Computer-Generated Minimal (and Larger) Response-Surface Designs: (I) The Sphere

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ABSTRACT

Computer-generated designs in the sphere are described which have the minimal (or larger) number of runs for a full quadratic response-surface design. In the case of 3 factors, the designs have 10 through 33 runs; for 4 factors, 15 through 28 runs; for 5 factors, 21 through 33 runs; etc. Some of these designs are listed here in full; the others can be obtained from the authors. The designs were constructed by minimizing the average prediction variance. No prior constraints — such as a central composite structure – are imposed on the locations of the points. The program itself determines the optimal number of runs to make at the center. The best designs found have repeated runs at the center and the remaining runs at points well spread out over the surface of the sphere. There is a simple lower bound on the average prediction variance; this bound is attained by many of the designs.

Key Words. Minimal designs; spherical designs; quadratic response surface; computer-generated designs; minimal variance designs; maximal volume designs.

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1 Introduction

A statistician in Seattle, David H. Doehlert (personal communication, Oct. 5, 1990) asked one of us if we could construct designs for a full quadratic response surface depending on k factors, for k between 3 and 14, in which the number of runs n is minimal or close to minimal.

The present paper (dealing with points in a sphere) and its sequel (dealing with points in a cube) describe the designs we found and the method used.

The chief merit of our designs when compared with classical ones such as fractional factorial designs, central composite designs (Box and Wilson, 1951), or uniform shell designs (Doehlert, 1970), lies in the fact that the number of runs is minimized, an important consideration when runs are expensive.

Designs with a small number of runs have been constructed in recent years by many authors (see for example Atkinson, 1973; Box and Behnken, 1960a, 1960b; Box and Draper, 1971, 1974; Draper and Lin, 1990; Hartley, 1959; Hartley and Rudd, 1969; Hoke, 1974; Pesotchinsky, 1975; Rechtschaffner, 1967; Roquemore, 1976; Westlake, 1990; and especially the surveys by Box and Draper, 1987, §15.5; Lucas, 1977; and Myers, Khuri and Carter, 1989). However, these have mostly been restricted to central composite designs, or to subsets of factorial designs or Plackett-Burman-Rao designs.

Although computers have of course been extensively used to construct designs (besides the references mentioned above, see Kennard and Stone, 1969; Galil and Kiefer, 1977a, 1977b; and the survey by Steinberg and Hunter, 1984), including the use of conjugate gradient methods to obtain D-optimal designs (see for example Cook and Nachtsheim, 1980; Johnson and Nachtsheim, 1983), the approach taken in the present paper appears to be new.

Out of all these earlier papers, the closest in spirit to ours seem to be those of Box and Draper (1971, 1974), who give several examples of designs in the k-dimensional cube obtained by maximizing the D-efficiency. (There appears to have been no comparable work for the sphere.) In Part II we compare the Box-Draper designs to ours. Besides having larger values of integrated variance, the arrangement of points in their designs seems to be less satisfactory than ours.

The reader may wonder (as we have frequently done in the past year) why our approach was not followed before. The most plausible explanation is that investigators were deterred by the thought of minimizing (e.g. in the case of a 5-factor 24-run design) a complicated function of 120 variables over a region defined by 36 inequalities in 120-dimensional space. We quote from Box and Draper (1971, p. 738): "The determination of the optimal design of 10 runs in 3 factors involves the selection of 30 coordinate values by computer search. With more runs and/or factors, the computing problem rapidly becomes prohibitive." Indeed, if it had not been for our successful application of similar techniques in constructing spherical codes (see Hardin, Sloane and Smith, 1991), we would probably not have tackled this problem ourselves. Our computations so far have been carried out on various very high speed computers, including a Cray X-MP and a MIPS R2000A/R3000 machine, but we are preparing a portable version of the program to run on work stations. This will be described elsewhere.

A second feature of our technique is that it can be used to produce minimal designs for other response surface models and in other convex regions, and so can be applied for example to mixture experiments on a simplex or mixtures with constraints.

Following Box and Draper (1959), Galil and Kiefer (1977a,b), and others, we have initially focused our attention on the sphere and the cube. The chief reasons for studying the sphere are that the design points then enclose the largest region of space (we discuss this aspect further in Section 5), and that in a high-dimensional cube some boundary points — when compared with a sphere of the same volume — are a long way from the center and may call for unacceptable operating conditions. Another reason is that good spherical designs tend to have larger symmetry groups than good cubical designs. Symmetry groups may be irrelevant to the person using these designs — although they may lead to designs which are easier to implement — but they are important when it comes to trying to understand what makes a good design.

We have recently used these methods to construct minimal variance designs for other situations, for example 3-factor third-order designs in the cube, 9-factor quadratic designs in which six factors belong to a six-dimensional cube and three are two-level variables, and a ten-factor design in which three variables form a mixture with a constraint, five other variables are continuous, one variable is 3-level and the last is 2-level. These are briefly described in Section 6, which mentions some applications.

2 The method of construction

We make three assumptions (all of which can however be varied).

(i) The quadratic response-surface model is of the form

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j + \epsilon \ . \tag{1}$$

Then the minimal number of runs needed is equal to the number of unknown parameters, which is

$$p = \frac{(k+2)(k+1)}{2} \ . \tag{2}$$

(ii) The design consists of n points

$$(x_{j1}, \ldots, x_{jk}), \quad \text{for} \quad 1 \le j \le n \ ,$$

where $n \geq p$, chosen from (in this paper) the unit ball defined by

$$x_1^2 + \cdots + x_k^2 \leq 1 \ . \tag{3}$$

In Part II we describe designs in which (3) is replaced by the cube

$$-1 \leq x_i \leq 1 \quad (1 \leq i \leq k) \ . \tag{4}$$

(iii) We assume that a design with the smallest integrated prediction variance (defined below) is likely to be generally acceptable. However, in view of the dangers in using any single number as a design criterion, we have also plotted *variance dispersion graphs* (Giovannitti-Jensen and Myers, 1989; Vining, 1990) for our designs; some examples are given in Figure 2 below.

Let X be the $n \times p$ design matrix, containing one row

$$f(x) \ = \ (1, x_1, \ldots, x_k, x_1^2, \ldots, x_k^2, x_1 x_2, \ldots, x_{k-1} x_k)$$

for each design point $x = (x_1, \ldots, x_k)$. The prediction variance at an arbitrary point x in the unit ball is

$$\text{var } \hat{y}(x) \ = \ \sigma^2 f(x)(X'X)^{-1} f(x)' \ , \tag{5}$$

if the errors ϵ in (1) are independent with mean 0 and variance σ^2.

As a figure of merit we use the *integrated prediction variance* (Box and Draper 1959, 1963), which is

$$\text{IV} \ = \ \int_{\text{ball}} \frac{1}{\sigma^2} \text{ var } \hat{y}(x) d\mu(x) \ ,$$

where μ is uniform measure on the unit ball (3),

$$= \ \int_{\text{ball}} f(x)(X'X)^{-1} f(x)' d\mu(x) \ . \tag{6}$$

This integral simplifies (cf. Box and Draper 1963, p. 341) to give

$$\text{IV} \ = \ \text{trace } \{M(X'X)^{-1}\} \ , \tag{7}$$

where

$$M \ = \ \begin{bmatrix} 1 & 0 & \alpha u & 0 \\ 0 & \alpha I & 0 & 0 \\ \alpha u' & 0 & \beta(2I + J) & 0 \\ 0 & 0 & 0 & \beta I \end{bmatrix} \tag{8}$$

is a matrix of moments of the ball. The blocks in (8) have sizes $1, k, k$ and $k(k-1)/2$, $u = (1, 1, \ldots, 1)$, I is an identity matrix, J is an all 1's matrix, $\alpha = 1/(k+2)$, and $\beta = 1/((k+2)(k+4))$. It is easy to see that IV is scale-invariant; in fact IV is unchanged even if each variable x_i is separately rescaled.

To summarize, we wish to choose n points (with $n \geq p$) from the unit ball so as to minimize the integrated prediction variance given by (7).

This formulation of the problem, which asks for the minimum of a smooth function of kn variables over a convex region (3), is well suited to computer solution. We make use of the *pattern search* optimization strategy of Hooke and Jeeves (1961), as described by Beightler et al. (1979) (although the conjugate gradient methods described for example in Press et al. (1986) might perform equally well).

A subroutine is used to evaluate IV for each trial design, and the region of interest (the ball) is defined in the calling program. Both the function to be minimized and the optimizing region can therefore easily be changed. Our only constraint is that the function to be minimized should be differentiable (so the technique could be used to find A- or D-optimal, but not E- or G-optimal designs). The partial derivatives of IV are obtained from the formula

$$\begin{aligned} \frac{\partial \, \mathrm{IV}}{\partial x} &= -\,\mathrm{trace}\left\{ M(X'X)^{-1} \frac{\partial \, X'X}{\partial x} (X'X)^{-1} \right\} \\ &= -\,\mathrm{trace}\left\{ B \frac{\partial \, X'X}{\partial x} \right\} , \end{aligned}$$

where $B = (X'X)^{-1} M (X'X)^{-1}$. In the present situation M is given by (8), but in more complicated problems (such as that described in Section 6) we use Monte Carlo methods to estimate M.

It is also necessary to specify starting points to initiate the search, and for this we use both random starts, as well as spherical codes that we have constructed while studying the packing problem on the k-dimensional sphere (Hardin, Sloane and Smith, 1991).

Our final designs are then obtained by taking the smallest IV that occurs over a number of tries. Designs have been constructed with the following parameters (the 2-factor case being trivial):

no. of factors (k)	no. of runs (n)	no. of factors (k)	no. of runs (n)
3	$10-33$	9	$55-62$
4	$15-28$	10	$65-74$
5	$21-33$	11	$78-86$
6	$28-39$	12	$91-99$
7	$36-43$	13	$104-111$
8	$45-52$	14	$120-128$

For the designs with up to 9 factors we have made over a thousand tries for each value of n. Numerical evidence, together with the fact that the integrated variance of many of our designs coincides with the conjectured lower bound of Eq. (11), strongly suggests that our designs have values of IV that are minimal (or very close to minimal).

Table 1, described in the next section, summarizes our designs. Note in particular the second column, which specifies the best number of replicates to run at the center of the sphere for a given total number of runs.

Table 1. For k factors and n runs, the table gives the best choices for c (runs at center) and b (runs at surface of sphere), and, if appropriate, the table where the design can be found, together with the corresponding value of the integrated prediction variance (IV).

$k=2$					$k=3$				
n	c	b	Table	IV	n	c	b	Table	IV
6	1	5	see text	0.7333	10	1	9	3a	0.7369
7	2	5	””	0.5667	11	2	9	3a	0.6226
8	2	6	””	0.5000	12	2	10	3b	0.5537
9	3	6	””	0.4444	13	2	11	3c	0.5154
10	3	7	””	0.3968	14	3	11	3c	0.4773
11	3	8	””	0.3611	15	3	12	see text	0.4405
12	4	8	””	0.3333	16	3	13	3d	0.4135
13	4	9	””	0.3056	17	3	14	3e	0.3884
14	4	10	””	0.2833	18	3	15		0.3679
15	4	11	””	0.2652	19	4	15		0.3488
16	5	11	””	0.2485	20	4	16		0.3304
$k=4$					$k=5$				
n	c	b	Table	IV	n	c	b	Table	IV
15	1	14	4a	0.7524	21	1	20	see text	0.7577
16	2	14	4a	0.6691	22	2	20	see text	0.6942
17	2	15	see text	0.5976	23	2	21	see text	0.6329
18	2	16	4b	0.5641	24	2	22	5a	0.6084
19	2	17	4c	0.5348	25	2	23	5b	0.5843
20	3	17	4c	0.5070	26	2	24		0.5615
21	3	18	4d	0.4820	27	2	25		0.5399
22	3	19		0.4591	28	3	25		0.5187
23	3	20		0.4389	29	3	26		0.5002
24	3	21		0.4206	30	3	27		0.4833
25	3	22		0.4040	31	3	28		0.4675
$k=6$					$k=7$				
n	c	b	Table	IV	n	c	b	Table	IV
28	1	27	see text	0.7333	36	1	35	see text	0.7616
29	2	27	see text	0.6833	37	2	35		0.7212
30	2	28	6a	0.6661	38	2	36		0.7042
31	2	29	6b	0.6479	39	2	37		0.6860
32	2	30		0.6285	40	2	38		0.6680
33	2	31		0.6073	41	2	39		0.6438
34	2	32		0.5855	42	2	40		0.6274
35	3	32		0.5688	43	2	41		0.6131
36	3	33		0.5523					
37	3	34		0.5365					
38	3	35		0.5220					
39	3	36	6c	0.5083					

Table 1 (cont.)

$k=8$				$k=9$				$k=10$			
n	c	b	IV	n	c	b	IV	n	c	b	IV
45	1	44	0.7892	55	1	54	0.8144	66	1	65	0.8472
46	2	44	0.7559	56	2	54	0.7865	67	2	65	0.8234
47	2	45	0.7384	57	2	55	0.7707	68	2	66	0.8043
48	2	46	0.7230	58	2	56	0.7513	69	2	67	0.7867
49	2	47	0.7033	59	2	57	0.7381	70	2	68	0.7699
50	2	48	0.6886	60	2	58	0.7212	71	2	69	0.7523
51	2	49	0.6701	61	2	59	0.7023	72	2	70	0.7380
52	2	50	0.6550	62	2	60	0.6906	73	2	71	0.7225

Remarks

(i) The running time of our program grows roughly as k^6, where k is the number of factors, and so for $k \geq 10$ we were not able to produce as many examples and there is less chance that we have found the best designs. A 9-factor design takes about 4 minutes on one processor of a MIPS R2000A/R3000 computer.

Of course for practical applications a design that is reasonably close to the best will serve almost as well. Such designs can be obtained by stopping the program before it runs to completion, and this will be an option in the portable version of the program. Nevertheless, for publication purposes we have attempted to find the best possible designs and to present them in as attractive a manner as possible (rather than simply listing the computer-generated coordinates). We were also interested to discover what geometrical structure these designs would have. The results can be seen in Section 4.

The value of IV for any of these spherical designs is unchanged when an orthogonal transformation is applied. In particular, the columns in Tables 3-6 may be freely permuted and their signs changed. (On the other hand the signs of the rows may not be changed.) Such transformations rotate (and possibly reflect) the underlying sphere. The coordinates may also be rescaled (replacing x_1 by $\alpha_1 x_1$, x_2 by $\alpha_2 x_2$, etc.), transforming the sphere into an ellipsoid, without changing the value of IV.

(ii) With a few exceptions (such as that shown in Table 8 of Part II), our designs generally have large numbers of levels, and are intended for use in situations where a small number of runs is more important than a small number of levels. This has certainly been the case in all the applications so far where we have supplied designs – these include detergent manufacture, the construction of diamond film, catalytic converters, protein crystals, and laser welding (see Section 6). Our program can also be used in situations where some (but not all) of the variables are constrained to have two or three (or more) levels, as mentioned at the end of Section 1.

(iii) Lucas (1977) has investigated the best number of measurements to make at the center of the sphere for a 4-factor central composite design, given that the other points are held fixed. In contrast our program simultaneously optimizes the location of the points and their multiplicities.

(iv) The analysis of a computer-generated design is facilitated by computation of its *symmetry group*: this is the largest subgroup of the full k-dimensional real orthogonal group that fixes the design. We used several programs to compute symmetry groups. The graph automorphism program "Nauty" of McKay (1987) was invaluable for handling large groups.

(v) Box and Draper (1959, 1963) observe that effects from inadequacy of the response surface model ("bias error") can be greater than the effects from sampling error ("variance error"). In this paper we have concentrated on minimizing the variance error, assuming that a quadratic model is correct. In fact for a design with a minimal number of runs it is difficult to see how else to proceed. Consider a 4-factor 15-run design, where there are 15 parameters in the quadratic model but 35 in the cubic model. It is hard to see how else to take account of the 20 unknown (and hopefully small) cubic terms other than by regarding them as causing random perturbations of the measurements.

(vi) Concerning the choice of optimality criterion: minimizing the maximal value of var $\hat{y}(x)$ (G-optimality) and minimizing the average value of var $\hat{y}(x)$ appear to be the two best single measures of performance, and good arguments exist in support of each. We have chosen to use the average variance, mostly because it is differentiable. The variance dispersion graphs mentioned above provide a important check on the distribution of var $\hat{y}(x)$ over the region.

We believe that our optimality criterion, minimizing IV $=$ trace$\{M(X'X)^{-1}\}$, is definitely superior to A-optimality (minimizing trace $(X'X)^{-1}$) and D-optimality (minimizing det $(X'X)^{-1}$), since these ignore the moment matrix M. This matrix measures the effects caused by the fact that the columns of the design matrix X for a quadratic model are dependent.

(vii) "Why don't you just choose the design points at random?", we are sometimes asked. The answer is that random designs with a small number of runs behave very poorly. A sample of 120 eight-factor 46-run designs, for example, each one obtained by taking the center and 45 randomly chosen points on the sphere, had a mean IV value of 299 and variance of 1.6×10^6, the smallest value found being 7.44. In contrast, the best design that we have constructed with these parameters has IV $= 0.7559$ (see Table 1).

3 Three types of designs

We consider three types of designs.

A. One run at center, $n-1$ runs on surface of sphere.

B. c (≥ 1) runs at center, $n-c$ runs on surface of sphere.

C. n runs at points anywhere in or on the sphere.

Type C designs. To our surprise, the computer found that the best type C designs coincide (for all practical purposes) with the best type B designs.

For example, the best 3-factor design with 14 runs has three runs at a point distance 0.003622 from the center and 11 runs on the surface of the sphere, and has IV=0.4773060. This is essentially the same as the best 14-run type B design, which has three runs exactly at the center and 11 runs on the surface, and has IV=0.4773084. In cases where the configuration of surface points is sufficiently regular the computer places the repeated points in the type C design exactly at the center.

Even after decades of using computers we were impressed: the computer starts from a random arrangement of points, and unerringly converges to a configuration with repeated points close to the center (agreeing with each other to five or more decimal places) with the other points well spread out over the surface. The program discovers for itself the notion of replicated runs! Noncentral interior points never occur.

We conclude that nothing is lost by restricting attention to designs of type A and B only. (In the case of the cube, however, as we shall see in Part II, the situation is reversed and type C designs dominate.)

Type B designs. There are two questions in choosing a type B design: what is the best value of c (the number of runs at the center), and what is the best placement of the other $b = n - c$ points $\xi_1, \ldots, \xi_b$ (say) on the surface of the sphere? In the Appendix we show that these two questions are *independent*. In fact

$$\mathrm{IV} = \frac{8}{c(k+2)(k+4)} + \Phi(\xi_1, \ldots, \xi_b) \ , \tag{9}$$

where Φ is independent of c. Thus the best type B design is obtained from some type A design by increasing the number of runs at the center.

It follows from (9) that increasing the number of runs at the center from c (≥ 1) to $c+1$ reduces IV by

$$\frac{8}{c(c+1)(k+2)(k+4)} \ . \tag{10}$$

Table 1, obtained by applying (10) to the IV values for the best type A designs (see Table 2), shows the optimal choices for c and b for various values of k and n.

An example will illustrate the use of Table 1. Suppose a 3-factor design with 14 runs is required. The $k = 3$, $n = 14$ entry in Table 1 specifies that $c = 3$ runs should be made at the center, and $b = 11$ runs at points on the sphere, these points being specified in Table 3c. (This is somewhat surprising, since one might have expected that it would be better to make two runs at the center and 12 runs at the vertices of the icosahedron. Not so!)

We also see from Table 1 that in the range of this table every optimal type A design is also an optimal type B design for some value of c. (When n is increased by 1, either c or b increases by 1.) None of them are wasted!

Remark. If a large number (b) of runs are made at points distributed uniformly over the surface of the sphere, and c runs are made at the center, then one can show that

$$\mathrm{IV} = \frac{1}{(k+2)(k+4)} \left\{ \frac{8}{c} + \frac{k^2(k^2+5k+10)}{2b} \right\} . \tag{11}$$

We conjecture that the right-hand side of (11) is a lower bound to IV for any design. The integrated variance of our designs is already within 0.001 of this value for all 2-factor designs, for 3-factor designs with $b \geq 12$, 4-factor designs with $b \geq 17$, 5-factor designs with $b \geq 25$, and 6-factor designs with $b = 27$ and $b \geq 33$. We call a design *perfect* if its integrated variance is given by (11). The following designs are perfect: the center of the sphere together with the vertices of any regular polygon with at least five sides, the icosahedron, the 24-cell, and the Schläfli polytope (see below). It is remarkable that (11) gives the exact value of IV for all these designs.

In the range when (11) applies, the optimal values of c and b are

$$c = \lambda n, \qquad b = (1-\lambda)n , \tag{12}$$

where

$$\lambda = \frac{4k\sqrt{k^2+5k+10} - 16}{(k-1)(k+2)(k^2+4k+8)} , \tag{13}$$

and then

$$\mathrm{IV} = \frac{\alpha}{n} , \tag{14}$$

where

$$\alpha = \frac{(k-1)^2(k+2)(k^2+4k+8)^2}{2(k+4)\{k\sqrt{k^2+5k+10} - 4\}^2} . \tag{15}$$

To summarize this section, we have shown that the problem of finding the best designs in or on the sphere reduces to the problem of finding the best type A designs. These are described in Section 4.

4 Type A designs

Tables 3-6 and the following paragraphs give examples of our type A designs with 3 to 7 factors. Others can be obtained from the authors – please write to N. J. A. Sloane,

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Of course a 2-factor type A design is trivial: measurements are made at equally spaced points around the circle. For a type B 2-factor design, $c = 0.29n$ runs should be made at the center of the circle (from Eqs. (12), (13)).

Table 2 gives an overview, showing the variation in the minimal IV found for a type A design, as a function of the number of factors and number of runs.

Table 2. Smallest integrated prediction variance (IV) for type A designs, as a function of number of factors (k) and number of runs (n).

$k=2$		$k=3$		$k=4$		$k=5$		$k=6$	
n	IV	n	IV	n	IV	n	IV	n	IV
6	0.7333	10	0.7369	15	0.7524	21	0.7577	28	0.7333
7	0.6667	11	0.6680	16	0.6809	22	0.6964	29	0.7161
8	0.6190	12	0.6297	17	0.6475	23	0.6719	30	0.6979
9	0.5833	13	0.5929	18	0.6181	24	0.6478	31	0.6785
10	0.5556	14	0.5659	19	0.5931	25	0.6250	32	0.6573
11	0.5333	15	0.5408	20	0.5702	26	0.6034	33	0.6355
12	0.5152	16	0.5202	21	0.5500	27	0.5849	34	0.6189
13	0.5000	17	0.5018	22	0.5317	28	0.5679	35	0.6032
14	0.4872	18	0.4857	23	0.5152	29	0.5522	36	0.5887
15	0.4762	19	0.4714	24	0.5000	30	0.5375	37	0.5750
16	0.4667	20	0.4586	25	0.4861	31	0.5238	38	0.5622
17	0.4583	21	0.4471	26	0.4733	32	0.5110	39	0.5500
18	0.4510	22	0.4367	27	0.4615	33	0.4990		
19	0.4444	23	0.4273	28	0.4506				
$k=7$		$k=8$		$k=9$		$k=10$		$k=11$	
n	IV	n	IV	n	IV	n	IV	n	IV
36	0.7616	45	0.7892	55	0.8144	66	0.8472	78	0.8796
37	0.7446	46	0.7718	56	0.7987	67	0.8281	79	0.8582
38	0.7264	47	0.7564	57	0.7792	68	0.8105	80	0.8394
39	0.7084	48	0.7367	58	0.7661	69	0.7937		
40	0.6842	49	0.7219	59	0.7491	70	0.7761		
41	0.6679	50	0.7034	60	0.7303	71	0.7619		
42	0.6535	51	0.6883	61	0.7186	72	0.7463		
43	0.6378	52	0.6680	62	0.7070	73	0.7380		
$k=12$		$k=13$		$k=14$					
n	IV	n	IV	n	IV				
91	0.9090	105	0.9385	120	0.9685				
92	0.8926	106	0.9220	121	0.9340				
93	0.8709	107	0.9020	122	0.9368				
94	0.8555	108	0.8878	123	0.9172				

The coordinates given here have been rounded to four decimal places (although our computations were usually accurate to at least six decimal places).

To conserve space, parentheses are used in the tables to indicate that all cyclic shifts of the enclosed coordinates are to be included. For example (abc) is an abbreviation for the three vectors abc, bca, cab. In the 6a-factor 29-point design in Table 6a, (a^2b^3) is an abbreviation for the ten vectors $aabbb, \ldots, bbbaa$. Square brackets have no special meaning and are used to group components; thus $\pm[a\,b]$ abbreviates the two vectors $+a \; +b$ and $-a \; -b$.

In many cases, analysis of the computer-generated coordinates (especially computation of the symmetry group of the design) reveals that the design has an elegant geometrical structure. The larger the group, the more structure, and the easier it is to specify the design. A few especially interesting examples are described below, while others can be seen in the tables.

To save space and display as much of the symmetry as possible, the 4-factor 19-run design in Table 4d is described using five coordinates $x_1x_2x_3x_4x_5$ satisfying $x_1+x_2+x_3=0$; the 5-factor 23-run design in Table 5a uses coordinates $x_1 \cdots x_7$ satisfying $x_1+x_2+x_3 = x_4+x_5+x_6 = 0$; and the 6-factor 29-run design in Table 6a uses coordinates $x_1 \cdots x_7$ satisfying $x_1 + \cdots + x_5 = 0$. (To obtain standard $(r-1)$-dimensional coordinates for a vector $v = (v_1, \ldots, v_r)$ with r components adding to 0, postmultiply v by the $r \times (r-1)$ matrix $A = (a_{ij})$, where $a_{ij} = 1/\sqrt{j(j+1)}$, $1 \le i \le j \le r-1$; $a_{j+1,j} = -\sqrt{j/(j+1)}$; $a_{ij} = 0$ otherwise. This transformation preserves lengths.)

In the worst case, when the design has no symmetry (as in the 3-factor 15-run design in Table 3e) there is no shorter description than a listing of the individual points.

Examples of 3-factor designs with 10 through 15 runs are shown in Table 3 and Figure 1. The 13-run design is omitted from the table, since it may be taken to consist of the twelve vertices

$$5^{-1/4}\tau^{-1/2}(\pm\tau,\ \pm 1,\ 0)$$

($\tau = (1+\sqrt{5})/2$) of a regular icosahedron together with its center (cf. Bose and Draper, 1959, p. 1101). The figures show the convex hulls of the points.

The 10-run design (Fig. 1a) consists of the origin, an equilateral triangle on the equator and inverted equilateral triangles above and below, and has a symmetry group of order 12. The 11- and 12-run designs (Figs. 1b,1c) are much less symmetric. There are unique minimal-IV designs for $n \le 12$ and for $n = 14$, but for $n = 13$ and $n \ge 15$ there many equally good designs. For 13 runs infinitely many designs with the same IV as the icosahedral design can be obtained by taking an icosahedron with vertices at the North and South poles and rotating the northern hemisphere by an arbitrary amount. It is worth mentioning that for 15 runs a central composite design for $k = 3$, which is the union of a cube and an octahedron projected onto the sphere, is not optimal, since it has IV $= 0.5413$, compared with 0.5408

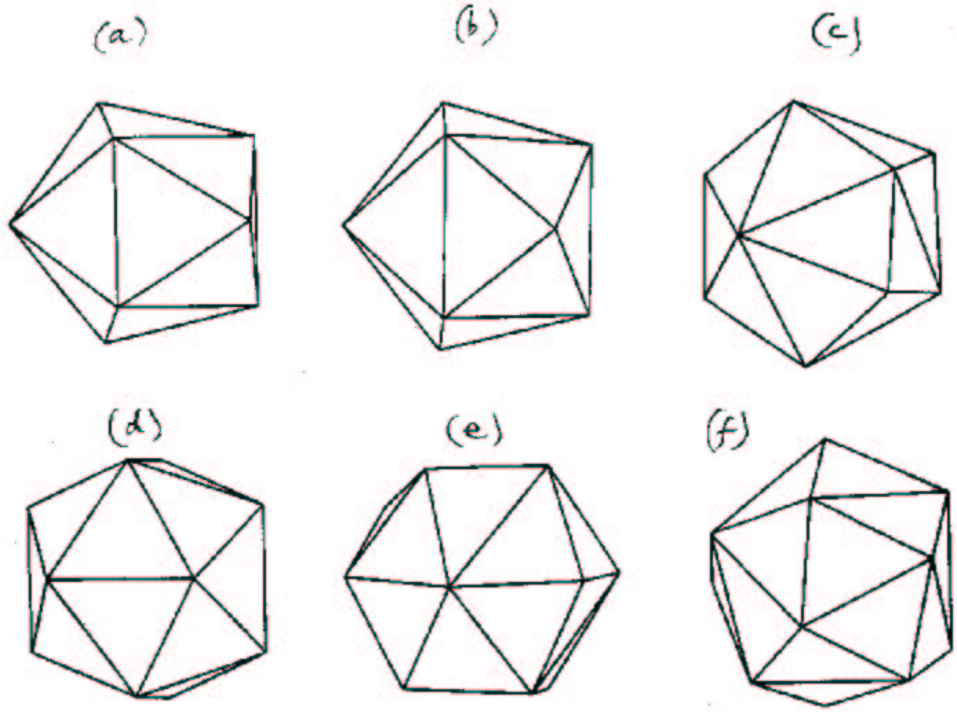

Figure 1: (a)–(f) Minimal-IV type A designs for 3 factors and 10 through 15 runs.

for the design given in Table 3e and Fig. 1f.

The best 4-factor 16-run design has a simple description by pairs of complex numbers. The design consists of the points $(0,0)$, $(\omega^r, 0)$, $(0, \omega^r)$, $2^{-1/2}(-\omega^r, -\omega^s)$, where $\omega = e^{2\pi i/3}$, $0 \le r$, $s \le 2$, and has a symmetry group of order 72. The best 4-factor 15-run design is also constructed from equilateral triangles, but is less symmetric – see Table 4a.

The designs with $k = 5$, 6 and 7 factors and the minimal number of runs (respectively 21, 28 and 36 runs) have a uniform construction, which we describe using $k+1$ coordinates, the first k of which add to zero. There is the origin, together with three layers of points, the heights of the layers being specified by the final coordinate. On the equatorial hyperplane there are $k(k-1)/2$ points of the form

$$c_1[(2-k, 2-k, 2, \ldots, 2);\ 0]\ ,$$

and above and below there are $2k$ points

$$c_2[(k-1, -1, -1, \ldots, -1);\ \pm h]\ ,$$

where $h = 3.5600$ (if $k = 5$), $h = 4.2426$ (if $k = 6$), $h = 4.8469$ (if $k = 7$), and c_1, c_2 are then determined by the condition that the sum of the squares of the coordinates is 1. In each case all permutations of the first k coordinates are included. In geometrical terms this design consists of the origin, the vertices of two regular $(k-1)$-simplices at heights $\pm h$, and on the equator the negatives of the midpoints of the edges of another regular $(k-1)$-simplex. (The 6-dimensional example is also known as the Schläfli polytope 2_{21} – see Coxeter, 1973; Conway and Sloane, 1991). Unfortunately, except in $5, 6$ and 7 dimensions, this design is inferior (from the point of view of IV) to others we have found.

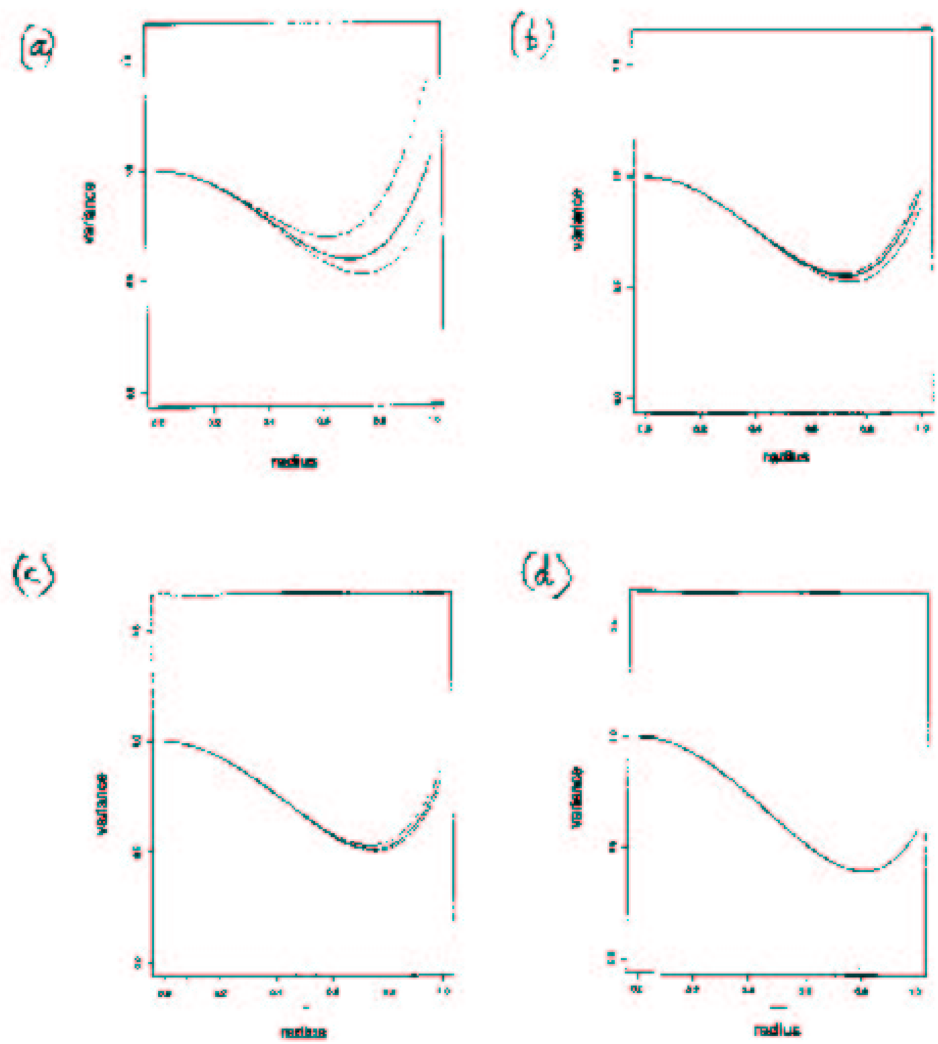

Figure 2: Variance dispersion graphs for 4-factor type A designs with (a) 15, (b) 16, (c) 18 runs, compared with that for (d) the classical 25-run central composite design projected onto the sphere.

The 5-factor, 22-run design consists of the 6 vertices of a regular five-dimensional simplex, the negatives of the 15 midpoints of the edges, and the center. The same construction yields $p+1$ points in any dimension, but except in five dimensions this is inferior to other designs.

The 6-factor 37-run design in Table 6c has been included because of its relatively large symmetry group, of order 36.

As mentioned in the previous section, we have also computed variance dispersion graphs (Giovannitti-Hensen and Myers, 1989; Vining, 1990) for many of these designs, using a program kindly supplied by Geoffrey Vining. These graphs show the lower limit, mean, and upper limit of $\frac{1}{\sigma^2} \operatorname{var} \hat{y}(x)$ (see (5)) over a spherical shell of radius r, for $0 \le r \le 1$.

Figures 2a,b,c show these graphs for our 4-factor designs with 15, 16 and 18 runs (see Table 4), and for comparison Figure 2d gives the corresponding graph for the classical 25 run design obtained by projecting the central composite design onto the sphere. As can be seen, although for the 15-run design there is wide fluctuation in the variance near the boundary of the sphere, the graphs for the designs with $n \ge 16$ runs are not too dissimilar from the classical design and are close to being rotatable.

5 Maximal volume designs on the sphere

David Doehlert also suggested to us that sets of points on the sphere enclosing as large a *volume* as possible would be useful designs for certain statistical applications. Similar design criteria have been recommended by Scheffé, 1963 and Kennard and Stone, 1969. The maximal volume problem arises in geometry, as a way of approximating a sphere by a polyhedron, and the optimal solutions were found for up to 8 points in three dimensions by Berman and Hanes (1970). We have used our methods to extend this work, obtaining what appear from numerical evidence to be maximal volume designs for up to 130 points in three dimensions and up to 24 points in four dimensions. With a few exceptions (such as the icosahedron) these maximal volume designs are different from the minimal integrated prediction variance designs described in Section 3. These results will be published elsewhere (Hardin, Sloane and Smith, 1991).

One additional result is worth mentioning here: the classical 24-run 4-dimensional central composite design, when projected onto a sphere, or in other words the vertices of the regular polytope called the 24-cell (Coxeter, 1973; Conway and Sloane, 1988) is *not* a maximal volume design. It has volume 2, whereas we have discovered a much less symmetrical design with volume 2.188188.

6 Applications

We shall describe (with the permission of the experimenters) three applications, only one of which has been completed.

(i) Keith Hovda at Chemithon Corporation in Seattle was faced with determining settings for sulfonation that would produce acceptable product (a detergent) from a particular feed stock of alkyl benzene. In a training course conducted in January 1991 by The Experiment Strategies Foundation, Hovda received one of our first designs, a 4-factor 19-run design. Without this design he would have had to use a central composite with 25 runs or a uniform shell design with 21 runs, both of which would have involved unacceptable expense. Another alternative would have been to use intuition and experience to select a smaller number of points. The designs with 15, 16, ... runs described in Table 1 would have been even less expensive than the 19-run design, but were not available at the time.

The 19-run design used was a forerunner of those given in Table 4. It was in fact formed from the best packing of 16 spherical caps on the four-dimensional sphere (Hardin, Sloane and Smith 1991) together with three runs at the center. We now know – see Table 1 – that for 19 runs it is better to take $c = 2$, $b = 17$ and use the design in Table 4c. Since the design that was used has been superseded and is not included in this paper, we do not give full details of the experimental results.

The process fed SO_3 in air and alkyl benzene into a continuous reactor held at a controlled temperature (X_1). After the reaction was complete the batch was drained into a digestor and sampled four times during digestion, at 0, 10, 35 and 120 minutes. All four times were needed to support certain reaction rate computations not of interest here.

The experimental variables are X_1, the reactor temperature (degrees Celsius); X_2, the percentage of SO_3 in the SO_3-air mixture; X_3, the digestion temperature (degrees Celsius); and X_4, the SO_3 to alkyl-benzene mole ratio. The primary response measured was Y_1, the percentage of active ingredient in the detergent, although three other responses (the percentage of H_2SO_4 and oils, and the Klett color) were also recorded.

Quadratic models were fitted to each of the responses and contour plots drawn. These showed that this feed stock would not make acceptable product at a setting within the factor limits studied. No catalyst had been used. Chemithon's client had hoped that no catalyst would be needed. This study showed that if this feed stock was to be used then a catalyst would be required. A new design has been planned to aid in selecting a catalyst.

Had Hovda used his 19 runs for a 2^4 factorial plus three runs at the center he would have been unable to compute the pure quadratic effects.

(ii) Linda S. Plano at Chrystallume Corporation in Menlo Park CA is using one of our designs to attempt to maximize the thermal conductivity of heat-spreading diamond film for AT&T. The thermal conductivity of this film is at least three times that of copper and is the highest presently known. The diamond film is made from methane and carbon monoxide using a plasma of atomic hydrogen (cf. Guyer and Koshland, 1990). There are six continuous and three discrete factors: X_1, flow rate of the reactant gases; X_2, percentage of methane; X_3, percentage of carbon monoxide; X_4, microwave power; X_5, gas pressure; X_6, spacing between substrate and plate; X_7, position of plasma ball relative to substrate; X_8, gas injection method; and X_9, low or high temperature. Here X_1 through X_6 range (after scaling) between -1 and $+1$, while X_7, X_8, X_9 are two-level factors. The primary response is thermal conductivity, as measured by Ramon spectroscopy; a secondary response Y_2 is growth rate. The model expresses Y_1 as a quadratic function of the X_i's, with 52 parameters to be determined. The design points lie in a space which is a disjoint union of eight 6-dimensional cubes. We used a more general version of the cube design program described in Part II of the paper to construct a minimal variance design for this situation. We placed seven points in each of the eight cubes, for a total of 56 runs. This experiment, like the following, has not yet been completed.

(iii) Kimberly Coombs at Corning Inc. in Corning NY is using another of our designs to study the flow behavior of a cellular ceramic substrate used in catalytic converters. There are 10 variables. Three variables, A, F and K, are different binders forming a mixture constrained by

$$A + F + K = 1 \ ,$$

with the additional requirement that

$$5A + 9F + 11K \geq 8 \ .$$

The binder level BL, lubricant level LL, mix time MT, water level W and temperature T all range (after scaling) between -1 and $+1$. Finally, the molecular weight of A, MWA, takes three values and the lubricant type LT takes two values. There are 54 parameters in the quadratic model.

We used this problem (involving a constrained mixture and a combination of continuous and discrete factors) as a test case for our general purpose program, which uses Monte Carlo methods to estimate the moment matrix M (see Eq. (7)). We produced designs with between 54 and 60 runs (taking the best of 40 tries for each number of runs). The smallest integrated variance found was as follows:

no. of runs (n)	IV
54	0.936
55	0.890
56	0.848
57	0.813
58	0.778
59	0.753
60	0.721

As can be seen, the 60-run design is appreciably better than the others, and is the one now being used.

We plan to discuss the designs in examples (ii) and (iii) in a later paper when the experiments are completed.

Acknowledgements

Our primary debt is to David Doehlert, of The Experiment Strategies Foundation in Seattle, who proposed this problem to us and has provided invaluable guidance and encouragement. We should also like to thank our colleagues John Conway, Colin Mallows and Vijayan Nair for many helpful discussions, and we are grateful to Geoffrey Vining of the Univ. of Florida for sending us a copy of his variance dispersion graph program. We also thank Kimberly Coombs, David Doehlert, Keith Hovda and Linda Plano for providing us with information about applications of these designs.

Appendix: Number of replications of center

In this Appendix we establish the expression (9) for the integrated variance of a type B design with c runs at the center and b runs at points $\xi_1, \ldots, \xi_b$ on the surface of the sphere. Let P be the matrix

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ -u' & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix} ,$$

where the blocks have the same shape as in (8). Then $P'X'XP$ has the form

$$\begin{bmatrix} c & 0 & 0 & 0 \\ 0 & Y_{11} & Y_{12} & Y_{13} \\ 0 & Y_{12}' & Y_{22} & Y_{23} \\ 0 & Y_{13}' & Y_{23}' & Y_{33} \end{bmatrix} = Q \text{ (say)} ,$$

where the Y_{ij} are independent of c. Then

$$\begin{aligned} \text{IV} &= \text{trace}\{M(X'X)^{-1}\} = \text{trace}\{MPQ^{-1}P'\} \\ &= \text{trace}\{P'MP.Q^{-1}\} = \text{trace}\{NQ^{-1}\} , \end{aligned}$$

where

$$N = P'MP = \begin{bmatrix} 8\beta & 0 & 2\beta u & 0 \\ 0 & \alpha I & 0 & 0 \\ 2\beta u' & 0 & \beta(2I+J) & 0 \\ 0 & 0 & 0 & \beta I \end{bmatrix},$$

and Eq. (9) follows.

Table 3. 3-factor type A designs (for $n = 13$ see text)

(a) $k = 3$, $n = 10$, $c = 1$, $b = 9$, IV = 0.7369

0.0000	0.0000	0.0000
1.0000	0.0000	0.0000
-0.5000	$\pm$0.8660	0.0000
-0.7018	0.0000	$\pm$0.7123
0.3509	$\pm$0.6080	$\pm$0.7123

(b) $k = 3$, $n = 11$, $c = 1$, $b = 10$, IV = 0.6680

0.0000	0.0000	0.0000
$\pm$[0.0616	-0.5312]	0.8450
$\pm$[0.8707	0.3746]	0.3186
$\pm$[0.7624	-0.6382]	0.1065
$\pm$[0.1673	0.9191]	-0.3566
$\pm$[0.5779	-0.0525]	-0.8144

(c) $k = 3$, $n = 12$, $c = 1$, $b = 11$, IV = 0.6297

0.0000	0.0000	0.0000
0.1079	0.4923	$\pm$0.8637
0.4481	-0.3268	$\pm$0.8321
-0.5166	-0.6771	$\pm$0.5240
-0.8250	0.2847	$\pm$0.4882
0.9517	0.3071	0.0000
0.0000	1.0000	0.0000
0.5255	-0.8508	0.0000

(d) $k = 3$, $n = 14$, $c = 1$, $b = 13$, IV = 0.5659

0.0000	0.0000	0.0000
$\pm$[0.0710	-0.5154]	0.8540
$\pm$[0.8468	-0.0891]	0.5245
$\pm$[0.6249	0.7463]	0.2293
$\pm$[0.5336	-0.8449]	-0.0379
$\pm$[0.8527	-0.0223]	-0.5219
$\pm$[0.1505	0.8133]	-0.5620
0.0000	0.0000	-1.0000

(e) $k = 3$, $n = 15$, $c = 1$, $b = 14$, IV = 0.5408

0.0000	0.0000	0.0000
-0.6518	0.5417	0.5308
-0.4608	0.3549	-0.8134
0.6562	-0.6539	0.3766
-0.2742	-0.4984	0.8224
-0.6426	-0.7458	0.1757
0.4094	-0.2267	-0.8837
0.2324	0.9141	0.3324
-0.0229	0.9004	-0.4344
-0.9805	0.1967	-0.0003
0.9243	0.1869	0.3328
0.8165	0.2972	-0.4950
0.3313	-0.9113	-0.2445
-0.5148	-0.5397	-0.6661
0.1773	0.1840	0.9668

Table 4. 4-factor type A designs (for $n = 16$ see text)

(a) $k = 4$, $n = 15$, $c = 1$, $b = 14$, IV= 0.7524			
0.0000	0.0000	0.0000	0.0000
0.6812	0.0000	0.7321	0.0000
-0.3406	±0.5900	0.7321	0.0000
0.9098	0.0000	-0.4151	0.0000
-0.4549	±0.7879	-0.4151	0.0000
-0.7249	0.0000	0.1044	±0.6809
0.3625	±0.6278	0.1044	±0.6809
0.0000	0.0000	-0.7853	±0.6191

(b) $k = 4$, $n = 17$, $c = 1$, $b = 16$, IV= 0.6475			
0.0000	0.0000	0.0000	0.0000
-0.3136	-0.2307	±[0.9117	-0.1314]
0.2734	-0.1764	±[0.5783	0.7481]
-0.3304	0.7766	±[0.5008	0.1920]
0.6876	0.5408	±[0.4719	0.1102]
0.7051	-0.4549	±[0.4304	-0.3327]
0.0809	0.3808	±[0.3569	-0.8492]
-0.8438	-0.0191	±[0.0596	0.5330]
-0.2093	-0.8494	±[0.0123	-0.4844]

(c) $k = 4$, $n = 18$, $c = 1$, $b = 17$, IV= 0.6181			
0.0000	0.0000	0.0000	0.0000
0.2185	-0.3304	±[0.8219	0.4093]
0.3049	0.2504	±[0.8122	-0.4298]
-0.7582	-0.3478	±[0.5283	0.1582]
-0.6046	0.6134	±[0.4873	-0.1438]
0.0305	0.5928	±[0.3736	0.7128]
0.0746	-0.8624	±[0.3012	-0.3999]
-0.3873	-0.1316	±[0.1480	-0.9004]
0.8393	-0.1840	±[0.0309	0.5106]
0.5719	0.8203	0.0000	0.0000

(d) $k = 4$, $n = 19$, $c = 1$, $b = 18$, IV= 0.5931, $x_1 + x_2 + x_3 = 0$				
0.0000	0.0000	0.0000	0.0000	0.0000
(0.7517	-0.3759	-0.3759)	0.3324	-0.2043
(-0.7496	0.3251	0.4245)	0.3324	0.2043
(0.5224	-0.1282	-0.3942)	-0.2993	0.6824
(-0.5326	0.3644	0.1682)	-0.2993	-0.6824
(0.4599	-0.4400	-0.0198)	-0.7711	0.0000
0.0000	0.0000	0.0000	1.0000	0.0000
0.0000	0.0000	0.0000	0.5648	±0.8253

Table 5. 5-factor type A designs (for $n = 21, 22$ see text)

(a) $k = 5$, $n = 23$, $c = 1$, $b = 22$, IV= 0.6719 $x_1 + x_2 + x_3 = x_4 + x_5 + x_6 = 0$						
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
(-0.5773	0.2886	0.2886)	(-0.5773	0.2886	0.2886)	0.0157
(-0.5773	0.2886	0.2886)	(0.2886	-0.5773	0.2886)	0.0157
(-0.5773	0.2886	0.2886)	(0.2886	0.2886	-0.5773)	0.0157
(0.7163	-0.3581	-0.3581)	0.0000	0.0000	0.0000	0.4800
(0.6370	-0.3185	-0.3185)	0.0000	0.0000	0.0000	-0.6256
0.0000	0.0000	0.0000	(0.7163	-0.3581	-0.3581)	0.4800
0.0000	0.0000	0.0000	(0.6370	-0.3185	-0.3185)	-0.6256
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000

(b) $k = 5$, $n = 24$, $c = 1$, $b = 23$, IV= 0.6478				
0.0000	0.0000	0.0000	0.0000	0.0000
0.0273	0.4823	0.3434	±[0.8054	0.0066]
-0.5072	-0.2455	-0.1183	±[0.7052	0.4137]
0.4006	-0.0361	-0.3423	±[0.6724	-0.5186]
0.0836	-0.5160	0.6511	±[0.5330	-0.1370]
0.6339	-0.4897	-0.0552	±[0.3739	0.4642]
-0.6896	0.2393	-0.3604	±[0.3596	-0.4560]
0.1142	0.3957	-0.6583	±[0.3589	0.5179]
-0.3456	-0.7344	-0.0274	±[0.2060	-0.5460]
0.0205	0.2377	0.4172	±[0.0367	0.8762]
0.8437	0.5117	-0.1622	0.0000	0.0000
0.6375	0.2242	0.7371	0.0000	0.0000
0.0113	-0.4868	-0.8734	0.0000	0.0000
-0.2106	0.9768	0.0379	0.0000	0.0000
-0.7296	0.0938	0.6774	0.0000	0.0000

Table 6. 6-factor type A designs (for $n = 28$ see text)

(a) $k = 6$, $n = 29$, $c = 1$, $b = 28$, IV= 0.7161, $x_1 + x_2 + x_3 + x_4 + x_5 = 0$

0.0000	0.0000^4	0.0000	0.0000
(0.5200^2	-0.3468^3)	-0.3140	0.0000
(0.6988	-0.1747^4)	0.6242	0.0000
(-0.7008	0.1752^4)	0.1792	±0.5950
0.0000	0.0000^4	-0.6091	±0.7931
0.0000	0.0000^4	-1.0000	0.0000

(b) $k = 6$, $n = 30$, $c = 1$, $b = 29$, IV= 0.6979

0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
(±0.8569	0.0000	0.0000)	-0.5127	0.0000	-0.0527
0.4554	0.4554	0.4554	0.2079	±0.5786	0.0000
(0.4554	-0.4554	-0.4554)	0.2079	±0.5786	0.0000
-0.4318	-0.4318	-0.4318	0.2044	0.0000	0.6316
(-0.4318	0.4318	0.4318)	0.2044	0.0000	0.6316
-0.4360	-0.4360	-0.4360	0.3100	0.0000	-0.5775
(-0.4360	0.4360	0.4360)	0.3100	0.0000	-0.5775
0.0000	0.0000	0.0000	0.8990	±0.4291	0.0875
0.0000	0.0000	0.0000	-0.3609	±0.8187	0.4466
0.0000	0.0000	0.0000	-0.4068	±0.5901	-0.6973
0.0000	0.0000	0.0000	-0.7090	0.0000	0.7052

(c) $k = 6$, $n = 37$, $c = 1$, $b = 36$, IV= 0.5750, $x_1 + x_2 + x_3 = x_4 + x_5 + x_6 = x_7 + x_8 + x_9 = 0$

0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
(0.8165	-0.4082	-0.4082)	(0.0000	0.0000	0.0000)	(0.0000	0.0000	0.0000)
(0.3764	-0.0132	-0.3631)	(0.1397	0.0762	-0.2159)	(-0.3302	0.6605	-0.3302)
(0.3764	-0.3631	-0.0132)	(-0.5841	0.0236	0.5605)	(0.1685	0.0336	-0.2021)
(0.2722	-0.1361	-0.1361)	(0.4386	-0.6173	0.1787)	(0.4315	-0.1699	-0.2616)
(0.2080	-0.0319	-0.1762)	(0.2517	0.2599	-0.5116)	(0.5871	-0.2072	-0.3800)
(0.2080	-0.1762	-0.0319)	(0.5098	-0.1798	-0.3300)	(-0.5585	0.1123	0.4462)
(0.0840	0.3815	-0.4654)	(0.6485	-0.3242	-0.3242)	(0.0000	0.0000	0.0000)
(-0.4285	0.2706	0.1579)	(0.2684	0.0621	-0.3304)	(0.4462	-0.5655	0.1193)
(-0.4285	0.1579	0.2706)	(0.4473	0.0489	-0.4961)	(0.0386	0.3464	-0.3850)
(-0.4654	0.3815	0.0840)	(0.0365	-0.2282	0.1917)	(0.4635	0.0986	-0.5622)
(-0.5425	0.2712	0.2712)	(-0.4692	0.5178	-0.0486)	(0.1522	-0.2048	0.0527)
(-0.5462	0.2731	0.2731)	(0.0306	0.0995	-0.1301)	(-0.5837	0.3748	0.2089)

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