number of factors. These values are similar to (though less than) the average absolute correlations between interaction and quadratic-effect pairs in column 4. In general, the magnitude of the average absolute correlations shown in Table 3 suggests that the designs will provide reasonable power for distinguishing between these effects pairs. We explore this in greater detail in our discussion of statistical power below.

Correlations Between Estimated Effects

Determination of the actual correlations between estimated effects can only be accomplished in the context of a specific model. To give some idea as to the level of correlation between estimated second-order terms that might be encountered in practice, we computed the correlations for the full second-order model, for all possible three-factor models involving 6 through 20 factors. Results are shown in Table 4. Our notation for correlations here is the same as above for column correlations, except that we use r^e to denote a correlation between estimated effects in place of r^c. Column 2 of Table 4 indicates that the average absolute correlations between pairs of estimated quadratic effects ($\overline{|r^e_{qq,ss}|}$ values) are all less than 0.10 and are generally decreasing with m. Note that r^e is decreasing with m for this particular class of models, even though r^c, as given by (4), increases monotonically to 1/3. This decrease underscores the point made earlier—that the column correlations and the estimated effects correlations are different measures of confounding. Average correlations between quadratic effects and an interaction involving the quadratic factor (column 4 $\overline{|r^e_{qq,qs}|}$ values) are all less than or equal to 0.129 and are also generally decreasing in m. Correlations between estimated quadratic effects and interactions not having a factor in common (Column 6 $\overline{|r^e_{qq,st}|}$ values) range from 0.483 for $m = 6$ to 0.220 for $m = 20$. Here we see that the estimated effects correlations agree (to perhaps a surprising extent) with the column correlations given by (6). Finally, average absolute correlations between any pairs of estimated interaction effects ($\overline{|r^e_{st,uv}|}$ values) are shown in Column 8. These values range from 0.405 for $m = 6$ to 0.022 for $m = 11$ without any apparent trend. One conclusion we draw from the table is that the highest correlations appear to occur between estimated quadratic effects and an estimated interaction effect that does not involve the quadratic factor. Nonetheless, for $m \geq 10$, all average correlations are less than 1/3.

Design Efficiency

The D-efficiency of any design d_1, relative to a nonsingular design d_2, is given by

$$D_e(d_1, d_2) = \left(\frac{|\mathbf{X}(d_1)'\mathbf{X}(d_1)|}{|\mathbf{X}(d_2)'\mathbf{X}(d_2)|}\right)^{1/p}, \qquad (7)$$

where $\mathbf{X}(d_i)$ is the design matrix of design d_i, for $i = 1, 2$, and p is the number of terms in the model. The model of interest here consists of the intercept term and all m linear effects. The (absolute) D-efficiency of any design d is given by $D_e(d, d_D)$, where d_D is the D-optimal design. In order to obtain the D-efficiencies of the proposed designs, it is necessary to obtain the D-optimal main effects design for $n = 2m + 1$. For consistency and comparability, we found the D-optimal designs for $n = 2m$ and augmented this design with a single center point. When m is even, orthogonal main effects plans for $n = 2m$, such as Plackett–Burman designs, are readily available and are known to be D-optimal. For m odd, we constructed D-optimal designs of size $n = 2m$ using the coordinate exchange algorithm in the JMP statistical software system. The resulting relative D-efficiencies of our designs, obtained via (7), are provided in column 2 of Table 5.

TABLE 5. Relative Efficiencies of the 3-Level Screening Designs and Average Increases in the Ratio of Coefficient Standard Errors when Compared with Standard Orthogonal Alternatives

Number of factors	D-efficiency (%)	Average percentage increase in standard errors
6	85.5	9.5
7	84.1	14.3
8	88.8	6.9
9	86.8	10.6
10	90.9	5.4
11	89.1	8.1
12	89.8	7.6

In every case, the relative D-efficiency of the three-level screening design exceeded 85%, with values typically near 90%. As we expected, the three-level screening design gives up some efficiency for the estimation of the main effects. In compensation for this slightly lowered efficiency, the proposed designs allow for the estimation of pure-quadratic effects of each factor as well as the main effects. Moreover, the main effects estimates are not biased by the presence of any active two-factor interaction. This is in contrast with the D-optimal designs for the main effects models, whose main-effect estimates can be substantially biased in the presence of real two-factor interactions.

Another measure of the design efficiency is given by the ratio of the standard errors of each of the coefficients for each of the two design alternatives. The averages of these ratios is provided in column 3 of Table 5. The values indicate that standard errors will be 5%–15% larger for the proposed designs than for the D-optimal main-effects plans. In general, when both designs are orthogonal, the percentage increase in this ratio is $100(\sqrt{1/(1-m^{-1})}-1)\%$, which approaches zero as m increases. We would again maintain that this is a very small price to pay for the many advantages associated with the proposed plans.

Power

As mentioned before, the use of designs in this class leads to nonzero correlation between interaction pairs and between interaction and quadratic effects pairs. In an effort to assess the impact that these correlations can have on model selection, we determined the power of these designs for rejecting the types of hypotheses that are frequently tested during the analysis phase of a study. In particular, we considered the six hypotheses listed in Table 6. Hypothesis 1 concerns linear main effects. Hypotheses 2–3 represent situations where the analyst might first fit first-order effects and then wonder if a second-order term might be present. Hypotheses 4–6 are intended to represent situations where only a few effects are active and the analyst now wishes to determine which effects from a full second-order model involving those active effects are present. Each hypothesis represents an entire family of tests, depending on the specific factors i, j involved and the number of factors, m. We provide the average power for all such tests with $|\beta|/\sigma = 1$, 2, and 3 and for designs with even numbers of factors ranging from $m = 6$ to $m = 12$.

TABLE 6. Hypotheses Tested in Power Study

Hypothesis number	Hypothesis tested	Other terms in full model
1	H_0: $\beta_i = 0$	Constant term
2	H_0: $\beta_{ii} = 0$	Constant and all linear effects
3	H_0: $\beta_{ij} = 0$	Constant and all linear effects
4	H_0: $\beta_i = 0$	Constant, β_j, β_{ii}, β_{jj}, and β_{ij}
5	H_0: $\beta_{ii} = 0$	Constant, β_i, β_j, β_{jj}, and β_{ij}
6	H_0: $\beta_{ij} = 0$	Constant, β_i, β_j, β_{ii}, and β_{jj}

Average power for rejecting hypotheses 1–6 are shown for the proposed three-level screening designs in columns 3 through 5 of Table 7. We make the following observations:

1. Power increases with the size of the design, $2m + 1$, and the size of the true regression coefficient, β. This is as expected.
2. Tests for linear effects have uniformly high power.
3. The power of tests for interaction effects is slightly less than that for linear main effects.
4. The least power is associated with tests for quadratic terms. This power is less than about 0.32 when $|\beta|/\sigma = 1$; however, if $|\beta|/\sigma \geq 2$, power is quite good, exceeding 0.68 in all cases.
5. In general, we can expect the power for tests of linear main effects and interactions to approach 1.0 as m increases for a given value of $|\beta|/\sigma$. This is not the case, however, for tests of quadratic effects. Each column designates exactly three runs at the center point of the factor range, and this does not increase with m. As a result, the extra sum of squares due to a quadratic effect in the numerator of the F-test will be approximately constant as m increases. The power of the tests for quadratic effects will increase only marginally as the denominator degrees of freedom increases with m. This pattern is clearly in evidence in the third column of Table 7, corresponding to $|\beta|/\sigma = 1$. As the number of factors increases from $m = 6$

TABLE 7. Average Power of Tests For Hypotheses 1–6

		3-Level screening designs			Orthogonal designs		
Effect	m	$\lvert\beta\rvert/\sigma = 1$	$\lvert\beta\rvert/\sigma = 2$	$\lvert\beta\rvert/\sigma = 3$	$\lvert\beta\rvert/\sigma = 1$	$\lvert\beta\rvert/\sigma = 2$	$\lvert\beta\rvert/\sigma = 3$
Hypothesis 1	6	0.821	0.999	1	0.883	1	1
(one linear effect)	8	0.937	1	1	0.962	1	1
	10	0.980	1	1	0.989	1	1
	12	0.994	1	1	0.997	1	1
Hypothesis 2	6	0.236	0.683	0.949	Aliased	Aliased	Aliased
(one quadratic effect)	8	0.275	0.769	0.980	Aliased	Aliased	Aliased
	10	0.300	0.814	0.989	Aliased	Aliased	Aliased
	12	0.317	0.840	0.993	Aliased	Aliased	Aliased
Hypothesis 3	6	0.623	0.993	1	0.548	0.982	1
(one interaction effect)	8	0.843	1	1	Aliased	Aliased	Aliased
	10	0.944	1	1	0.794	0.999	1
	12	0.982	1	1	0.993	1	1
Hypothesis 4	6	0.774	0.999	1	N.E.	N.E.	N.E.
(one linear effect	8	0.925	1	1	N.E.	N.E.	N.E.
in two-factor full	10	0.977	1	1	N.E.	N.E.	N.E.
quadratic model)	12	0.993	1	1	N.E.	N.E.	N.E.
Hypothesis 5	6	0.257	0.734	0.970	N.E.	N.E.	N.E.
(one quadratic effect	8	0.292	0.802	0.987	N.E.	N.E.	N.E.
in two-factor full	10	0.310	0.832	0.992	N.E.	N.E.	N.E.
quadratic model)	12	0.322	0.848	0.994	N.E.	N.E.	N.E.
Hypothesis 6	6	0.681	0.998	1	N.E.	N.E.	N.E.
(one interaction effect	8	0.883	1	1	N.E.	N.E.	N.E.
in two-factor full	10	0.962	1	1	N.E.	N.E.	N.E.
quadratic model)	12	0.988	1	1	N.E.	N.E.	N.E.

NOTE: "Aliased" indicates that the test could not be conducted due to direct aliasing of the effect with other second-order effects; "N.E." indicates that the full second-order model could not be estimated and the test could therefore not be conducted.

to $m = 12$, the power for the test of a linear main effect increases from 0.821 to 0.994, while the power for the test of an interaction increases from 0.623 to 0.982. In contrast, the power of the test for a quadratic effect increases only marginally, from 0.236 to 0.317. In summary, as m increases, we can anticipate that the power for tests for quadratic effects will continue to increase, but only very slightly beyond the numbers reported in Table 7 for $m = 12$.

We also compared the power of the proposed designs with that of standard two-level alternatives. For $m = 6$, $m = 10$, and $m = 12$, we chose Plackett–Burman designs with one added center point. For $m = 8$, we chose a resolution IV factorial design, also with one added center point. Power calculations for these designs are shown in columns 6 through 8 of Table 7. In examining columns 6 through 8, the first thing we notice is that many of the tests cannot be conducted due to estimability or aliasing issues. Consider, for example, hypothesis 2. For the orthogonal designs, the test for a specific quadratic effect (H_0: $\beta_{ii} = 0$) cannot be conducted because all of the quadratic effects are mutually aliased. Similarly, hypothesis 3 (H_0: $\beta_{ij} = 0$) cannot be tested for $m = 8$. The resolution IV fractional factorial design used in this case aliases each two-factor interaction with three other two-factor interactions. For the same reason, none of hypotheses 4 through 6—where full second-order models are employed for specific pairs of active factors—can be tested for the orthogonal designs. For those cases where hypotheses can be tested and comparisons between the orthogonal designs and the proposed designs can be made, we have two observations:

1. For testing linear effects (hypothesis 1), use of the three-level designs leads to a slight decrease in power for $|\beta|/\sigma = 1$ relative to the orthogonal designs. The losses range from about 0.003 ($m = 12$) to about 0.062 ($m = 6$). It is easy to show that this difference approaches zero as the number of factors grows. For $|\beta|/\sigma = 2$ or 3, the power values are nearly identical.
2. Somewhat surprisingly, the power for tests of interactions (hypothesis 3) is slightly larger for the three-level designs for $m = 6$ and $m = 10$. The orthogonal designs and the three-level designs appear to perform comparably for tests of this hypothesis for $m = 12$.

Projective Properties

In this section, we examine the characteristics of the two- and three-dimensional projections of the proposed designs.

In two dimensions, by construction, the designs project to the support of the 3×3 factorial design. For any design in the class, the projection consists of one overall center point, four edge center points and $2m-4$ corner points. The corner-point design will be balanced if the design distributes the $2m - 4$ points equally to the four corners, and from this observation it is easy to see that corner-point balance can only occur if m is even. It turns out that, in every case we have examined having six or more factors, corner-point balance occurs for all two-dimensional projections of our designs when m is even. When m is odd, all corner-point designs are *nearly balanced*, in the sense that the number of replications of any corner point for any projection is $(m/2-1) \pm 1/2$. Thus, for even m, the two-dimensional projections are central composite designs having $m/2 - 1$ replicates of the corners, one center point, and α (the length of the star point projection) equal to one. For odd m, the corner points are replicated as equally as possible.

In three dimensions, the designs do not fully project to the support of a $3 \times 3 \times 3$ factorial design. However, for every design we have examined, and for every projection, the full three-factor quadratic model is estimable and the design represented by the projection exhibits a very high level of D-efficiency for this model. This is demonstrated in Table 8, where we show, for $6 \leq m \leq 12$, the average, minimum, and maximum D-efficiencies, taken over all possible three-dimensional projections of the designs in Figure 1. From column 3 of the table, we observe that the average D-efficiency ranges from 91%, for $m = 7$, to 97%, for $m = 8$. Another interesting finding was that, in every case in which the three-level design was orthogonal (i.e., for $m = 6$, $m = 8$, and $m = 10$), every projection led to the same D-efficiency. For example, for the 10-factor design, we see that there were 120 three-dimensional projections. The D-efficiency for every one of these projections was 95% for estimation of the full quadratic model. These results indicate that, if the analysis indicates that only two or three factors are active, a

TABLE 8. Average, Minimum and Maximum D-Efficiencies for Estimation of Full Quadratic Model for All Three-Dimensional Projections of Designs with m Factors ($6 \leq m \leq 12$)

Number of factors (m)	Number of projections	Average D-efficiency	Minimum D-efficiency	Maximum D-efficiency
6	20	0.92	0.92	0.92
7	35	0.91	0.81	0.97
8	56	0.97	0.97	0.97
9	84	0.95	0.88	0.95
10	120	0.95	0.95	0.95
11	165	0.94	0.89	0.95
12	220	0.93	0.90	0.94

full quadratic polynomial in those factors can be estimated with a very high level of efficiency.

Suggestions for Analysis

The analysis of these designs is straightforward if only main effects or main and pure-quadratic effects are active. Then a multiple regression model containing the main effects only or a saturated model containing both main and pure-quadratic effects will produce coefficients that are unbiased assuming no third- or higher-order effects.

The analysis becomes more challenging if both two-factor interactions and pure-quadratic effects are active because these may be correlated, as shown previously. Figure 3 shows the column correlations for the design shown in Table 2. Columns labeled "X1*X1" through "X6*X6" represent the pure-quadratic terms. Columns "X1*X2" through "X5*X6" show the correlations for the two-factor interaction columns. Note that the main effects are uncorrelated with each other and all second-order effects.

The properties of the design do not depend on the response y_i, but in order to illustrate how the analysis might proceed, we generated entries in the response column $\mathbf{y}$ in Table 2 using the formula

$$y_i = 20 + 4x_{i,1} + 3x_{i,2} - 2x_{i,3} - x_{i,4} + 5x_{i,2}x_{i,3} + 6x_{i,1}^2 + \varepsilon_i, \quad (8)$$

where the errors, ε, are independently normally distributed with mean zero and variance 1.

Following Hamada and Wu (1992), we performed forward stepwise regression in JMP using the "Combine" option for the choice of rules and a p-value to enter of 0.1. We considered all terms up through second order for our "full model". In JMP, the "Combine" option for the choice of rules requires that the test for entering any higher order term must include all lower order terms. This rule enforces models with strong heredity. For example, in the second step of the forward stepwise algorithm, the $\mathbf{x}_{23}$ term is added along with $\mathbf{x}_2$ and $\mathbf{x}_3$ because the three-degree-of-freedom test for all three terms is the most significant of all possible tests at this stage. The final model found by the forward stepwise procedure in JMP added the effects $\mathbf{x}_4$ and $\mathbf{x}_{44}$, resulting in a Type I error from including the $\mathbf{x}_{44}$ term and having $AICc = 83.72$. Note that this model correctly identifies the active *factor set*, namely, factors one through four.

Another standard approach employs best-subsets regression, based on the corrected Akaike's information criterion, $AICc$ (Hurvich and Tsai, 1989). We fit all possible models involving first- and second-order terms having 10 or fewer predictors. (With $n = 13$, 10 is the maximum number of predictors that can be included with $AICc$). The best model included columns $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, $\mathbf{x}_{23}$, and $\mathbf{x}_{11}$, with $AICc = 70.63$. Thus, minimizing the $AICc$ criterion results in a model exhibiting strong heredity with one Type II error due to missing the term $\mathbf{x}_4$. Running the true model (8) leads to $AICc = 71.25$. Note that the true, normalized effect of term $\mathbf{x}_4$ is $|\beta|/\sigma = 1$. Our power study indicated that the probability of detecting such an effect is 0.821, so finding it was not guaranteed.

Generally, we recommend using forward stepwise regression (or some other modern and commercially available model-selection tool) where the full set of model terms consists of all first- and second-order effects and with provisions to ensure models with strong heredity. Note that, if there are multiple active pure-quadratic and two-factor interaction terms, there may be model confounding. That is, two or more models may yield identical $\hat{\mathbf{y}}$-vectors. In such cases, the all-subsets regression will identify the confounded models and additional runs will be necessary to resolve the confounding.

Discussion and Conclusions

We have introduced a class of economical three-level designs for screening quantitative factors in the presence of active second-order effects. These designs provide a definitive approach to screening in that main effects are not biased by any second-order effect and all quadratic effects are estimable. Moreover, in the presence of sparsity in the number of active factors, our designs project to highly efficient response surface designs. We have also provided an algorithm for generating these designs for any number of factors. Our designs have the minimum possible number of runs for estimating both the main and pure-quadratic effects of the factors.

These designs need not be limited to exactly $2m + 1$ runs. Designs having larger numbers of runs can be derived from the $(2m + 1)$-run designs in Table 1 (or generated by the algorithm) while maintaining basic properties. For example, for odd numbers of factors, it follows from our discussion of two-dimensional projections that our designs cannot be orthogonal for the main effects. For investigators who require orthogonal designs, we can suggest the following. At the expense of two extra runs, orthogonal designs for five, seven, or nine factors can be obtained by dropping a column from our 6, 8, and 10-factor designs, respectively. Alternatively, a design having more than $2m+1$ runs may be required for increased power. In this case, a design based on $2m+1+2k$ runs can be obtained by dropping any k columns from the existing design for $m+k$ factors.

This work can be extended in a number of directions. Planned future work includes the modification of the design to accommodate two-level categorical factors. Other useful areas of inquiry include the development of augmentation strategies in the presence of many active effects, the development of effective blocking schemes, the development of combinatorial construction methods, and the assessment of new estimation strategies, such as the Lasso (Tibshirani (1996)) and the Dantzig selector (Candes and Tao (2007)) when used in connection with these designs.

Appendix 1
Pseudocode for Algorithm

```
m = number of factors
n = number of runs = 2m + 1
s = number of random starts

1) for start = 1 to s do 2) and 3)
2) Create starting design
   a. F = mxn matrix of zeros
   b. for row = 1 to n−1 by 2
        for column = 1 to m
          if column ~= 2*row−1 &
             column ~= 2*row do
              set F[row,column] = 2*uniform random
                − 1
              set F[row+1,column] = 2*uniform
                random − 1
          end if
        end for
      end for

3) Improve starting design
   a. X = column of ones prepended to F
   b. dCurrent = determinant of X
   c. set iteration counter to 1
   d. set maximum number of iterations (maxiter)
   e. set madeswitch to true
   f. while madeswitch & iteration counter <
        maxiter do
  set madeswitch to false
  for row = 1 to n−1 by 2
    for column = 1 to m
      Z = X
      if column ~= 2*row−1 & column ~=
         2*row do
         if Z[row,column+1] = 1
            set Z[row,column+1] = −1
         set Z[row+1,column+1] = 1
         dTemporary = determinant of Z
         if dTemporary > dCurrent
            dCurrent = dTemporary
            set X[row,column+1] = −1
            set X[row+1,column+1] = 1
            set madeswitch to true
         end if
         else if Z[row,column+1] = −1
            set Z[row,column+1] = 1
            set Z[row+1,column+1] = −1
            dTemporary = determinant of Z
            if dTemporary > dCurrent
               dCurrent = dTemporary
               set X[row,column+1] = 1
               set X[row+1,column+1] = −1
               set madeswitch to true
            end if
         else
            set Z[row,column+1] = 1
            set Z[row+1,column+1] = −1
            dTemporary1 = determinant of Z
            set Z[row,column+1] = −1
            set Z[row+1,column+1] = 1
            dTemporary2 = determinant of Z
            if dTemporary1 > dTemporary2
               dCurrent = dTemporary1
               set X[row,column+1] = 1
               set X[row+1,column+1] = −1
               set madeswitch to true
            else
               dCurrent = dTemporary2
               set X[row,column+1] = −1
               set X[row+1,column+1] = 1
               set madeswitch to true
            end if
         end if
      end if
    end for
  end for
  increment iteration counter
end while
```

Appendix 2
Justification of Correlations (4)–(6)

In this appendix, we provide justifications for correlation expressions (4), (5), and (6). Let $\bar{x}_{qq}(m)$ denote the average of column $\mathbf{x}_{qq}$ for an m-factor design. The correlation between any two quadratic columns is (all sums range from $i = 1$ to $i = 2m+1$)

$$r^c_{qq,ss} = \frac{\sum[x_{i,qq} - \bar{x}_{qq}(m)][x_{i,ss} - \bar{x}_{ss}(m)]}{\sqrt{\sum[x_{i,qq} - \bar{x}_{qq}(m)]^2 \sum[x_{i,ss} - \bar{x}_{ss}(m)]^2}}. \tag{9}$$

We first note that, for $q = 1, \ldots, m$, the column $\mathbf{x}_{qq}$ consists of 3 zeros and $(2m+1)-3$ ones. As a result, we have $\bar{x}_{qq}(m) = 2(m-1)/(2m+1)$. Then $\sum[x_{i,qq} - \bar{x}_{qq}(m)]^2 = 3[0-\bar{x}_{qq}(m)]^2 + [(2m+1)-3][1-\bar{x}_{qq}(m)]^2$, again for any q. Denote this sum of squares term by $SS_{qq}(m)$. Expression (9) becomes

$$\begin{aligned} r^c_{qq,ss} &= \frac{\sum[x_{i,qq} - \bar{x}_{qq}(m)][x_{i,ss} - \bar{x}_{qq}(m)]}{\sqrt{SS^2_{qq}(m)}} \\ &= \frac{\sum x_{i,qq}x_{i,ss} - 2\bar{x}_{qq}(m)\sum x_{i,qq}}{SS_{qq}(m)} \\ &\quad + \frac{\sum[\bar{x}_{qq}(m)]^2}{SS_{qq}(m)} \\ &= \frac{[(2m+1)-5] - 2\bar{x}_{qq}(m)[(2m+1)-3]}{SS_{qq}(m)} \\ &\quad + \frac{(2m+1)[\bar{x}_{qq}(m)]^2}{SS_{qq}(m)}. \end{aligned}$$

Substituting the expressions for $\bar{x}_{qq}(m)$ and $SS_{qq}(m)$ into the above and simplifying yields (4).

To obtain (5) and (6), we assume m is even and that the interaction column sums to zero. For $s \neq q$, we have

$$\begin{aligned} r^c_{qq,qs} &= \frac{\sum[x_{i,qq} - \bar{x}_{qq}(m)][x_{i,qs} - 0]}{\sqrt{SS_{qq}(m)\sum[x_{i,qs} - 0]^2}} \\ &= \frac{\sum x_{i,qq}x_{i,qs}}{SS_{qq}(m)[(2m+1)-3]^2}. \end{aligned} \tag{10}$$

Because $x_{i,qs} \neq 0 \Rightarrow x_{i,qq} = 1$, the numerator is $\sum x_{i,qq}x_{i,qs} = \sum x_{i,qs} = 0$; hence, $r^c_{qq,qs} = 0$, as required by (5).

To obtain (6) for $s \neq q$, $t \neq q$, and $s \neq t$, we have, from (10),

$$r^c_{qq,st} = \frac{\sum x_{i,qq}x_{i,st}}{SS_{qq}(m)[(2m+1)-3]^2}. \tag{11}$$

The column $\mathbf{x}_{qq}$ consists of all ones with three zeros—one in the row corresponding to the overall center point and two in the two rows of one foldover pair. For this pair, the two entries in $\mathbf{x}_{st}$ are either identically +1 or identically −1. Because $\sum x_{i,st} = 0$ by assumption, it follows that the numerator in (11) is $\sum x_{i,qq}x_{i,qs} = \pm 2$. Simplification yields (6).

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