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SOME NEW THREE-LEVEL RESPONSE SURFACE DESIGNS

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New three-level designs for fitting second-order response surfaces are obtained by three methods. New designs for 9, 10, and 13 factors are obtained by combining two-level factorial designs and incomplete block designs. New designs for 6, 8 and 10 factors are obtained by design rotation; these designs are rotations of central composite designs. Two sequences of design (for 7, 11 and 15 factors) are obtained by using a Hadamard matrix to reduce $v+1$ linearly dependent variables to a design for v factors. One of these sequences of design corresponds to a rotation of uniform shell designs; the other sequence is complementary to the rotated uniform shell designs in the sense that the 0's and ± 1's of the design points are interchanged.

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PREFACE

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SOME NEW THREE-LEVEL RESPONSE SURFACE DESIGNS

1. INTRODUCTION

In many experiments, both the dependent variable y and the independent variables or factors $x_1, x_2, \ldots, x_v$ are quantitative variables, but the mathematical function relating y to the x's is unknown. In such cases the unknown function may be approximated by a low-order polynomial. Designs for collecting data to estimate the coefficients of the polynomial are called response surface designs. These designs specify the settings of the x's at which the dependent variable y is measured. A design for v factors is written as an $N \times v$ design matrix $\mathbf{D}$, where N is the number of design points or experimental runs required. For analysis of the data, the design matrix is expanded into an $N \times p$ model matrix $\mathbf{X}$ that has one column for each coefficient of the polynomial model.

Designs for fitting the second-order polynomial

$$y_n = \beta_0 + \sum_{i=1}^{v} \beta_i x_{i,n} + \sum_{i=1}^{v} \beta_{ii} x_{i,n}^2 + \sum_{i=1}^{v-1} \sum_{j=i+1}^{v} \beta_{ij} x_{i,n} x_{j,n} + e_n, \qquad (1)$$

where the errors e_n $(n = 1, 2, \ldots, N)$ are independently distributed with common variance σ^2, must have at least three levels of each factor. Designs with three levels of each factor may be preferred for ease of experimentation, or may be required because the levels of one or more factors can not be set accurately. When the factor level settings are only approximate, it does not seem appropriate to use an experimental design that requires setting the factors to many levels that differ from each other by a small amount. Designs with three levels of the factors are not necessarily inferior to designs with more levels by other criteria (such as the number of experimental runs required). Box and Behnken[1] have provided three-level designs for fitting second-order response surfaces over a spherical region for v = 3, 4, 5, 6, 7, 9, 10, 11, 12 and 16 factors. This report presents three-level designs for fitting second-order response surfaces for v = 6, 7, 8, 9, 10, 11, 13, and 15 factors.

2. BACKGROUND AND NOTATION

The Box-Behnken designs[1] are obtained by combining two-level factorial designs[2] and balanced incomplete block (BIB) or partially balanced incomplete block (PBIB) designs[2,3] in a manner best explained by an example. The three-factor Box-Behnken design is obtained by combining the 2^2 factorial design with the BIB design in Table 1.

Table 1. A Balanced Incomplete Block Design

Block	Treatments	
1	1	2
2	1	3
3	2	3

The design columns of the factorial design are assigned to the treatments of the BIB design in a block, while the treatments not occurring in that block are assigned columns of zeros. Center points (0,...,0) must be added to the design points generated by this process; the number of center points is denoted n_0. Box-Behnken designs are often written in a shorthand notation in which, for example, (±1, 0, ±1) indicates a two-level factorial design for factors 1 and 3, and a column of 0's for factor 2. The Box-Behnken design for three factors in shorthand notation is given in Table 2.

Table 2. Three-Factor Design in Shorthand Notation

Group	Count	x_1	x_2	x_3
1	4	±1	±1	0
2	4	±1	0	±1
3	4	0	±1	±1
4	n_0	0	0	0

Tables 1 and 2 provide essentially the same information, and the forms of Tables 1 and 2 will be used to specify designs.

To facilitate discussion of both incomplete block designs and response surface designs, it is helpful to adopt the notation frequently used to parameterize incomplete block designs: v treatments (from varieties in agricultural applications),

b blocks of size k, with r replications of each treatment. The response surface designs are then for v factors, and k is the number of ± 1's in the design points (except center points). In a BIB design each treatment occurs together with each other treatment exactly λ times—that is, each pair of treatments occur together in λ blocks. In a PBIB design two treatments that are uth associates occur together in λ_u blocks.

Box and Behnken[1] provide formulas for the least-squares estimates b of the coefficients β of the second-order polynomial (1), the variance of the estimates, and the sums of squares for an analysis of variance table. Although such formulas were useful in 1960, the availability of statistical software packages and electronic computers for the analysis of data make such analysis by hand unnecessary now. Further, doing the analysis by hand restricts the designs that can be used to those that have nearly all terms of the second-order polynomial orthogonal to each other. The variances of the estimates of the coefficients of the second-order polynomial will be used to compare the new designs to the Box-Behnken designs. The formula for Covariance(b_0, b_{ii}) in Box and Behnken[1] should have s, not s^2, in the denominator (s is the block size, as given in their Table 5c). The formula for Variance(b_{ii}) in Box and Behnken[1] does not yield correct values for all the designs; the problem is not in the formula itself but in the value of the constant B in their Table 5c. For the 3-, 5-, 7-, and 11-factor designs, the value of B is too low by C_1 (so that B+C_1 should be substituted for B). The correct values of Var(b_{ii}) and Covar(b_0, b_{ii}) were obtained from a regression analysis (see, for example, Montgomery[2], pages 420-424). The regression analyses, as well as the formulas of Box and Behnken, assume that the low, middle, and high levels of the independent variables are coded as -1, 0, and 1 for the analysis.

The formula for Var(b_0) given by Box and Behnken[1] must be generalized to be applicable to all the designs in this report; further it is helpful to rewrite some of the formulas to show the relationships among the quantities. The rewritten and generalized formulas are

$$\mathrm{Var}(b_0) = \frac{h\,\sigma^2}{g + h\,n_0} \tag{2}$$

$$\mathrm{Var}(b_i) = A\,\sigma^2 \tag{3}$$

$$\mathrm{Var}(b_{ii}) = \left[B + \frac{1}{k^2 n_0}\right] \sigma^2 \tag{4}$$

$$\mathrm{Var}(b_{ij}) = D_u \sigma^2 \qquad (u\text{th associates}) \tag{5}$$

$$\mathrm{Covar}(b_0, b_{ii}) = \left[\frac{-1}{k}\right] \mathrm{Var}(b_0) \tag{6}$$

$$\mathrm{Covar}(b_{ii}, b_{jj}) = C_u \sigma^2 + \frac{1}{k^2} \mathrm{Var}(b_0) \quad (u\text{th assoc.}) \tag{7}$$

and

$$\mathrm{Covar}(b_{ij}, b_{mn}) = E_{ij,mn} \sigma^2. \tag{8}$$

Table 3 gives the constants for equations (3)-(8) for the designs discussed in this report; the correct value of B is given for the 3-, 7-, and 11-factor Box-Behnken designs. In Table 3, the designs are indicated by the number of factors and a letter for the method of construction or the sequence that the design belongs to. The letter code is B for designs constructed from BIB designs, P for designs constructed from PBIB designs, C for rotated central composite designs (section 4), U for rotated uniform shell designs (section 5), and S for simplex-shell designs (section 6). The designs given by Box and Behnken[1] are marked with an asterisk. The block size k is not an integer for the rotated central composite designs because it is ̄ average of different block sizes. The constants g and h in equation (2) are 0 and 1 respectively for all designs except the rotated central composite design.

Comparisons of design efficiencies are usually made by scaling the designs to have the same diameter. It is on the basis of equal design diameters that Lucas[4], for example, assigns the same design efficiency to the four-factor central composite design and the four-factor Box-Behnken design. In practice, however, response surface designs are applied by scaling the coded factor ranges (often -1 to 1, or $-\alpha$ to α) to the ranges of the actual factors as specified by the experimenter. The four-factor Box-Behnken design has a ratio of design diameter to factor range of $2^{1/2}$, but the four-factor central composite design has a diameter/range ratio of 1. Therefore, if the central composite design varies pressure from 30 psi (pounds per square inch) to 50 psi, the Box-Behnken design would have to vary pressure from 32.9 psi to 47.1 psi to have the same diameter as the central composite design. In practice the pressure would be varied from 30 psi to 50 psi for the Box-Behnken design as well as for the central composite design. The effect of common practice in applying response surface designs is to make some of the traditional design efficiency calculations irrelevant and to make the diameter/range ratio an important characteristic of a response surface design.

Table 3. Constants for Equations (3)-(8)

Design	$N-n_0$	k	A	B	C_1	C_2	D_1	D_2	$E_{ij,mn}$
3U*	12	2	1/8	3/16	−1/16		1/4		0
6C	44	14/5	1/20	17/224	3/224	−4/224	1/4	1/8	0
6P*	48	3	1/24	17/216	−10/216	−1/216	1/16	1/8	0
7S*	56	3	1/24	1/18	−1/144		1/8		0
7U	56	4	1/32	7/128	−1/128		3/32		0,−1/32
8C	80	34/9	1/36	69/1088	35/1088	−1/68	1/4	1/16	0
9B	96	3	1/32	11/288	−1/288		1/8		0
9P*	120	3	1/40	1/30	−1/120	−1/720	1/16	1/8	0
10P*	160	4	1/64	17/512	1/512	−7/512	1/16	1/32	0
10P	160	5	1/80	73/2000	−13/500	−1/1000	1/64	1/32	0
10C	148	82/17	1/68	305/5248	223/5248	−1/82	1/4	1/32	0
11S	132	5	1/60	23/900	−1/450		7/144		0,±1/432
11U	132	6	1/72	11/432	−1/432		15/324		0,±1/324
11B*	176	5	1/80	23/1200	−1/600		1/32		0
13B	208	4	1/64	5/256	−1/768		1/16		0
15S	240	7	1/112	23/1568	3/3136		1/36		0,−1/288
15U	240	8	1/128	15/1024	−1/1024		7/256		0,−1/256

3. DESIGNS FROM INCOMPLETE BLOCKS

The designs in this section are typical of the designs given by Box and Behnken[1] and are obtained by a straightforward application of the their method of combining incomplete block designs and two-level factorial designs.

3.1 *Nine-Factor Design.*

A design for nine factors that has fewer design points ($N=96+n_0$) than the nine-factor Box-Behnken design ($N=120+n_0$) can be obtained by combining the 2^3 factorial with a BIB design ($v=9$, $r=4$, $b=12$, $k=3$, $\lambda=1$). The blocks of this BIB design can be divided into replication groups—sets of blocks in which all the treatments occur the same number of times. The replication groups of the BIB design can be used to block the response surface design, which is given in Table 4. Table 3 allows a comparison of the new design and the nine-factor Box-Behnken design by the variance of the estimated model coefficients. The Box-Behnken design yields better estimates of the coefficients because it has more design points. The nine-factor Box-Behnken design is based on a PBIB design so that the variances of the interaction coefficients and the covariances between squared-term coefficients depend on whether the factors are first- or second-associates. The Box-Behnken design can be divided into 5 or 10 blocks, so Box and Behnken[1] suggested 10 center points for their design. The new design has 4 blocks, so it would have 8 center points (2 per block) if blocked.

Table 4. Design for Nine Factors

Group	Count	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	Block
1	8	±1	±1	±1	0	0	0	0	0	0	1
2	8	0	0	0	±1	±1	±1	0	0	0	1
3	8	0	0	0	0	0	0	±1	±1	±1	1
4	8	±1	0	0	±1	0	0	±1	0	0	2
5	8	0	±1	0	0	±1	0	0	±1	0	2
6	8	0	0	±1	0	0	±1	0	0	±1	2
7	8	±1	0	0	0	±1	0	0	0	±1	3
8	8	0	±1	0	0	0	±1	±1	0	0	3
9	8	0	0	±1	±1	0	0	0	±1	0	3
10	8	±1	0	0	0	0	±1	0	±1	0	4
11	8	0	±1	0	±1	0	0	0	0	±1	4
12	8	0	0	±1	0	±1	0	±1	0	0	4
13	n_0	0	0	0	0	0	0	0	0	0	1-4

3.2 *Ten-Factor Design.*

An alternative to the 10-factor Box-Behnken design can be obtained by combining the cyclic PBIB design in Table 5 ($v=b=10$, $r=k=5$, $\lambda_1=4$, and $\lambda_2=2$) with the 2^{5-1} fractional factorial design defined by $\mathbf{5}=\mathbf{1234}$ (the fifth factor is set equal to the product of the first four factors). This alternative design has a larger diameter than the Box-Behnken design. Both designs have $160+n_0$ design points. The choice for the number of center points depends on the goals of the experimenter. Box and Behnken[1] selected the number of center points for their designs to make the prediction variance approximately uniform within a sphere of radius 1 when the factors are coded −1, 0, and 1; except for their 16-factor design, which has 12 center points, this choice led to $v-1 \leq n_0 \leq v+1$.

Table 5. A PBIB Design for 10 Treatments

Block	Treatments				
1	1	2	3	6	8
2	2	3	4	7	9
3	3	4	5	8	10
4	4	5	6	9	1
5	5	6	7	10	2
6	6	7	8	1	3
7	7	8	9	2	4
8	8	9	10	3	5
9	9	10	1	4	6
10	10	1	2	5	7

The cyclic PBIB design in Table 5 can be obtained from any one block by repeatedly adding one to the treatment numbers in that block and restarting at one whenever a treatment number exceeds the number of treatments. This process is known as ***developing*** an initial block and allows cyclic incomplete block designs to be specified by a single block.

3.3 *Thirteen-Factor Design.*

A design for 13 factors can be obtained by combining the 2^4 factorial design with the cyclic BIB design ($v=b=13$, $r=k=4$, and $\lambda=1$) obtained by developing the initial block 1, 2, 4, 10. The 13-factor design has $208+n_0$ design points, which is a reasonable increase from the $192 + n_0$ design points of the 12-factor design given by Box and Behnken[1]. Box and Behnken give the ***redundancy factor*** (equal to the number of design points divided by the number of parameters to be estimated) for each of their designs; they calculate the redundancy factors using $n_0 = 0$. Thus, the 13-factor design has redundancy factor $R = 208/105 = 1.98$, which compares favorably to the redundancy factors of Box-Behnken designs with more than seven factors (R's>2). The design for 13 factors can be orthogonally blocked by using the four-factor interaction of the 2^4 factorial design to separate the design points into two blocks and using the same number of center points with each block.

4. ROTATED CENTRAL COMPOSITE DESIGNS

4.1 *Central Composite Designs.*

Central composite designs[2] consist of three types of design points: factorial points, star (or axial) points, and center points. In the usual orientation and scaling, the factorial points are a 2^{v-f} factorial design of at least resolution V with levels ± 1, the star points have each factor in turn at its high and low level ($\pm\alpha$) and the other factors at their middle level (zero), and the center points have all factors at zero. When $\alpha = 1$, the designs cover a cuboidal region and are sometimes called face-centered cube designs; when $\alpha = v^{1/2}$ the designs are spherical, but to make the precision of the model predictions equal on a sphere α must be equal to the fourth root of the number of factorial points. Designs that yield equally precise predictions in all directions are called ***rotatable*** designs; the prediction variance of a rotatable design is a function only of the distance of the prediction point from the center of the design region. As it refers only to a property of prediction variance, the term ***rotatable*** is misleading: designs that are not rotatable can be rotated. Hence I coin the term ***isospheric*** to replace the misused ***rotatable***.

Design rotations are accomplished by post-multiplying the design matrix by an orthogonal matrix. Box and Behnken[1] give the orthogonal matrix that rotates the four-factor central composite design to their four-factor design. The orthogonal matrix is

$$\mathbf{P} = 2^{-1/2} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix}. \tag{9}$$

The factors are thus rotated in pairs. This method of rotating a central composite design can be generalized to any even value of v. When the rotated designs are scaled so that the rotated factorial points have levels -1, 0, and 1, the rotated star points have levels $-\alpha/2$, 0, and $\alpha/2$. Hence the rotation produces a three-level design for $\alpha = 2$. The two-factor central composite design with $\alpha = 2$ covers a square region and the rotation merely produces the usual face-centered cube design.

4.2 *Six-Factor Design.*

The rotation of the six-factor central composite design with $\alpha=2$ is given in Table 6.

Table 6. Six-Factor Rotated Central Composite Design ($\alpha=2$)

Group	Count	x_1	x_2	x_3	x_4	x_5	x_6
1	8	±1	0	±1	0	±1	0
2	8	±1	0	0	±1	0	±1
3	8	0	±1	±1	0	0	±1
4	8	0	±1	0	±1	±1	0
5	4	±1	±1	0	0	0	0
6	4	0	0	±1	±1	0	0
7	4	0	0	0	0	±1	±1
8	n_0	0	0	0	0	0	0

The region covered by the design is intermediate between a cube and a sphere. Table 3 gives the constants for calculating the variances of the coefficients for both this design and the six-factor Box-Behnken design. The constants g and h of equation (2) are 8 and 7 respectively for the rotated six-factor central composite with $\alpha=2$. The rotated central composite design in Table 6 is nonsingular even when $n_0 = 0$, but the use of center points is recommended.

4.3 *Eight-Factor Design.*

The rotated eight-factor central composite design is presented in Table 7. The constants g and h of equation (2) are 64 and 17 respectively for the eight-factor design in Table 7. There is no eight-factor Box-Behnken design to compare this new design to. The design has a redundancy factor of $80/45 = 1.78$, which is comparable to 1.75, the redundancy factor of the new nine-factor design.

Table 7. Eight-Factor Rotated Central Composite Design ($\alpha = 2$)

Group	Count	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
1	8	±1	0	±1	0	±1	0	1	0
2	8	0	±1	±1	0	±1	0	−1	0
3	8	±1	0	0	±1	0	±1	−1	0
4	8	0	±1	0	±1	0	±1	1	0
5	8	±1	0	0	±1	±1	0	0	−1
6	8	0	±1	0	±1	±1	0	0	1
7	8	±1	0	±1	0	0	±1	0	1
8	8	0	±1	±1	0	0	±1	0	−1
9	4	±1	±1	0	0	0	0	0	0
10	4	0	0	±1	±1	0	0	0	0
11	4	0	0	0	0	±1	±1	0	0
12	4	0	0	0	0	0	0	±1	±1
13	n_0	0	0	0	0	0	0	0	0

The factorial points of the unrotated design are a 2^{8-2} fractional factorial design with **7 = 1234** and **8 = 1256**.

4.4 *Ten-Factor Design.*

The rotated ten-factor central composite design is given in Table 8; it requires 12 fewer design points than the ten-factor Box-Behnken design or the new ten-factor design of the previous section. The constants g and h are 288 and 41 respectively for this design. The variance of the estimated interaction coefficients depends heavily on whether the two factors are first- or second-associates. The poor estimation of β_{ij} when i and j are first-associates suggests that this type of rotation of central composite designs becomes less desirable as the number of factors increases. Central composite designs with small values of the axial point distance—that is, $\alpha \ll v^{1/2}$ —give poor estimates of the squared-term coefficients β_{ii}; the rotation has merely moved the poor estimation to some of the interaction coefficients.

Table 8. Ten-Factor Rotated Central Composite Design ($\alpha=2$)

Group	Count	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}
1	8	±1	0	1	0	±1	0	±1	0	a	0
2	8	±1	0	0	1	±1	0	±1	0	$-a$	0
3	8	0	±1	−1	0	0	±1	±1	0	$-b$	0
4	8	0	±1	0	−1	0	±1	±1	0	b	0
5	8	±1	0	−1	0	±1	0	0	±1	a	0
6	8	±1	0	0	−1	±1	0	0	±1	$-a$	0
7	8	0	±1	1	0	0	±1	0	±1	$-b$	0
8	8	0	±1	0	1	0	±1	0	±1	b	0
9	8	0	±1	−1	0	±1	0	±1	0	0	$-c$
10	8	0	±1	0	−1	±1	0	±1	0	0	c
11	8	±1	0	1	0	0	±1	±1	0	0	d
12	8	±1	0	0	1	0	±1	±1	0	0	$-d$
13	8	0	±1	1	0	±1	0	0	±1	0	$-c$
14	8	0	±1	0	1	±1	0	0	±1	0	c
15	8	±1	0	−1	0	0	±1	0	±1	0	d
16	8	±1	0	0	−1	0	±1	0	±1	0	$-d$
17	4	±1	±1	0	0	0	0	0	0	0	0
18	4	0	0	±1	±1	0	0	0	0	0	0
19	4	0	0	0	0	±1	±1	0	0	0	0
20	4	0	0	0	0	0	0	±1	±1	0	0
21	4	0	0	0	0	0	0	0	0	±1	±1
22	n_0	0	0	0	0	0	0	0	0	0	0

$a=x_1x_5$; $b=x_2x_6$; $c=x_2x_5$; $d=x_1x_6$.

The factorial points of the unrotated design are a 2^{10-3} fractional factorial design with **8=1237**, **9=2345**, and **10=1346**.

An alternative to the available three-level designs is to use a design with five levels such as a central composite design in standard orientation. If a five-level design is to be used, the rotated central composite design is preferable to the standard orientation design; even with five levels, the rotated central composite designs keep their diameter/range ratio of $2^{1/2}$ (as opposed to a diameter/range ratio of 1 for the standard orientation). For the ten-factor design in Table 8, the isospheric $\alpha = 128^{1/4} = 3.3636$ of the central composite design in standard orientation changes the ± 1 of groups 17-21 to $\pm\alpha/2 = \pm 1.6818$. The use of ± 1.6818 for the rotated star points will cause all the β_{ij}'s to be estimated with equal precision. The moment matrix $\mathbf{X'X}$ of the isospheric design is typical of response surface designs constructed from BIB designs rather than from PBIB designs.

5. ROTATED UNIFORM SHELL DESIGNS

5.1 *Uniform Shell Designs.*

Doehlert[5] obtained the uniform shell designs by starting with a regular simplex that has one vertex at the origin; by subtracting each vertex from all other vertices the complete set of design points is obtained. This process generates $v(v+1)$ points on the surface of a sphere and a center point; in practice, $n_0 > 1$ center points would be used.

Doehlert and Klee[6] show how to rotate the uniform shell designs to minimize the number of factor levels that the designs require. The uniform shell design for v factors as is written as an $N \times (v+1)$ matrix $\mathbf{M}$; the rows of $\mathbf{M}$ are all permutations of $(-1, 1, 0, \ldots, 0)$ and a row of 0's for the center point. Note that the $v+1$ columns of $\mathbf{M}$ are linearly dependent and sum to zero. The matrix $\mathbf{M}$ is then reduced to a design for v factors and a column of 0's by post-multiplying $\mathbf{M}$ by an orthogonal matrix that has a constant column. Doehlert and Klee[6] give the orthogonal matrices that yield designs with the minimum number of factor levels. For $k = 3$, 7, 11, and 15, three-level rotations of uniform shell designs can be obtained by using a Hadamard matrix (a square matrix of 1's and -1's that has orthogonal columns[7]) to reduce the $v+1$ linearly dependent variables to a design for v factors[6]. This process and the scaling to achieve a design with levels -1, 0, and 1 can be written in matrix notation as

$$\left[\mathbf{D}\,|\,\mathbf{0}\right] = c\,\mathbf{MH}, \tag{10}$$

where **H** is a Hadamard matrix and c is a scaling constant. The three-factor rotated uniform shell design is the same design as the three-factor Box-Behnken design (Table 2).

5.2 *Seven-Factor Design.*

The seven-factor rotated uniform shell design is presented in Table 9. A word of caution is required. The design is described as a combination of a BIB design ($v = b = 7$, $r = k = 4$, $\lambda = 2$) and the 2^{4-1} fractional factorial design defined by $\mathbf{4} = \mathbf{123}$; the use of the other half fraction, defined by $\mathbf{4} = -\mathbf{123}$, will result in a singular design.

Table 9. Seven-Factor Rotated Uniform Shell Design

Group	Count	x_1	x_2	x_3	x_4	x_5	x_6	x_7
1	8	±1	±1	±1	0	0	0	±1
2	8	0	±1	±1	±1	±1	0	0
3	8	±1	0	±1	±1	0	±1	0
4	8	0	0	±1	0	±1	±1	±1
5	8	±1	±1	0	0	±1	±1	0
6	8	0	±1	0	±1	0	±1	±1
7	8	±1	0	0	±1	±1	0	±1
8	n_0	0	0	0	0	0	0	0

The four ±1's in each row are a 2^{4-1} design with $\mathbf{4} = \mathbf{123}$.

The seven-factor rotated uniform shell design might be described as the complement of the seven-factor Box-Behnken design: the rotated uniform shell design has three 0's and four ±1's in each row, whereas the Box-Behnken design has three ±1's and four 0's in the corresponding positions in each row. Thus the design points of the seven-factor rotated uniform shell design lie on a sphere of larger diameter than the design points of the seven-factor Box-Behnken design when both designs are scaled to have a range of ±1 for each factor.

Some of the interaction coefficients of the seven-factor design are correlated with each other. The 21 interaction coefficients can be divided into 7 sets of 3 coefficients that are correlated with one another, but not correlated with the coefficients in any other set. (Thus each interaction coefficient is correlated with two other interaction coefficients.) The correlations among the interaction coefficients are not serious, as indicated by a variance inflation factor (VIF) of 1.5 for each interaction coefficient. The VIF is a measure of the linear dependence of a term of the model on the other terms of the model; VIF's less than five are considered acceptable—see, for example, Montgomery and Peck[8].

5.3 *Eleven-Factor Design.*

Doehlert and Klee[6] do not give a table of the three-level rotation of the 11-factor uniform shell design "because of considerations of space." The design can be described as a combination of various 2^{6-5} fractional factorials and a BIB design ($v=11$, $r=36$, $b=66$, $k=6$, $\lambda=18$). The 132 design points on the shell can be grouped into 66 pairs; each member of a pair is the reflection of the other through the origin—that is, obtained by multiplying the other by -1. Each of the 66 pairs has a distinct assignment of 0's and ±1's to the 11 factors, but these 66 assignments can be obtained from cyclic permutation of 6 different assignments. Table 10 gives the cyclic permutations of the first assignment (rows 1-11) and then the first row of the remaining five cyclic groups (rows 12, 23, 34, 45, and 56). Each row of Table 10 has either six 1's or three 1's and three -1's; of course the negatives of these points will contain rows with six -1's. The six cyclic groups represent replication groups in the BIB design, but the replication groups may *not* be used to block the rotated uniform shell design.

Box and Behnken give an 11-factor design with $176+n_0$ design points. The 11-factor rotated uniform shell design has $132+n_0$ design points, which is 44 fewer design points than the Box-Behnken design.

Like the 7-factor design, the 11-factor rotated uniform shell design has correlations among some of the interaction coefficients. Each interaction coefficient has a negative correlation with 12 other interaction coefficients, a positive correlation with 24 other interaction coefficients, and is uncorrelated with the remaining 18 interaction coefficients. There is a simple (but counter-intuitive) rule for identifying the uncorrelated interaction coefficients: the estimates b_{ij} and b_{mn} are uncorrelated if b_{ij} and b_{mn} have a subscript in common—that is, if $i=m$, $i=n$,

$j = m$, or $j = n$. The VIF for the interaction terms is 1.67.

Table 10. Eleven-Factor Rotated Uniform Shell Design

Row	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}
1	1	−1	−1	−1	1	0	1	0	0	0	0
2	0	1	−1	−1	−1	1	0	1	0	0	0
3	0	0	1	−1	−1	−1	1	0	1	0	0
4	0	0	0	1	−1	−1	−1	1	0	1	0
5	0	0	0	0	1	−1	−1	−1	1	0	1
6	1	0	0	0	0	1	−1	−1	−1	1	0
7	0	1	0	0	0	0	1	−1	−1	−1	1
8	1	0	1	0	0	0	0	1	−1	−1	−1
9	−1	1	0	1	0	0	0	0	1	−1	−1
10	−1	−1	1	0	1	0	0	0	0	1	−1
11	−1	−1	−1	1	0	1	0	0	0	0	1
12	1	0	1	1	0	1	1	1	0	0	0
23	1	1	0	0	−1	−1	1	−1	0	0	0
34	1	−1	1	0	−1	1	0	0	−1	0	0
45	1	−1	0	1	0	−1	−1	0	1	0	0
56	1	0	−1	0	−1	0	−1	1	1	0	0

Cyclically permute to obtain 66 rows; add negatives and center points.

5.4 *Fifteen-Factor Design.*

The 15-factor rotated uniform shell design can be described as a combination of a 2^{8-4} fractional factorial design and a BIB design ($v = b = 15$, $r = k = 8$, $\lambda = 4$) and is given in Table 11. Note that the factor numbers in the rows or groups of Table 11 are not in numerical order and they must not be put into numerical order; to do so would result in a singular design. The design uses $240 + n_0$ design points to estimate 136 parameters; thus, the design has a redundancy factor of 1.76. The interaction coefficients of the 15-factor design can be grouped into 15 sets of 7 coefficients that are correlated with one another but not with the coefficients in any other set. The VIF for the interaction terms is 1.75.

The 3-level rotation of the 8-factor uniform shell design given by Doehlert and Klee[6] is erroneous [Doehlert, personal communication, 1991]; the last factor should have five levels. There is also an error (the 1 should be a zero) in the last row of the 6-factor design in Table 4 of Doehlert and Klee[6]. As a general warning, all designs should be checked (by doing the intended analysis with random numbers for the response) before they are used.

Table 11. Fifteen-Factor Rotated Uniform Shell Design

		Columns of a 2^{8-4} Fractional Factorial Design							
Group	Count	1	2	3	4	123	124	134	234
1	16	3	4	6	8	7	9	11	12
2	16	2	4	5	8	7	10	11	13
3	16	2	3	5	9	6	10	12	13
4	16	1	4	5	6	9	10	11	14
5	16	1	3	5	7	8	10	12	14
6	16	1	2	6	7	8	9	13	14
7	16	1	2	3	4	11	12	13	14
8	16	1	2	3	7	11	9	10	15
9	16.	1	2	4	6	12	8	10	15
10	16	1	3	4	5	13	8	9	15
11	16	1	5	6	7	11	12	13	15
12	16	2	3	4	5	14	6	7	15
13	16	2	5	8	9	11	12	14	15
14	16	3	6	8	10	11	13	14	15
15	16	4	7	9	10	12	13	14	15
16	n_0								

Table entries are the factors to which the columns of a 2^{8-4} design are to be assigned; factors not listed in a group are assigned zeros.

6. SIMPLEX-SHELL DESIGNS

6.1 *Generation.*

Simplex-shell designs are obtained by using all permutations of $(v-1,\ v-1,\ -2,\ -2, \ldots, -2)$, their negatives, and a row of 0's for the center point for the matrix **M** in equation (10). When reduced to v functionally independent variables by a Hadamard matrix, the simplex-shell designs have a simple interpretation: they are the complements of the rotated uniform shell designs. Like the uniform shell designs, the simplex-shell designs have $N = v(v+1) + n_0$ design points.

Only the simplex-shell designs for $v = 3,\ 7,\ 11,\ \ldots,$ are three-level designs and will be considered in this report. The 3-factor simplex-shell design is singular because the 12 design points on the sphere are two replications of six points (which are the axial or star points of a composite design). The 7-factor simplex-shell design is the 7-factor Box-Behnken design, so only the 11-factor and 15-factor designs need to be tabled.

6.2 *Eleven-Factor Design.*

The 11-factor design can be described as a combination of several 2^{5-4} fractional factorials and a BIB design ($v = 11,\ r = 30,\ b = 66,\ k = 5,\ \lambda = 12$) that has cyclic replication groups. The design is presented in Table 12. The 11-factor simplex-shell design is very similar to the 11-factor rotated uniform shell design in its structure and properties. Some of the interaction coefficients are correlated in the 11-factor simplex-shell design and the same rule—that b_{ij} and b_{mn} are uncorrelated if they have a subscript in common—applies to the simplex-shell design as well as to the rotated uniform shell design. The VIF for the interaction coefficients is 1.17 for the 11-factor simplex-shell design. Like its complementary uniform shell design, the 11-factor simplex-shell design cannot be blocked by utilizing the replication groups of its underlying BIB design. But the 11-factor simplex-shell design can be orthogonally blocked into two blocks: one block consists of the 66 rows formed by cyclic permutation of the six rows given in Table 12; the negatives of these points form the other block. The center points must be evenly divided between the two blocks.

Table 12. Eleven-Factor Simplex-Shell Design

Row	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}
1	0	0	0	0	0	−1	0	1	−1	1	1
12	0	−1	0	0	−1	0	0	0	−1	−1	−1
23	0	0	1	−1	0	0	0	0	1	1	−1
34	0	0	0	1	0	0	1	1	0	−1	−1
45	0	0	1	0	1	0	0	−1	0	−1	1
56	0	1	0	−1	0	1	0	0	0	−1	1

Cyclically permute to obtain 66 rows; add negatives and center points.

In the theory of constructing response surface designs by combining BIB designs and two-level factorials, it is well known[9] that the response surface design will be isospheric if the BIB design has $r = 3\lambda$. The uniform shell designs for $k = 7$, 11, and 15 are based on BIB designs that have $r = 2\lambda$; the corresponding simplex-shell designs are constructed from BIB designs that have $2\lambda < r \leq 3\lambda$. Thus the contours of equal prediction variance are more nearly spherical for the simplex-shell designs than for the uniform shell designs.

The 11-factor shell designs may be used as designs for 10 factors by ignoring one design column; the point of using an 11-factor design for 10 factors is to obtain a design with as few design points as possible.

6.3 *Fifteen-Factor Design.*

The 15-factor simplex-shell design can be described as a combination of a 2^{7-3} fractional factorial and a BIB design with parameters $v = b = 15$, $r = k = 7$, $\lambda = 3$. The design is given in Table 13. The pattern of correlated interaction coefficients is the same for the 15-factor simplex-shell design as for the 15-factor rotated uniform shell design, but the amount of correlation is less for the simplex-shell design: the VIF for its interaction coefficients is 1.33. The 15-factor simplex-shell design can be divided into two orthogonal blocks. The design points (rows of Table 13) that have seven 1's or three 1's and four −1's form one block, and the design points with seven −1's or three −1's and four 1's form the other block. The same number of center points must be used with each block.

Table 13. Fifteen-Factor Simplex-Shell Design

		Columns of a 2^{7-3} Fractional Factorial Design						
Group	Count	**1**	**2**	**3**	**4**	**124**	**134**	**234**
1	16	5	13	14	15	1	2	10
2	16	6	12	14	15	1	3	9
3	16	7	11	14	15	1	4	8
4	16	8	12	13	15	2	3	7
5	16	9	11	13	15	2	4	6
6	16	10	11	12	15	3	4	5
7	16	8	9	10	15	5	6	7
8	16	8	12	13	14	5	6	4
9	16	9	11	13	14	5	7	3
10	16	10	11	12	14	6	7	2
11	16	8	9	10	14	2	3	4
12	16	10	11	12	13	8	9	1
13	16	6	7	10	13	1	3	4
14	16	5	7	9	12	1	2	4
15	16	5	6	8	11	1	2	3
16	n_0							

Table entries are the factors to which the columns of a 2^{7-3} design are to be assigned; factors not listed in a group are assigned zeros.

Box and Behnken[1] do not give a design for 15 factors, but Raghavarao[10] does; his design has $512+n_0$ design points. The much smaller size ($240+n_0$ points) of the 15-factor shell designs may be interpreted as a benefit of using two-level fractional factorial designs of less than resolution V in the construction of response surface designs from two-level factorials and incomplete block designs. In the terminology of incomplete block designs, it is the recovery of interblock information that allows the use of fractional factorials of less than resolution V. It is the use of interblock information that makes $\mathbf{4}=-\mathbf{123}$ not equivalent to $\mathbf{4}=\mathbf{123}$ in the 7-factor uniform shell design, that prevents the blocking of the 11-factor shell designs by the replication groups of the BIB designs, and that prevents reordering of the factors within the groups of the 15-factor shell designs.

7. THE GEOMETRY OF THE SHELL DESIGNS

Both the uniform shell designs and the simplex-shell designs can be constructed from two regular simplexes that are centered at the origin. Denote the vertices of one of the simplexes by $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, ... ; the vertices of the other simplex are $-\mathbf{a}$, $-\mathbf{b}$, $-\mathbf{c}$, ... —that is, the second simplex must be the negative of the first. The symbols $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, ... , may be interpreted as points (the vertices of a simplex) or as vectors from the origin to those points. The statement that the vectors $\mathbf{a}$ and $\mathbf{b}$ are the same length is equivalent to the statement that the vertices $\mathbf{a}$ and $\mathbf{b}$ are the same distance from the origin.

The design points of the simplex-shell designs are the origin and the midpoints of the edges of the two oppositely oriented simplexes; this construction can be readily verified by writing out the coordinates of the vertices of the simplexes and averaging pairs of them to obtain (after rescaling) the matrix $\mathbf{M}$ for a simplex-shell design. In terms of $v+1$ linearly dependent variables the vertices of one simplex may be written as all permutations of $(v, -1, -1, \ldots, -1)$ and the vertices of the other simplex as all permutations of $(-v, 1, 1, \ldots, 1)$. The midpoints of the edges of the first simplex will be $(\mathbf{a}+\mathbf{b})/2$, $(\mathbf{a}+\mathbf{c})/2$, etc., and the midpoints of the edges of the second simplex will be $(-\mathbf{a}-\mathbf{b})/2$, $(-\mathbf{a}-\mathbf{c})/2$, etc.

The design points of the uniform shell designs are the midpoints of lines drawn from the vertices of one simplex to the vertices of the other simplex. The midpoints of the vertex connectors will be $(\mathbf{a}-\mathbf{b})/2$, $(\mathbf{a}-\mathbf{c})/2$, ... , $(-\mathbf{a}+\mathbf{b})/2$, $(-\mathbf{a}+\mathbf{c})/2$, etc. There are also $v+1$ vertex connectors between opposite (reflected) vertices, such as $\mathbf{a}$ and $-\mathbf{a}$, $\mathbf{b}$ and $-\mathbf{b}$, etc. Hence this construction of the uniform shell designs generates $v+1$ center points.

The complementary nature of the uniform shell designs and the simplex-shell designs may be explained by noting that for every point in a uniform shell design, there is a point in the simplex-shell design that is orthogonal to it. For example, the point $(\mathbf{a}-\mathbf{b})/2$ of the uniform shell design is orthogonal to the point $(\mathbf{a}+\mathbf{b})/2$ of the simplex-shell design. Using the dot product of vector notation, $(\mathbf{a}-\mathbf{b})\cdot(\mathbf{a}+\mathbf{b}) = \mathbf{a}\cdot\mathbf{a}+\mathbf{a}\cdot\mathbf{b}-\mathbf{b}\cdot\mathbf{a}-\mathbf{b}\cdot\mathbf{b} = \mathbf{a}\cdot\mathbf{a}-\mathbf{b}\cdot\mathbf{b} = 0$ because $\mathbf{a}$ and $\mathbf{b}$ are the same length.

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