Computer-Generated Minimal (and Larger) Response-Surface Designs: (II) The Cube

R. H. Hardin and N. J. A. $Sloane^1$

Mathematical Sciences Research Center AT&T Bell Laboratories 600 Mountain Avenue Murray Hill, New Jersey 07974

This paper and its companion (Part I) were written in 1991 but never published. They are now (August, 2001) being published electronically on N. J. A. Sloane's home page, http://www.research.att.com/~njas/.

ABSTRACT

Computer-generated designs in the cube are described which have the minimal (or larger) number of runs for a full quadratic response-surface design. Examples of 2-factor designs are included with 6 to 20 runs, 3-factor designs with 10 to 20 runs, 4-factor designs with 15 to 20 runs, 5-factor designs with 21 to 25 runs, 6-factor designs with 28 to 31 runs, and 7-factor designs with 36 and 39 runs. The designs were constructed by minimizing the average prediction variance, and without imposing any prior constraints – such as a central composite structure – on the locations of the points.

Key Words. Minimal designs; cube designs; quadratic response surface; computer-generated designs; minimal variance designs.

¹Present address: AT&T Shannon Labs, Florham Park, NJ 07932-0971

1 Introduction

In Part I (Hardin and Sloane, 1991) we constructed designs for a quadratic responsesurface model in which the runs are made at points in or on a sphere. The present paper uses the same techniques to construct designs in which the runs are at points (x_1, \ldots, x_k) in or on the cube defined by

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

The reader is referred to Part I for details of the method, discussion of earlier work, and applications. There are k factors,

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

unknown parameters in the quadratic response-surface model (Eq. (1) of Part I), and the design contains n runs, with $n \ge p$.

The designs are constructed by minimizing the *integrated prediction variance* (Box and Draper 1959, 1963), which in the case of a cube is given by

IV = trace{
$$M(X'X)^{-1}$$
}, (2)

where X is the $n \times p$ design matrix and

$$M = \begin{bmatrix} 1 & 0 & \frac{1}{3}u & 0\\ 0 & \frac{1}{3}I & 0 & 0\\ \frac{1}{3}u' & 0 & \frac{1}{45}(4I+5J) & 0\\ 0 & 0 & 0 & \frac{1}{9}I \end{bmatrix}$$
(3)

is now a matrix of moments of the cube (compare Eqs. (7), (8) of Part I). Again IV is scale-invariant.

Designs were constructed with the following parameters:

no. of factors
$$(k)$$
 no. of runs (n)
2 $6-20$
3 $10-20$
4 $15-22$
5 $21-31$
6 $28-42$
7 $36-54$
8 $45-67$

and in some cases with larger numbers of runs. (We have also constructed other types of designs, for example 3-factor designs for a third-order response surface, and 9-factor quadratic designs in which six factors are continuous and three are two-level factors. These will be described elsewhere.) As in Part I, numerical evidence strongly suggests that the designs obtained have values of IV that are minimal (or very close to minimal). We initially considered two types of designs: (type B) those in which at least one run is made at the center of the cube, and (type C) those where all runs can be anywhere in the cube. As discussed in Part I, for the sphere there is essentially no difference between the types. For the cube, in contrast, the best designs of type C often do not include runs at the center. This is especially true of designs with the minimal number of runs, as can be seen from Table 1. Since our main goal is to construct designs with small numbers of runs, we have therefore concentrated on type C (or unrestricted) designs, and it is these that are described in Section 2. (It is also easy to modify our program to find minimal variance designs with a pre-specified number of runs at the center of the cube.)

Table 1 contains a summary of our designs, and gives the smallest integrated prediction variance (IV) found for each number of factors (k) and runs (n), as well as the number of runs (c) made at or close to the center of the cube and the number of runs (b) near the boundary of the cube. (Points neither near the center nor near the boundary never occur – either all the coordinates of a point are small, or at least one coordinate is close to 1.)

The program itself determines the best number of runs to make at or near the center (discovering on its own the notion of replicated runs!). Note that for $k \ge 3$ factors and the minimal number of runs (as well as for 3 factors and 20 runs), *all* the runs are made at points on the boundary of the cube.

We have found no simple formula for IV for the cube, analogous to that for the sphere given in Eq. (11) of Part I.

As we mentioned in Part I, of the innumerable earlier papers on the construction of designs, the closest in spirit to ours seem to those of Box and Wilson (1971, 1974). These two papers contain several examples of designs in the k-dimensional cube, obtained by maximizing D-efficiency. As we shall see in the next section, however, there are significant differences between their designs and ours.

Other designs with small numbers of points in the k-dimensional cube have been constructed by Atkinson (1973), Draper and Lin (1990), Hartley (1959), Hoke (1974), Pesotchinsky (1975), Rechtschaffner (1967), Westlake (1965), and others, but these have almost always been found by optimizing over a restricted family of designs (central composite designs, or subsets of factorial designs or Plackett-Burman-Rao designs). Surveys of these designs can be found in Box and Draper (1987, §15.5), Lucas (1976).

In contrast, we impose no constraints on the locations of the points and let the computer find the optimal arrangement.

| | | k = 2 | 2 | | | k = 3 | 3 | | | k = 4 | 1 |
|----|---|--------------|--------|----|---|-------|--------|----|---|-------|--------|
| n | c | b | IV | n | c | b | IV | n | С | b | IV |
| 6 | 1 | 5 | 0.7657 | 10 | 0 | 10 | 0.6856 | 15 | 0 | 15 | 0.6471 |
| 7 | 2 | 5 | 0.5736 | 11 | 1 | 10 | 0.5500 | 16 | 2 | 14 | 0.5451 |
| 8 | 2 | 6 | 0.4888 | 12 | 2 | 10 | 0.4897 | 17 | 2 | 15 | 0.4766 |
| 9 | 2 | 7 | 0.4265 | 13 | 2 | 11 | 0.4488 | 18 | 3 | 15 | 0.4388 |
| 10 | 2 | 8 | 0.3659 | 14 | 3 | 11 | 0.4065 | 19 | 3 | 16 | 0.4173 |
| 11 | 3 | 8 | 0.3260 | 15 | 1 | 14 | 0.3676 | 20 | 3 | 17 | 0.3894 |
| 12 | 4 | 8 | 0.3028 | 16 | 2 | 14 | 0.3405 | | | | |
| 13 | 4 | 9 | 0.2840 | 17 | 2 | 15 | 0.3220 | | | | |
| 14 | 4 | 10 | 0.2651 | 18 | 1 | 17 | 0.3005 | | | | |
| 15 | 4 | 11 | 0.2468 | 19 | 2 | 17 | 0.2839 | | | | |
| 16 | 4 | 12 | 0.2318 | 20 | 0 | 20 | 0.2667 | | | | |
| | | $k = {$ | 5 | | | k = 6 | 3 | | | k = 7 | 7 |
| n | С | b | IV | n | c | b | IV | n | С | b | IV |
| 21 | 0 | 21 | 0.6094 | 28 | 0 | 28 | 0.5824 | 36 | 0 | 36 | 0.5496 |
| 22 | 2 | 20 | 0.5361 | 29 | 1 | 28 | 0.5114 | 37 | 1 | 36 | 0.5060 |
| 23 | 3 | 20 | 0.4832 | 30 | 3 | 27 | 0.4661 | 38 | 3 | 35 | 0.4644 |
| 24 | 3 | 21 | 0.4499 | 31 | 3 | 28 | 0.4331 | 39 | 3 | 36 | 0.4232 |
| 25 | 2 | 23 | 0.4196 | 32 | 4 | 28 | 0.4129 | 40 | 4 | 36 | 0.3959 |
| 26 | 4 | 22 | 0.3979 | 33 | 4 | 29 | 0.3985 | 41 | 5 | 36 | 0.3791 |
| | | $k = \delta$ | 3 | | | | | | | | |
| n | С | b | IV | | | | | | | | |
| 45 | 0 | 45 | 0.5413 | | | | | | | | |
| 46 | 1 | 45 | 0.5090 | | | | | | | | |
| 47 | 3 | 44 | 0.4779 | | | | | | | | |
| 48 | 4 | 44 | 0.4504 | | | | | | | | |
| 49 | 4 | 45 | 0.4359 | | | | | | | | |
| 50 | 4 | 46 | 0.3956 | | | | | | | | |

Table 1. Minimal integrated variance (IV) as a function of number of factors (k) and number of runs (n); c is the number of points near center of cube, b is number near boundary.

2 The designs

Tables 2-6 give examples of our designs. The others mentioned in Section 1 can be obtained from the authors – please write to N. J. A. Sloane, Room 2C-376, AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, New Jersey 07974; electronic mail address njas@research.att.com .

The format of the tables is the same as in Part I. Parentheses are used to indicate that the permutation defined by the parentheses is to be applied repeatedly. For example (abcd)is an abbreviation for the four vectors abcd, bcda, cdab, dabc; while (ab)(cd) abbreviates abcd, badc. 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.

The coordinates given in the tables are essentially those found by the computer, except that some reordering and sign-changing has been carried out to reveal hidden symmetries. (Permuting the coordinates and changing their signs does not affect the value of IV. On the other hand the signs of the rows may not be changed.)

Since these designs are constrained to lie in the cube, a less symmetrical region than the sphere, they are generally less symmetrical than those found in Part I, and with some exceptions are of less geometrical interest.

The 2-factor designs are described in Table 2 and Figure 1. In the figure the box specifies the region $-1 \le x_1, x_2 \le 1$, and when necessary points are labeled by the number of replications. We have not given coordinates for the larger 2-factor designs since they can be found from the figure.

| (a) $k = 1$ | $2, \ n = 6,$ | (b) k | $x = 2, \qquad n$ | = 7, | (c) $k = 2, n = 8,$ | | | |
|-------------|---------------|------------|-------------------|-------|----------------------|----------|-------|--|
| c=1, | b=5, | c=2, b=5, | | | c=2, b=6, | | | |
| IV = | 0.7657 | IV | V = 0.5736 | | IV = 0.4888 | | | |
| 1.0000 | 1.0000 | 1.0000 | 1.0000 | | $\pm [1.0000$ | 1.0000] | | |
| (1.0000 | -0.7075) | (1.0000 | -0.7969) | | (1.0000 | -0.7683) | | |
| 0.1449 | 0.1449 | 0.1479 | 0.1479 | twice | 0.0949 | 0.0949 | twice | |
| (-1.0000 | -0.2764) | (-1.0000 | -0.3105) | | (-1.0000 | 0.0039) | | |

Table 2. 2-factor designs

| (d) <i>i</i> | k=2, n | = 9, | | | |
|--------------|--------------|-------|---------------|--------------|-------|
| <i>c</i> = | = 2, b = 7 | , | (e) k | = 2, n = | = 10, |
| Г | V = 0.4265 | | c = | = 2, b = 8, | |
| 1.0000 | ± 1.0000 | | IV | r = 0.3659 | |
| 1.0000 | 0.0000 | | ± 1.0000 | ± 1.0000 | |
| -0.0442 | ± 1.0000 | | $(\pm 1.0000$ | 0.0000) | |
| -0.0447 | 0.0000 | twice | 0.0000 | 0.0000 | twice |
| -1.0000 | ± 0.8367 | | | | |

| (f) k | x = 2, n | = 13, |
|--------------|--------------|----------|
| c : | = 4, b = 9 | 9, |
| I | V = 0.2840 |) |
| ± 1.0000 | ± 1.0000 | |
| 1.0000 | 0.0000 | |
| 0.0567 | 0.0000 | 4 times |
| -0.0437 | ± 1.0000 | |
| -1.0000 | ± 0.1941 | |



Figure 1: Minimal variance 2-factor designs for 6 through 20 runs. Points are labeled with their multiplicities when these exceed one.

As can be seen from the figure, there is no uniform geometrical description of these 2-factor designs. Even the symmetry group changes with the number of runs. There is also no general rule for obtaining the best design with n+1 runs from the best with n runs. The best 10-run design is a central composite with 2 runs at the center, and the 11- and 12-run designs just add more center points; but the best 9- and 13-run designs are not of this type. The less symmetrical designs (e.g. the 13- and 16-run designs) are especially striking.

It is interesting to compare our designs with the D-optimal designs constructed by Box and Draper (1971). Their designs with two factors and from 6 to 13 runs are shown in Figure 2; the corresponding IV values (which are considerably larger than ours) are

| no. of runs | IV |
|-------------|-------|
| 6 | 0.817 |
| 7 | 0.660 |
| 8 | 0.553 |
| 9 | 0.450 |
| 10 | 0.433 |
| 11 | 0.416 |
| 12 | 0.399 |
| 13 | 0.381 |
| | |

The chief difference between their designs and ours is that theirs have multiple runs at boundary points, whereas ours have multiple runs of the central point. Our program seems to produce designs which are more intuitively appealing (although our 3-factor 20-run design mentioned below is a surprise).





Some of our 3-factor designs are shown in Table 3. Again, sometimes only a small change occurs when the number of runs increases by 1, sometimes not. For example, one can see that the 12-run design is close to the 11-run design with an extra central point. The 15-run design is a central composite, the 16-run design (omitted from the table) simply adds a central point, while the 17-run design (which is shown) has a quite different structure. The best 20-run design, a central composite consisting of the vertices of the cube and two replications of each of the midpoints of its faces, but with no interior point, is particularly interesting.

The groups of the best 3-factor designs range from cyclic groups of order 3 (for n =10, 11, etc.) to the octahedral group of order 48 (for n = 15, 16).

| (a) $k = 3$, $n = 10$, | (b) $k = 3, n = 11,$ |
|--|------------------------------------|
| c = 0, b = 10, IV = 0.6856 | c = 1, b = 10, IV = 0.5500 |
| | 1.0000 1.0000 1.0000 |
| (0.9605 - 0.1025 - 0.1025) | (1.0000 - 0.1905 - 0.1905) |
| (0.3000 - 0.1020 - 0.1020) | (0.2349 - 1.0000 - 1.0000) |
| (0.2333 - 1.0000 - 1.0000) | 0.0589 0.0589 0.0589 |
| (-1.0000 1.0000 1.0000) | (-1.0000 1.0000 1.0000) |
| ſ | |
| (c) $k = 3$, $n = 12$, | (d) $k = 3, n = 14,$ |
| c = 2, b = 10, IV = 0.4897 | c = 3, b = 11, IV = 0.4065 |
| 1,0000, 1,0000, 1,0000 | $\pm [1.0000 1.0000] -0.6585$ |
| $(1\ 0\ 0\ 0\ -0\ 3119\ -0\ 3119)$ | $\pm (1.0000 0.1423) 1.0000$ |
| (0.1685 1.0000 - 0.0119 - 0.0119) | (1.0000 - 1.0000) 0.3261 |
| (0.1085 - 1.0000 - 1.0000) | (1.0000 - 1.0000) - 1.0000 |
| (1,0000, 1,0000, 1,0000) | 0.0000 0.0000 -0.0516 3 times |
| (-1.0000 1.0000 1.0000) | 0.0000 0.0000 -1.0000 |
| Ľ | |
| Г | (f) $k = 3$, $n = 17$, |
| (e) $k = 3, n = 15,$ | c = 2, b = 15, IV = 0.3220 |
| c = 1, b = 14, IV = 0.3676 | $\pm 1.0000 \pm 1.0000 \pm 1.0000$ |
| $\pm 1.0000 \pm 1.0000 \pm 1.0000$ (3) | ± 1.0000 0.0000) 0.0030 |
| (±1.0000 0.0000 0.0000) | 0.0000 0.0000 1.0000 twice |
| 0.0000 0.0000 0.0000 | 0.0000 0.0000 -0.0512 twice |
| | 0.0000 0.0000 -1.0000 |
| L | |

Table 3. 3-factor designs

| () | g) $k = 3$, | n = 20, | |
|---------------|--------------|--------------|-------|
| c = 0 | , b = 20, | IV = 0.266 | 57 |
| ± 1.0000 | ± 1.0000 | ± 1.0000 | |
| $(\pm 1.0000$ | 0.0000 | 0.0000) | twice |

Box and Draper (1971) give a D-optimal 10-run design which is very similar to the

design in Table 3a, and has integrated variance IV = 0.708. They terminated their search for optimal designs at this point, finding that the computing problem was becoming prohibitive. For larger numbers of runs only restricted classes of designs have been studied up to now, and it is perhaps unfair to compare their IV values with ours. We give just one example. For 3 factors and 11 runs, the best design found by Lucas (1974) consists of the vertices of the cube plus three face-center (or star) points. This has IV = 0.775, considerably worse than our value of 0.550. It is worth remarking that Lucas' design does not make any measurements at the center of the cube.

Some of our 4-factor designs are shown in Table 4. The 18-run design (not shown) is close to the 17-run design with an extra central point. The groups of these designs are usually cyclic of orders 2 or 3 (although the 19-run design, not shown, has no group).

Tables 5-7 give further examples. The 6-factor 32-run design (not shown) is close to the 31-design with an extra central point. The 7-factor 36-run design in Table 7b is noteworthy for its large symmetry group, of order 21.

Finally, we mention an even more remarkable 7-factor 36-run design with just three levels that was found by one of our programs (Table 8). It was designed for fitting a quadratic response surface, but has IV = 0.672 and is inferior from that point of view to the design shown in Table 7a. The design in Table 8 has the property that every pair of columns of the design matrix X are orthogonal, although it is not an orthogonal array. Of course designs with this number of factors, runs and levels can be obtained from the orthogonal array OA(36, 13, 3, 2) of Seiden (1954) (see also Taguchi, 1987, Vol. 2, p. 1175), but these would not be suitable for fitting a quadratic response surface. It turns out that our new design is based on the binary Hamming code of length 7 (MacWilliams and Sloane, 1977, p. 24), although of course it was not constructed that way. The code consists of the eight vectors 0000000, (0010111), and the design can be seen to be a union of vectors of this form. It has a symmetry group of order 1344, generated by the permutations of PSL_2 (7) and sign-changes on Hamming codevectors. We find it remarkable that the computer discovered this design.

Table 4. 4-factor designs

| | 1 | | | | | | 1 2 | | 1 | | |
|---|--------------|--------|-----------------|------------------------|----------------|-----------------|--------------|--------------|------------|------|--------------|
| | | | (| a) k | =4, | n = | 15, | 4 1 1 | | | |
| | | 1.0 | c = 0 | $b, b = \frac{1}{100}$ | = 15, | IV = | = 0.6 | 471 | 10 | | |
| | | 1.0 | 000 | 1.00 | 00 | 1.000 | JU 24) | 1.00 | s19 | | |
| | | (1.0) | 000 | -0.47 | 34 | -0.473 | (54) | 1.00 | | | |
| | | (1.0) | 000 | -1.00 | 00 | -1.000 |)U) | -1.00 |)UU | | |
| | | (-0.4) | 082 | 1.00 | 00 | 1.000 | JU) 27) | -0.90 |)18 325 | | |
| | | (-1.0 | 000 | 0.20 | 137 171 | 0.203 | 5() 71 | 1.00 | 030 | | |
| | | -0.2 | 000 | -0.28 | 000 | -0.28 | 11 | -1.00 | | | |
| | | -1.0 | 000 | -1.00 | 100 | -1.000 | 10 | 1.00 | 000 | | |
| | | | (| D K | = 4, | n = | 10, | 451 | | | |
| | 1 | 0000 | c = 2 | $\frac{1}{0000}$ | = 14, | 1V = 0000 | = 0.5 | 401 | | | |
| | | .0000 | 1. | 0000 | 1. | 0000 | 1.0 | 2000 | | | |
| | | .0000 | 1. | 0000 | -0. | 2354 | 0.0 | 5294 | | | |
| | (1) | 0000 | -0.0 | 0207) 0000) | -1. 1 | 0000 | 0.0 | 1502 | | | |
| | | .0000 | -1.0 | 2017 | 1. 1 | 0000 | -0. | 1090 | | | |
| | | 02917 | 0. | 2917 0997 | 1. | 0000 | -1.0 | 1965 | + | 00 | |
| | -0 | 7380 | -0. | 7380 | 0. | 0024 | -0.0 | 0200 | UW | lce | |
| | -0 | 0000 | -0. | 7300 5482) | 1. 1 | 0000 | 1.0 | 0000 | | | |
| | (-1) | .0000 | 0.0 | 5402) | -1. | 2200 | -1.0 | 0000 | | | |
| | (-1 | .0000 | 0.0 | 0042) | -0. | 2099 1200 | 1.0 | 0000 | | | |
| | -1 | .0000 | -1. 1 | 0000 | 0. 1 | 4300 | -1.0 | 0000 0001 | | | |
| ſ | -1 | .0000 | -1. | | -1. | 0000 | 17 | 2021 | | | 1 |
| | | | (a — 9 | $(c) \kappa$ | = 4, | n = W_{-} | 17, - 0.4 | 766 | | | |
| ł | ⊥[1 | | c = 2 | $\frac{1}{0}, 0 = 0$ | = 10, | 1 v = | = 0.4 | 7280 | | | |
| | ل] ت 1 (1 | | 1. | 0000 | 1.0 | 0000 | 0. 1 | 1209 | | | |
| | (1 | | 0. | 0000 | -1.0 | (000) | 1. | 2254 | | | |
| | () | 1 1282 | -1. 1 | 0000 | 0.0 | (000) | 0. | 0000 | | | |
| | ((|) 0000 | -1. | 0000 | -1.0 |)000))000 | -1. 1 | 0000 | | | |
| | |) 0000 | 0. | 0000 | 0.0 | 0000 | 1. | 1918 | t | ico | |
| | |) 1283 | 0. 1 | 0000 | 0.0 |)000 | -0. 1 | 0000 | 6.00 | ice | |
| l | (-(| .4000 | 1. | $\frac{(d)}{(d)}$ | 1.0 | ,000) m – | - 20 | 0000 | | |] |
| | | | <i>c</i> — | (a) k 3 h | = 4 - 17 | n = 1 | = 20, 0' | 3804 | | | |
| | 1 (| 000 | $\frac{c}{1.0}$ | 000 | $\frac{-1}{1}$ | $\frac{1}{000}$ | - 0.0 1 (| 0004 | | | |
| | 1.0 | 0000 | 1.0 | 000 | (_1) | 0000 | 0.0 |)840) | | | |
| | (1.0 | 0000 | -0.0 | 208) | 0.0 | 0118 | 0.0 |)110 | | | |
| | (1.0) | 0000 | -1.00 | (00) | (1) | 0000 | -0.4 | 1076 | | | |
| | (1.0 | 0000 | -1 00 | 000) | (-0 4 | 4076 | 1.0 |)000) | | | |
| | 0.1 | 2251 | 0.2° | 251 | (1) | 0000 | -1.0 |)000) | | | |
| | -0.0 | 0850 | -0.0 | 850 | -0.0 | 0111 | -0.0 |)111 | 3 1 | time | \mathbf{s} |
| | (-1.0 | 0000 | 0.5' | 736) | -1.0 | 0000 | -1.0 | 0000 | 0 | | |
| | (-1.0 | 0000 | -0.0' | 762) | 1.0 | 0000 | 1.0 | 0000 | | | |
| | -1.(| 0000 | -1.0 | 000 | (-1.0 | 0000 | 0.4 | 1354) | | | |
| | | • | | | · -·· | • | | / | | | |

Table 5. 5-factor designs

| | | , | | | | | | | | 1 |
|-----|----------|-----------|------------|--------|------------|-------------------|------|-------|---------------------|-----|
| | | (8 | a) k = | = 5, | <i>n</i> = | = 21, | | | | |
| | | c = 0, | b = | : 21, | IV | = 0.60 | 94 | | | |
| | 1.000 | 00 1.000 | 00 | 1.00 | 000 | 1.00 | 00 | 1.00 | 000 | |
| | 1.000 | 00 1.000 | 00 | (-1.00 | 000 | 0.222 | 24) | 1.00 | 000 | |
| | 1.000 | 00 1.000 | 00 | -0.04 | 41 | -0.04 | 41 | -0.96 | 697 | |
| | (1.000) | 00 -0.340 |)0) | (1.00) | 000 | -0.42 | 03) | 0.05 | 553 | |
| | (1.000) | 00 -0.340 |)0) (| (-0.42 | 203 | 1.00 | (00) | 0.05 | 553 | |
| | (1.000) | 00 -1.000 |)0) | -1.00 | 000 | -1.00 | 00 | -1.00 | 000 | |
| | -0.142 | -0.141 | 19 (| (-1.00 | 000 | 0.45 | 78) | -1.00 | 000 | |
| | -0.243 | -0.243 | 36 | -1.00 | 000 | -1.00 | 00 | 0.42 | 224 | |
| | -0.541 | 13 -0.541 | 13 | 1.00 | 000 | 1.00 | 00 | 0.53 | 313 | |
| | (-1.000) | 0.775 | 58) | 1.00 | 000 | 1.00 | 00 | -1.00 | 000 | |
| | (-1.000) | 0.374 | 41) | -0.01 | 17 | -0.01 | 17 | 1.00 | 000 | |
| | -1.000 | 00 -1.000 | 00 | (1.00) | 000 | -1.00 | (00) | 1.00 | 000 | |
| | -1.000 | 00 -1.000 | 00 | -0.08 | 391 | -0.08 | 91 | -0.42 | 292 | |
| | | (1 | o) $k =$ | = 5, | <i>n</i> = | = 22, | | | | |
| | | c=2, | <i>b</i> = | 20, | IV | = 0.53 | 61 | | | |
|] | 1.0000 | 1.0000 | 1.0 | 000 | 1.(| 0000 | 1. | 0000 | | |
| (1 | 1.0000 | 1.0000 | -0.2 | 440 | -1.(| (0000 | 0. | 4046 | | |
| (1 | 1.0000 | 1.0000 | -0.9 | 647 | 0.1 | 1933) | -1. | 0000 | | |
| (1 | 1.0000 | -0.5251) | (1.0 | 000 | -0.5 | 5251) | -0. | 3460 | | |
| (| 0.0040 | 0.0040 | 0.0 | 040 | 0.0 | 0040 | -0.2 | 2369 | twi | ce |
| (-] | 1.0000 | -0.1190 | -0.0 | 687 | 0.9 | 9478) | 1. | 0000 | | |
| (-] | 1.0000 | -1.0000 | -1.0 | 000 | 0.6 | 5248) | -1. | 0000 | | |
| -] | 1.0000 | -1.0000 | -1.0 | 000 | -1.(| 0000 | 0. | 5378 | | |
| | | (| (c) k | = 5, | n = | = 25, | | | | |
| | | c = 2 | 2, b = | = 23, | IV | v = 0.4 | 196 | | | |
| | 1.0000 | 1.0000 | 1.(| 0000 | 1. | 0000 | 1 | .0000 | | |
| (| 1.0000 | 1.0000 | -1.(| 0000 | 0. | 1776) | -0 | .6060 | | |
| (| 1.0000 | 0.1907 | -0.0 |)009 | -1. | 0000) | 0 | .0812 | | |
| (| 1.0000 | 0.0041) | (1.0 | 0000 | 0. | 0041) | -1 | .0000 | | |
| (| 1.0000 | -1.0000) | (1.0 | 0000 | -1. | 0000) | 1 | .0000 | | |
| (| 1.0000 | -1.0000 | -1.(| 0000 | 0. | 3900 [°] | 1 | .0000 | | |
| - | 0.0034 | -0.0034 | -0.0 |)034 | -0. | 0034 | 1 | .0000 | | |
| _ | 0.0525 | -0.0525 | -0.0 |)525 | -0. | 0525 | 0 | .0973 | tw | ice |
| (- | 1.0000 | -1.0000 | -1.(| 0000 | 0. | 6157) | -1 | .0000 | | |
| - | 1.0000 | -1.0000 | -1.(| 0000 | -1. | 0000 | 0 | .5263 | | |

| | | (a) $k = 6$, | n = 28, | | |
|----------|----------|---------------|-----------|--------------|----------|
| | c = | 0, b=28, | IV = 0.5 | 824 | |
| 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 1.0000 | 1.0000 | -1.0000 | -1.0000 | 0.0637 | -1.0000 |
| (1.0000 | -0.2928) | (0.2928) | -1.0000) | 0.0050 | 1.0000 |
| (1.0000 | -1.0000) | (1.0000 | 0.4438) | -0.0056 | 0.1090 |
| (1.0000 | -1.0000) | (1.0000 | -1.0000) | ± 1.0000 | -1.0000 |
| (1.0000 | -1.0000) | (-1.0000 | 1.0000) | -1.0000 | 1.0000 |
| 0.9507 | 0.9507 | 0.0712 | 0.0712 | -1.0000 | 0.1869 |
| (0.9240) | -0.0902) | (-0.9433) | 0.0888) | 1.0000 | 0.1919 |
| (0.0975) | 0.8211) | (1.0000 | -0.1040) | -0.0054 | -1.0000 |
| 0.0346 | 0.0346 | 1.0000 | 1.0000 | -1.0000 | 0.9093 |
| -0.0577 | -0.0577 | -0.9782 | -0.9782 | -1.0000 | 0.1773 |
| -0.9387 | -0.9387 | -0.0235 | -0.0235 | -1.0000 | 0.8732 |
| (-1.0000 | 0.1009) | (-0.1047) | -0.8306) | 0.0018 | -1.0000 |
| (-1.0000 | 0.0089) | (1.0000 | -0.0022) | 1.0000 | 0.9181 |
| (-1.0000 | -0.4427) | (-1.0000 | 1.0000) | 0.0067 | 0.1099 |
| -1.0000 | -1.0000 | 1.0000 | 1.0000 | -0.0583 | -1.0000 |
| -1.0000 | -1.0000 | -1.0000 | -1.0000 | 1.0000 | 1.0000 |
| | | (b) $k = 6$ | , n = 29, | | |
| | c = | 1, $b = 28$ | IV = 0.5 | 5114 | |
| (1.0000) | 1.0000 | -0.0063) | (-1.0000 | 1.0000 | -1.0000) |
| (1.0000 | 1.0000 | -0.0909) | (0.0243) | -1.0000 | 0.0243) |
| (1.0000 | 1.0000 | -1.0000) | (1.0000 | 0.1631 | -1.0000) |
| (1.0000 | 1.0000 | -1.0000) | (-1.0000 | 0.1631 | 1.0000) |
| 0.8313 | 0.8313 | 0.8313 | 1.0000 | 1.0000 | 1.0000 |
| -0.0561 | -0.0561 | -0.0561 | -0.0243 | -0.0243 | -0.0243 |
| (-0.9326 | -0.9326 | 0.9618) | -1.0000 | -1.0000 | -1.0000 |
| (-1.0000 | 0.1451 | 0.1451) | (-0.0880 | -0.0880 | 1.0000) |
| (-1.0000 | 0.1414 | 0.1414) | (1.0000 | 1.0000 | -1.0000) |
| (-1.0000 | -1.0000 | 1.0000) | 1.0000 | 1.0000 | 1.0000 |
| (-1.0000 | -1.0000 | -1.0000) | (-1.0000) | -1.0000 | 0.7178) |

Table 6.6-factor designs

| () | c) $k = 6$, | n = 30, | c=3, | b = 27, 1 | IV = 0.4661 | |
|----------|---------------|---------|---------|-----------|-------------|----------|
| 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | |
| (1.0000 | 1.0000 | 1.0000 | 1.0000 | -0.6747) | -1.0000 | |
| (1.0000 | -0.0100 | -1.0000 | -1.0000 | -0.0100) | -1.0000 | |
| 0.0414 | 0.0414 | 0.0414 | 0.0414 | 0.0414 | 0.2441 | 3 times |
| (-1.0000 | 1.0000 | 1.0000 | -1.0000 | 0.0064) | 0.2178 | |
| (-1.0000 | 1.0000 | -1.0000 | -0.0115 | -0.0115) | -1.0000 | |
| (-1.0000 | -1.0000 | 0.9719 | -0.0484 | 0.9719) | 1.0000 | |
| -1.0000 | -1.0000 | -1.0000 | -1.0000 | -1.0000 | 0.7262 | |
| (| (d) $k = 6$, | n = 31, | c=3, | b = 28, | IV = 0.433 | 1 |
| 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | |
| (1.0000 | 1.0000 | 1.0000 | 1.0000 | -0.7208) | -1.0000 | |
| (1.0000 | -1.0000 | -1.0000 | 1.0000 | -0.0525) | 1.0000 | |
| 0.0921 | 0.0921 | 0.0921 | 0.0921 | 0.0921 | 0.0139 | 3 times |
| -0.0976 | -0.0976 | -0.0976 | -0.0976 | -0.0976 | 1.0000 | |
| (-1.0000 | 1.0000 | 1.0000 | -1.0000 | 0.0087) | 0.2936 | |
| (-1.0000 | 1.0000 | -1.0000 | -0.0109 | -0.0109) | -1.0000 | |
| (-1.0000 | -1.0000 | -0.0093 | 1.0000 | -0.0093) | -1.0000 | |
| -1.0000 | -1.0000 | -1.0000 | -1.0000 | -1.0000 | 0.5946 | |

Table 6.6-factor designs cont.

| 1 | | (a) $k = 7$, | n = 36, | c=0, b | 0 = 36, IV | V = 0.5496 | |
|-----|-----------|---------------|-----------|-------------|------------|------------|---------------------|
| | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| | 1.0000 | 1.0000 | 1.0000 | 1.0000 | -1.0000 | -1.0000 | -1.0000 |
| | 1.0000 | 1.0000 | 0.0502 | 0.0502 | -0.7799 | -1.0000 | 1.0000 |
| | 1.0000 | 1.0000 | -1.0000 | -1.0000 | 1.0000 | -1.0000 | 0.5606 |
| | 1.0000 | 1.0000 | -1.0000 | -1.0000 | -0.1029 | 1.0000 | -1.0000 |
| | (1.0000 | 0.3223) | (1.0000 | -0.9006) | 0.1793 | -0.2102 | -0.1615 |
| | (1.0000 | -0.0367) | (-0.4081) | 0.7365) | -1.0000 | 0.7890 | -0.1520 |
| | (1.0000 | -0.8780) | (0.3849) | 1.0000) | 0.2512 | -1.0000 | 0.1160 |
| | (1.0000 | -1.0000) | (1.0000 | -1.0000) | -1.0000 | 1.0000 | 1.0000 |
| | (1.0000 | -1.0000) | (-0.4103) | -1.0000) | -1.0000 | -0.4971 | -1.0000 |
| | (1.0000 | -1.0000) | (-1.0000 | 1.0000) | 1.0000 | 1.0000 | -1.0000 |
| | (0.8976) | -0.5034) | (-1.0000 | -0.1168) | 0.2900 | 0.1209 | 1.0000 |
| | (0.4868) | -0.6186) | (0.0523) | -1.0000) | 1.0000 | 0.9624 | -0.0262 |
| | (0.3987) | -0.9650) | (1.0000 | 0.0607) | -0.1557 | 0.8604 | -1.0000 |
| | 0.1784 | 0.1784 | 0.1006 | 0.1006 | 1.0000 | -0.7590 | -1.0000 |
| | 0.0082 | 0.0082 | 1.0000 | 1.0000 | -1.0000 | -0.1433 | 1.0000 |
| | -0.0607 | -0.0607 | -1.0000 | -1.0000 | -1.0000 | -1.0000 | 0.6340 |
| | -0.9379 | -0.9379 | -1.0000 | -1.0000 | -1.0000 | 1.0000 | -0.9818 |
| | (-1.0000) | 0.0536) | (-0.8773) | 1.0000) | 1.0000 | -1.0000 | 1.0000 |
| | (-1.0000) | -0.1711) | (1.0000 | -0.3517) | 0.1572 | 1.0000 | 0.8744 |
| | (-1.0000) | -0.3850) | (1.0000 | -1.0000) | -1.0000 | -1.0000 | -1.0000 |
| | -1.0000 | -1.0000 | 1.0000 | 1.0000 | 1.0000 | -0.0018 | -0.5782 |
| | -1.0000 | -1.0000 | -0.0644 | -0.0644 | -0.9996 | -0.3290 | 0.5602 |
| | -1.0000 | -1.0000 | -1.0000 | -1.0000 | 0.5721 | -0.9967 | -0.7783 |
| | | (b) $k = 7$, | n = 39, | c = 3, | b = 36, I | V = 0.4232 | 2 |
| (| 1.0000 | 1.0000 1.0 | 0000 1.0 | 000 1.0 | 000 1.00 | 000 -0.87 | (42) |
| (| 1.0000 | 1.0000 -1.0 | 0000 1.0 | 000 -1.0 | 000 -1.00 | 000 -0.19 | 950) |
| (| - 00000 | 1.0000 0.1 | 1911 -1.0 | 000 1.0 | 000 -1.00 | 000 -0.18 | 319) |
| (-] | L.0000 - | 1.0000 -1.0 | 0000 1.0 | 000 0.1 | 911 1.00 | 000 -0.18 | 319) |
| (-] | 1.0000 | 1.0000 1.0 |)000 -1.0 | 000 -1.0 | 000 0.19 | 011 -0.18 | 319) |
| -1 | L.0000 - | 1.0000 -1.0 | 0000 -1.0 | 000 -1.0 | 000 -1.00 | 000 -1.00 | 000 |
| (|).0442 | 0.0442 0.0 |)442 0.0 | 0.0442 0.04 | 442 0.04 | 142 0.04 | $142 3 	ext{ tin}$ |

Table 7. 7-factor designs

Table 8. A 7-factor 36-run design with 3 levels; IV=0.6719

| 1 | 1 | 1 | 1 | 1 | 1 | 1 |
|-----|----|----|----|----|----|-----|
| (1 | 1 | -1 | 1 | -1 | -1 | -1) |
| (1 | 1 | 0 | -1 | 0 | 0 | 0) |
| (1 | -1 | 0 | 1 | 0 | 0 | 0) |
| (-1 | 1 | 0 | 1 | 0 | 0 | 0) |
| (-1 | -1 | 0 | -1 | 0 | 0 | 0) |

Acknowledgments

We thank Indra Chakravarti, David Doehlert, Anne Freeny, James Lucas, Colin Mallows and Vijay Nair for very helpful comments on the two manuscripts.

References

- Atkinson, A. C. (1973), "Multifactor Second Order Designs for Cuboidal Regions," *Biometrika*, 60, 15-19.
- Box, G. E. P., and Draper, R. N. (1959), "A Basis for the Selection of a Response Surface Design," J. American Statistical Association, 54, 622-654.
- Box, G. E. P., and Draper, R. N. (1963), "The Choice of a Second Order Rotatable Design," *Biometrika*, 50, 335-352.
- Box, G. E. P. and Draper, N. R. (1987), Empirical Model-Building and Response Surfaces, New York: Wiley.
- Box, M. J., and Draper, N. R. (1971), "Factorial Designs, the |X'X| Criterion, and Some Related Matters," *Technometrics*, 13, 731-742.
- Box, M. J., and Draper, N. R. (1974), "On Minimum-Point Second-Order Designs," Technometrics, 16, 613-616.
- Draper, N. R., and Lin, D. K. J. (1990), "Small Response-Surface Designs," Technometrics, 32, 187-194.
- Hardin, R. H., and Sloane, N. J. A. (1991), "Computer-Generated Minimal (and Larger) Response-Surface Designs: (I) The Sphere", preprint.
- Hartley, H. O. (1959), "Smallest Composite Designs for Quadratic Response Surfaces," *Biometrics*, 15, 611-624.
- Hoke, A. T. (1974), "Economical Second-Order Designs Based on Irregular Fractions of the 3ⁿ Factorial," *Technometrics*, 16, 375-384.
- Lucas, J. M. (1976), "Which Response Surface Design is Best," Technometrics, 18, 411-417.
- MacWilliams, F. J., and Sloane, N. J. A. (1977), *The Theory of Error-Correcting Codes*, Amsterdam: North-Holland.
- Pesotchinsky, L. L. (1975), "D-Optimum and Quasi-D-Optimum Second-Order Designs on a Cube," *Biometrika*, 62, 335-340.
- Rechtschaffner, R. L. (1967), "Saturated Fractions of 2^n and 3^n Factorial Designs," *Technometrics*, 9, 569-575.
- Seiden, E. (1954), "On the Problem of Construction of Orthogonal Arrays," Ann. Math. Stat., 25, 151-156.
- Taguchi, G. (1987), System of Experimental Design, White Plains: UNIPUB/Krause.
- Westlake, W. J. (1965), "Composite Designs Based on Irregular Fractions of Factorials," *Biometrics*, 21, 324-336.