Small Response-Surface Designs

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Standard composite designs for fitting second-order response surfaces typically have a fairly large number of points, especially when k is large. In some circumstances, it is desirable to reduce the number of runs as much as possible while maintaining the ability to estimate all of the terms in the model. We first review prior work on small composite designs and then suggest some alternatives for $k \le 10$ factors. In some cases, even minimal-point designs are possible.

KEY WORDS: Center points; Composite designs; Plackett and Burman designs; Small composite designs; Two-level fractional designs.

1. INTRODUCTION

Consider the situation in which a *response* y depends on k factors, coded as $x_1, x_2, \ldots, x_k$. The true response function is unknown, and we shall approximate it over a limited experimental region by a polynomial representation. If a first-order fitted model $\hat{y} = b_0 + b_1x_1 + b_2x_2 + \cdots + b_kx_k$ suffers from lack of fit arising from the existence of surface curvature, the first-order model can be upgraded by adding higher-order terms to it. We might then wish to fit, by least squares, a quadratic response-surface model of the form

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum\sum_{i>j=1}^{k} \beta_{ij} x_i x_j + \varepsilon. \quad (1)$$

The quadratic model has a constant term, k first-order terms, k quadratic terms, and $k(k - 1)/2$ interaction terms and thus has a total of $p = (k + 1)(k + 2)/2$ terms.

Many possible second-order designs may be used to obtain the data for such a model fitting. The specific choice of design would depend on the relative importance to the experimenter of various design features (see Box and Draper 1987, pp. 502–503). In this work, we specifically look for small designs of *composite design form* (see Sec. 2) such that the number of runs is as little in excess of p as possible. In addition, of course, the corresponding $X'X$ matrix must be nonsingular. A minimal-point design is one with exactly p runs.

2. SMALL COMPOSITE DESIGNS

Composite designs for fitting second-order surfaces were first introduced by Box and Wilson (1951) and followed up by Box and Hunter (1957). A composite design consists of a 2^k factorial or a 2^{k-q} fractional factorial portion (conventionally called a *cube*), with runs selected from the 2^k runs $(x_1, x_2, \ldots, x_k) = (\pm1, \pm1, \ldots, \pm1)$ usually of resolution V or higher, plus a set of $2k$ axial points at a distance α from the origin, plus n_0 center points. Thus we have a total of $2^{k-q} + 2k + n_0$ points. In general, the 2^{k-q} portion or cube may be repeated c times and the axial points or star may be repeated s times. The values of α, n_0, c, and s are to be selected by the experimenter (see Box and Draper 1987, pp. 477–478). Composite designs are extremely useful for sequential experimentation in which the cube portion is used to allow estimation of the first-order effects and the later addition of the star points permits second-order terms to be added to the model and estimated. If desired, a blocking variable can be added as well, if the number of runs permits it.

When experimentation is expensive, difficult, or time-consuming, small designs might be appropriate, especially when an independent estimate of experimental error is available. Hartley (1959) pointed out that, for estimation of the quadratic surface, the cube portion of the composite design need not be of resolution V. It could be of resolution as low as III, provided that two-factor interactions were not aliased with other two-factor interactions. Hartley employed a smaller fraction of the 2^k factorial than is used in the original Box–Wilson designs and so reduced the total number of design points. Hartley's cubes may be designated *resolution III**, meaning a design of resolution III but with no words of length four in the defining relation; see Draper and Lin (in press). Hartley thus obtained minimal- or near-minimal-point second-order designs for k = 2, 3, 4, and

6. For $k = 5, 7, 9$, and higher numbers, there was then the possibility that a worthwhile improvement could be made.

Westlake (1965) provided a method for generating composite designs based on irregular fractions of the 2^k factorial system (see Addelman 1961) rather than using the complete factorials or regular fractions of factorials employed by Box and Wilson (1951) and Hartley (1959). Westlake gave designs for the following:

1. $k = 5$, based on a 3/8 fraction of the 2^5 factorial
2. $k = 7$, based on a 13/64 fraction of the 2^7 factorial
3. $k = 9$, based on an 11/128 fraction of the 2^9 factorial.

An alternative approach to obtaining small composite designs was used by Draper (1985), who employed columns of the Plackett and Burman designs rather than regular or irregular fractions. [Plackett and Burman (1946) provided orthogonal designs for N equal to a multiple of 4 and for all such $N \leq 100$ (except 92). The missing $N = 92$ case was later given by Baumert, Golomb, and Hall (1962).] An advantage of this Plackett and Burman type of approach is that the designs are easy to construct. Specifically, (a) we can use, for the cube portion of the design, k columns of a Plackett and Burman (1946) design, and (b) where repeat runs exist, we can remove one of each set of duplicates if we wish to reduce the number of runs required.

Applying this method, Draper (1985) used 12-run, 28-run, and 44-run Plackett and Burman designs and obtained second-order response-surface designs with 22, 42, and 62 total runs (i.e., cube plus star points) for $k = 5, 7$, and 9, respectively. Deleting one of each duplicate pair gave 21 runs for $k = 5$ (a minimal-point design, beating Westlake's design by one run), 39 runs for $k = 7$ (again, one run fewer than Westlake's), and 60 runs for $k = 9$ (two runs fewer than Westlake's designs).

Table 1 shows the total number of points in cube plus star, excluding center points, in the various composite designs discussed previously. We next give this method more detailed scrutiny and discuss the extension into higher dimensions.

3. CHARACTERIZING DESIGNS

For our cube, we choose k columns from an n_{pb}-run Plackett and Burman design. A question of interest is how many such designs there are for given k and n_{pb}. We need to be able to distinguish designs that are intrinsically different and designs that are obtainable from others via sign changes in the columns, rearrangement of rows (points), and rearrangement of columns (renaming of variables). There are several methods of characterizing designs.

1. *Sign Pattern*. To obtain the so-called *sign pattern*, one counts the occurrences of +'s and −'s in each run and summarizes their pattern over the whole design.

2. *Repeat and Mirror-Image Pattern*. (For convenience, we shorten this to *repeat patterns* only.) We record how many repeat pairs are in the design, how many triple runs are in the design, how many mirror-image pairs are in the design, how many singles are in the design (i.e., neither pair nor mirror-image involved), how many triples that are such that two are a pair and the third a mirror-image or vice versa, and so on. For examples, see Table 2. The repeat-pattern characterization is invariant not only under changing column order but also under the switching of signs in any set of columns. Therefore, it provides a better criterion than the sign pattern to characterize a design. Obviously, identical designs give the same repeat pattern. Whether the same repeat pattern implies identical designs is not known, however, and needs further study. This is particularly true when a design consists of all single runs (i.e., no repeats and no mirror images).

3. *D Value*. The D value $= |X'X|/n^p$, which describes the "information per point" for the design, is often used to make comparisons among designs. When we have a number of designs of similar type—as we shall when we pick k columns with all coordinates ± 1 from a Plackett and Burman design—it makes sense to use the D values as one basis for

Table 1. Total Points Excluding Center Points in Some Small Composite Designs

	Factors, *k*							
	2	3	4	5	6	7	8	9
Coefficients, *p*	6	10	15	21	28	36	45	55
Points in Box–Hunter (1957) design	8	14	24	26	44	78	80	146
Hartley's number of points	6	10	16	26	28	46	80	82
Westlake's number of points	—	—	—	22	—	40	—	62
Draper's number of points	—	—	—	22	—	42	—	62

NOTE: Hartley's number of points for $k = 8$ should be the 80 shown, not the 48 in Westlake's paper (see Draper and Lin, in press).

Table 2. Sign and Repeat Patterns for Choice of Columns (1, 2, 3, 4, 5) From a 24-Run Plackett and Burman Design

Run number	*1*	*2*	*3*	*4*	*5*	*No. of +'s*	*Repeat and mirror*
1	+	+	+	+	+	5	Mirror of 24
2	+	+	+	+	−	4	Mirror of 20
3	+	+	+	−	+	4	
4	+	+	−	+	−	3	Mirror of 15
5	+	−	+	−	+	3	Mirror of 16
6	−	+	−	+	+	3	Mirror of 17
7	+	−	+	+	−	3	
8	−	+	+	−	−	2	Mirror of 10 and identical to 12
9	+	+	−	−	+	3	Mirror of 11 and identical to 13
10	+	−	−	+	+	3	Mirror of 8 and 12
11	−	−	+	+	−	2	Mirror of 9 and 13
12	−	+	+	−	−	2	Mirror of 10 and identical to 8
13	+	+	−	−	+	3	Mirror of 11 and identical to 9
14	+	−	−	+	−	2	
15	−	−	+	−	+	2	Mirror of 4
16	−	+	−	+	−	2	Mirror of 5
17	+	−	+	−	−	2	Mirror of 6
18	−	+	−	−	−	1	
19	+	−	−	−	−	1	Mirror of 23
20	−	−	−	−	+	1	Mirror of 2
21	−	−	−	+	+	2	
22	−	−	+	+	+	3	
23	−	+	+	+	+	4	Mirror of 19
24	−	−	−	−	−	0	Mirror of 1

NOTE: The sign pattern is 1-3-8-8-3-1, and the repeat pattern is 6-4-0-12-2.

comparison. In this way, we shall find the design that is most spread out in the ±1 coordinate space we are working with.

We feel, however, that it can be a mistake to use this D value as a method for absolute comparison among designs of different types constructed for different purposes. We initially did this ourselves in an earlier version of this article, causing the referees to comment that our new designs were not as good (smaller D value) as some previous ones constructed on a different basis for other reasons. If these are regarded as designs whose points must be restricted to the coded unit cube, this criticism is certainly valid; our designs are not the best way to fill the unit cube if the largest D value is required. It must be remembered that the D criterion is just one aspect of a design. Using it involves the assumption that the model is correct as well as having a precisely defined region to work within. No account is taken of the fact that the model may not be perfect, which is the normal situation in practice. Even a modest amount of model bias would require the design to be shrunk away from the edges of the region, for example, forcing the choice of a reduced D value (e.g., see Box and Draper 1959, 1963).

We thus do not claim that the designs we shall give have the highest D values possible for all designs within or on the unit cube. We claim only that our designs are small designs of composite type and that, of the possible ways of choosing the factorial points for these designs from the Plackett and Burman columns, we have examined all possibilities for $k \le 8$ and many of the possibilities for $k = 9$ and 10 and have exhibited the best relative choices. Our improvements over Draper (1985) are (a) we now have designs for higher values of k and (b) we have also reduced the number of design points in certain cases by finding designs that the previous article conjectured did not exist in a nonsingular version.

4. *Partition Method.* The Plackett and Burman designs have special cyclic structures. For example, in the 12-run case, we always have $(c_1, c_2, \ldots, c_k) = (c_1 + i, c_2 + i, \ldots, c_k + i) \bmod 11$ for $i = 1, 2, 3, \ldots, 10$, where $c_1, c_2, \ldots, c_k$ are column numbers. This leads to the fact that, *for any combination of column numbers, we can always find another design-equivalent combination with $c_1 = 1$.* Thus to choose k columns from an n_{pb}-run Plackett and Burman design with the first column fixed as number 1 is equivalent to partitioning an integer $n_{pb} - 1$ into k parts (see Andrews 1976). This greatly reduces the number of combinations to check for any specified criterion.

5. *Structure of $X'X$.* If we rearrange the order of terms in Model (1), the X matrix can be recast with column headings $(1, x_1^2, x_2^2, \ldots, x_k^2, x_1, x_2, \ldots, x_k, x_1x_2, x_1x_3, \ldots, x_{k-1}x_k)$ and can be split into the three portions headed by $(1, x_1^2, x_2^2, \ldots, x_k^2)$, $(x_1, x_2, \ldots, x_k)$, and $(x_1x_2, x_1x_3, \ldots, x_{k-1}x_k)$; note that $(x_1, x_2, \ldots, x_k)$

are the k columns chosen from an n_{pb}-run Plackett and Burman design with $2k$ star points added. The form of $X'X$ is then

$$X'X = \begin{bmatrix} Z & O & O \\ O & D_1 & A \\ O & A' & D_2 \end{bmatrix},$$

where $D_1 = \text{diag}(n_{pb} + 2a^2, n_{pb} + 2a^2, \ldots, n_{pb} + 2a^2)$ and $D_2 = \text{diag}(n_{pb}, n_{pb}, \ldots, n_{pb})$. Note that Z, D_1, and D_2 are not affected by the choice of the specific columns from the Plackett and Burman designs. The A matrix, however, depends on the specific k columns chosen.

4. CHOOSING THE COLUMNS

When n_{pb} is a power of 2, the Plackett and Burman designs are equivalent to 2^{k-r} fractional factorial designs. Thus choosing k columns from the Plackett and Burman design is now equivalent to choosing the defining relation for a 2^{k-r} fractional factorial design. (It might be of resolution as low as III.) This leads to the following fact: All the designs provided by Hartley (1959) and by Box and Hunter (1957) can be obtained by choosing columns from appropriately sized Plackett and Burman designs. Examples are $k = 4$, in which Hartley's design is equivalent to choosing columns (1, 2, 3, 6) of the eight-run Plackett and Burman design; $k = 5$, in which Hartley's design is equivalent to choosing columns (1, 2, 3, 4, 7) of the 16-run Plackett and Burman design; and $k = 6$, in which Hartley's design is equivalent to choosing columns (1, 2, 3, 4, 5, 14) of the 16-run Plackett and Burman design.

This is not true for Westlake's designs, which do not have the *equal occurrence* property; that is, each level does not occur the same number of times. Moreover, some of his designs are not orthogonal (e.g., see Westlake 1965, p. 333).

Minimal-point designs can be obtained when the minimal number of points required for the cube portion is a multiple of 4—namely, $p - 2k = (k + 2)(k + 1)/2 - 2k \equiv 0 \pmod 4$. Solutions for this equation are either $k \equiv 3 \pmod 8$ or $k \equiv 6 \pmod 8$. Therefore, minimal-point designs can be automatically obtained when $k = 3, 6, 11, 14, \ldots$. Note that for $k = 3$ and 6, this will produce Hartley's (1959) results.

An elaborate computer search was done for all possible choices of selecting k columns from certain n_{pb}-run Plackett and Burman designs. A detailed list of results was given by Draper and Lin (1988). In Table 3, we summarize the major results related to fitting a second-order model, listing the cube points needed for the composite designs discussed previously. In all cases, center points and star points have been omitted from the table. New designs are given for $k = 7$, 8, 9, and 10. Note that, for both cases $k = 7$ and $k = 9$, Draper's (1985) results have been improved.

Comments on Table 3

Case k = 3. As discussed previously, the four-run Plackett and Burman design is a minimal-point design. It is equivalent to Hartley's design and is a $2^{3-1}_{\text{III*}}$ design.

Case k = 4. The minimum possible number of cube points required is 7, so the eight-run Plackett and Burman design is considered. Columns (1, 2, 3, 6) give the highest D value. This $2^{4-1}_{\text{III*}}$ design is equivalent to Hartley's design. There is one run more than the minimum number required in the cube.

Case k = 5. Five columns of the 12-run Plackett and Burman design are used, because 11 is the minimum possible number of cube points required. As

Table 3. Numbers of Cube Points in Some Small Composite Designs

	Factors, k							
	3	*4*	*5*	*6*	*7*	*8*	*9*	*10*
Coefficients								
$p = (k + 1)(k + 2)/2$	10	15	21	28	36	45	55	66
Star points $2k$	6	8	10	12	14	16	18	20
Minimal points in cube	4	7	11	16	22	29	37	46
Box and Hunter (1957)	8	16	16	32	64	64	128	128
	(2^3)	(2^4)	(2^{5-1}_{V})	(2^{6-1}_{V})	(2^{7-1}_{V})	(2^{8-2}_{V})	(2^{9-2}_{V})	(2^{10-3}_{V})
Hartley (1959)	4	8	—	16	32	—	64	—
	($2^{3-1}_{\text{III*}}$)	($2^{4-1}_{\text{III*}}$)		($2^{6-2}_{\text{III*}}$)	($2^{7-2}_{\text{III*}}$)		($2^{9-3}_{\text{III*}}$)	
Westlake (1965)	—	—	12	—	26	—	44	—
			($3/8 \times 2^5$)		($13/64 \times 2^7$)		($11/128 \times 2^9$)	
Draper (1985)	—	—	12	—	28	—	44	—
Minimal runs via Plackett and Burman	4	8	12	16	24	36	40	48
After elimination of repeat	4	8	11	16	22	30	38	46

Draper (1985, p. 174) showed, there are two basic types of designs, one with a repeat pair and one with a mirror-image pair. All other choices are equivalent to one of these. The columns (1, 2, 3, 7, 11) produce a mirror-image pair and the higher D value. The columns (1, 2, 3, 9, 11) produce a repeat pair, leading to a minimal-point design with 11 runs in the cube portion after removal of a duplicate run.

Case k = 6. Again, a minimal-point design is automatically obtained when six appropriate columns are chosen from a 16-run Plackett and Burman design. Based on the D criterion, the choice of columns (1, 2, 3, 4, 5, 14) is recommended. This is equivalent to Hartley's $2^{6-2}_{\text{III}^*}$ design.

Case k = 7. There are 36 coefficients to estimate and 14 star points. Thus a minimum of 22 cube points is required. The smallest Plackett and Burman design that can be used is thus the one with 24 runs. We wish to pick seven columns. Draper (1985) tried four different combinations, all of which produced singular $X'X$ matrices, and conjectured that all of the other 245,153 possible column choices would also produce a singular $X'X$ matrix, necessitating his use of the 28-run Plackett and Burman design. In fact, this conjecture is not true. There are 12 possible repeat patterns, 5 of which produce nonsingular second-order $X'X$ matrices (see Draper and Lin 1988). The choice of columns (1, 2, 3, 5, 6, 7, 9) will give the highest D value. The choice of columns (1, 2, 5, 6, 7, 9, 10), however, will produce two repeat pairs, permitting the elimination of two runs, one from each pair. This minimal-point 22-run design is not only smaller than Hartley's 32-run design, but it is also smaller than Westlake's 26-run design.

Case k = 8. There are 45 coefficients to estimate, and 16 star points, so a minimum of 29 cube points is required. The 32-run Plackett and Burman design thus suggests itself. The choice of eight columns from this design constitutes a 2^{8-3} design. There is no 2^{8-3} design of resolution III*, however. [The table by Westlake (1965, p. 325) incorrectly suggested that there is.] The minimum so far consists of the 64-run design, 2^{8-2}_{V}, of Box and Hunter (1957). Fewer runs can be obtained by using the 36-run Plackett and Burman design. Columns (1, 3, 4, 5, 6, 7, 8, 9) will give the highest D value. Columns (1, 3, 4, 6, 8, 10, 16, 17) will produce six repeat pairs, of which one run each can be eliminated to obtain only 30 runs in the cube portion, one run more than the minimum number required.

Case k = 9. There are 55 coefficients to estimate and 18 star points. Thus a minimum of 37 cube points is required. This suggests use of nine columns of the 40-run Plackett and Burman design. Draper (1985) found that two tries with columns (1–9) and (2–9, 39) failed, producing a singular $X'X$ matrix, and conjectured that all of the other 211,915,130 possible choices would fail similarly. Again, this is not true. There are at least 50 different repeat patterns (see Draper and Lin 1988). Because of the enormous amount of computing time required, we have carried out only a partial investigation. The highest D value found is obtained by choosing columns (1, 2, 5, 6, 8, 21, 22, 23, 26). Columns (1, 2, 3, 33, 34, 35, 36, 37, 38) provide two repeat pairs, however, in each of which one run could be eliminated to give a two-level design of 38 points. This compares with 128 runs for Box and Hunter (1957, p. 233), 64 runs for Hartley (1959), and 44 runs for Westlake (1965, p. 331) and Draper (1985, p. 179). Columns (1, 8, 15, 19, 21, 24, 25, 26, 30) will produce three repeat pairs but lead to a singular $X'X$ matrix.

Case k = 10. For $k = 10$ factors, the smallest 2^{k-p}_{V} design requires 128 runs, as does the smallest $2^{k-p}_{\text{III}^*}$ design (see Draper and Lin 1990, table 4). The former was thus the best choice known to date. There are 66 coefficients to estimate and 20 star points, so a minimum of 46 cube points is required. The obvious choice is to try 10 columns of the 48-run Plackett and Burman design; this, in fact, works. Because of the enormous amount of computing time required, we have carried out only a partial investigation. Thirty-two types of design were found according to their repeat patterns, and the highest D value among them was obtained by choosing the columns (1, 2, 3, 4, 5, 6, 8, 9, 17, 18). Choice of the columns (1, 4, 5, 7, 10, 11, 14, 16, 17, 20), however, produces two repeat pairs, permitting elimination of one run from each pair to obtain a minimal-point design.

Table 4 summarizes, for $3 \le k \le 10$, those column choices already described that provide the highest relative D values.

5. DELETING REPEAT RUNS

Repeat runs provide information on pure error. Some repeat runs can be eliminated, however, if reduction in the total number of runs is critical. Table 5 shows the column choices based on deleting repeat

Table 4. Columns That Provide the Highest Relative D Values Found

k	p	n_{pb}	Columns chosen	Total points N
3	10	4	(1, 2, 3)	10
4	15	8	(1, 2, 3, 6)	16
5	21	12	(1, 2, 3, 4, 5)	22
6	28	16	(1, 2, 3, 4, 5, 14)	28
7	36	24	(1, 2, 3, 5, 6, 7, 9)	38
8	45	36	(1, 3, 4, 5, 6, 7, 8, 9)	52
9	55	40	(1, 3, 5, 6, 8, 21, 22, 23, 26)	58
10	66	48	(1, 2, 3, 4, 5, 6, 7, 11, 12, 25)	68

Table 5. Columns Chosen to Obtain Minimum Number of Runs

k	p	n_{pb}	Columns chosen	Run no. deleted	Total points N
3	10	4	(1, 2, 3)	None	10*
4	15	8	(1, 2, 3, 6)	None	16
5	21	12	(1, 2, 3, 5, 8)	7	21*
6	28	16	(1, 2, 3, 4, 5, 14)	None	28*
7	36	24	(1, 2, 5, 6, 7, 9, 10)	3, 20	36*
8	45	36	(1, 3, 4, 6, 8, 10, 16, 17)	1, 5, 10 16, 20, 29	46
9	55	40	(1, 2, 3, 33, 34, 35, 36, 37, 38)	10, 18	56
10	66	48	(1, 4, 5, 7, 10, 11, 14, 16, 17, 20)	5, 15	66*

*Obtaining minimal-point design.

runs to obtain the minimum total number of runs after elimination of repeats, N being the reduced number of runs in cube plus star but without center points. Note that for $k = 3$ and 6, minimal-point designs occur directly, for $k = 5$, 7, and 10, they can be obtained by deleting repeats, and for $k = 4$, 8, and 9, almost minimal-point designs are obtained. When repeat runs are eliminated, the orthogonality is lost, causing correlations among the estimates.

6. COMPARISONS WITH MINIMAL-POINT DESIGNS NOT OF COMPOSITE FORM

Attention has been focused in Section 4 on finding *minimal-point designs*, because they require only as many runs as there are parameters to be estimated. They do not, however, provide an estimate of experimental error and so require a prior estimate of that error. We now compare our minimal-point designs of composite type to others that are not of composite type. We restrict all design points to the unit cube for this particular comparison.

Lucas (1974) gave minimal-point designs not of composite type that he called "smallest symmetric composite designs," which consist of one center point, $2k$ star points, and $\binom{k}{2}$ "edge points." An edge point is a $k \times 1$ vector having ones in the ith and jth location and zeros elsewhere. Note that the edge point designs do not contain any two-level factorial points. For this design, $|X'X| = 2^{2k}a^{6k}$; therefore, its D value is $2^{2k}a^{6k}/p^p$.

Rechtschaffner (1967) used four different so-called *design generators* (actually point sets) to construct minimal-point designs for estimating a second-order surface (see Table 6). The signs of design generators I, II, and III can be varied to get a higher D value (e.g., we may have one -1 and all other $+1$ in design generator II, say). Rechtschaffner's designs are available for $k = 2, 3, 4, \ldots$, but, as pointed out by Notz (1982), they have an asymptotical D efficiency of 0 as $k \to \infty$ with respect to the class of saturated designs.

Box and Draper (1971, 1974) provided other minimal-point designs for $k = 2$, 3, 4, and 5, made up from the design generators (point sets) shown in Table 7. The best λ and μ (to give a maximized D value) were tabulated in the 1974 article. Kiefer, in unpublished correspondence, established, via an existence result, that this type of design cannot be D optimal for $k \geq 7$, however. Box and Draper's designs were given for $k \leq 5$, though they can be generated for any k.

Mitchell and Bayne (1976) used a computer algorithm called DETMAX that Mitchell (1974) developed earlier to find an n-run design that maximizes $|X'X|$, given n, a specified model, and a set of "candidate" design points. For each value of $k = 2$, 3, 4, and 5, they ran the algorithm 10 times, each time starting with a different randomly selected initial n-run design. The algorithm then improved the starting design by adding or removing points according to a so-called "excursion" scheme until no further improvement was possible. Because of the large amounts of computer time needed, Mitchell and Bayne carried out these calculations only for $k \leq 5$.

Table 6. Rechtschaffner's (1967) Point Sets

Number	Points	Design generator (point set)	Typical point
I	1	$(+1, +1, \ldots, +1)$ or $(-1, -1, \ldots, -1)$	$(+1, +1, \ldots, +1)$
II	k	One $+1$ and all other -1	$(+1, -1, \ldots, -1)$
III	$k(k-1)/2$	Two $+1$ and all other -1	$(+1, +1, -1, \ldots, -1)$
IV	k	One $+1$ and all other 0	$(+1, 0, \ldots, 0)$

Table 7. Point Sets of Box and Draper (1972, 1974)

Number	Points	Design generator (point set)	Typical point
I	1	(+1, +1, ..., +1) or (−1, −1, ..., −1)	(−1, −1, ..., −1)
II	k	One +1 and all other −1	(+1, −1, −1, ..., −1)
III	$k(k-1)/2$	Two λ and all other −1	(λ, λ, −1, ..., −1)
IV	k	One μ and all other 1	(μ, 1, ..., 1)

Notz (1982) studied designs for which $p = n$. He partitioned X so that

$$X = \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} = \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix},$$

where Z_1 is $(p - k) \times p$ and Z_2 is $k \times p$.

Note that Y_{11} is $(p - k) \times (p - k)$, Y_{12} is $(p - k) \times k$, Y_{21} is $k \times (p - k)$, and Y_{22} is $k \times k$, and we can think of Z_1 as representing the cube points and Z_2 the star points; Y_{12} over Y_{22} consists of the columns $(x_1^2, x_2^2, \ldots, x_k^2)$. Thus (a) all elements in Y_{11} are either +1 or −1, (b) all elements in Y_{22} are either 1 or 0, and, more important, (c) all elements in Y_{12} are +1. It follows that $|X| = |X'X|^{1/2} = |Y_{11}| \cdot |Y_{22} - J_{k,k}|$, where $J_{k,k}$ is a $k \times k$ matrix with all of its elements equal to 1. Maximization of $|X'X|$ is now equivalent to maximization of $|Y_{11}|$ and $|Y_{22} - J_{k,k}|$ separately. Notz found new saturated designs for $k \le 5$ and extended his results to the $k = 6$ case.

The minimal-point designs previously available elsewhere for $k \ge 7$ comprise the extensions of Lucas's (1974) or Rechtschaffner's (1967) or Box and Draper's (1971, 1974) designs. New minimal-point designs can be obtained by using our method for $k = 3, 5, 6, 7$, and 10. A comparison of the $D^{1/p}$ values for all of the designs we have discussed in this section is made in Table 8. As discussed in Section 3, paragraph 3, our designs do not do well in this comparison. They have other virtues, however. They are easy to construct and of composite form, providing orthogonal or near orthogonal designs and including other previously known small composite designs as special cases.

Note that we have only partially enumerated the designs for $k = 9$ and 10 because of the high computing costs. Thus it is possible that higher $D^{1/p}$ values exist for designs that we did not explore. *If* such values exceeded those of Rechtschaffner (1967), they would represent the best $D^{1/p}$ choice for these larger k. This question is unanswered and needs to be investigated.

A referee suggests the possibility

> that the Draper and Lin designs, the designs of Notz (1982), and the designs of Rechtschaffner (1967) share a common structure. The majority of points (at least $k(k + 1)/2$) are "cube" points. In all three cases these cube points actually come from balanced arrays, assuming Plackett and Burman designs are indeed balanced arrays. The remaining points are not cube points but their number, on the order of k, is a fraction of the total number of runs which tends to zero as k goes to infinity. This common structure might be worth noting and, perhaps, investigating since the properties of balanced arrays are fairly well known (see the paper by Srivastava and Chopra in the 1971 *Annals of Mathematical Statistics*, vol. 42, pp. 722–734).

This seems eminently sensible.

ACKNOWLEDGMENTS

Draper gratefully acknowledges partial support from National Science Foundation Grants DMS-8701027 and DMS-8900426. We are grateful for the use of the research computer in the Department of Statistics, University of Wisconsin–Madison. We are most grateful to the two referees, whose sharply focused comments were extremely helpful.

[*Received September 1988. Revised August 1989.*]

Table 8. Comparisons of $D^{1/p}$ for Selected Minimal-Point Designs (α = 1)

k	Draper and Lin (1988)	Lucas (1974)	Notz (1982)	Mitchell and Bayne (1976)	Box and Draper (1974)	Rechtschaffner (1967)
3	.303	.152	.400	.410	.423	.400
4	(.308)	.096	.392	.425	.423	.392
5	.241	.066	.459	.456	.374	.450
6	.263	.048	.446	ND	.317	.428
7	.196	.036	ND	ND	.227	.383
8	(.321)	.028	ND	ND	.193	.336
9	(.200)	.023	ND	ND	.167	.293
10	.165	.018	ND	ND	.146	.255

NOTE: ND indicates no design. Parentheses indicate one run more than the minimal-point design.

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