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FURTHER SECOND ORDER ROTATABLE DESIGNS

BY NORMAN R. DRAPER[1] AND AGNES M. HERZBERG[2]

University of Wisconsin and Imperial College, London

0. Summary. This note provides some new second order rotatable designs. The method of construction used is an extension of one introduced by Bose and Draper (1959). Further extensions of the method are briefly suggested.

1. Introduction. The technique of fitting a response surface to data resulting from experiments has gained wider and wider acceptance since its introduction by G. E. P. Box and co-authors in the early 1950's. A comprehensive bibliography of response surface methodology is given by Hill and Hunter (1966). A great many response surface designs are now available. Some of these (like the original 'cube' plus 'star' type designs given by Box, see for example Cochran and Cox, (1957) or Davies, (1956)) are frequently used and are sensible from a practical viewpoint. Other designs are of theoretical interest only at the moment and the chance of their being used in an experimental investigation is currently small, due to the number of points involved and/or the multiplicity of levels. However, developments may make the latter useful at some future time, just as large two-level fractional factorial designs suddenly became useful in coding theory.

A particularly useful type of response surface design is the *rotatable design* which, once the scales and the "center" of the experimental variables have been determined, provides equal information in all directions at any specified distance from the center of experimentation. While rotatable designs are by no means essential, it is generally better to use a rotatable design rather than a non-rotatable design, all things being otherwise equal.

The conditions for second order rotatability are given by Bose and Draper ((1959), pp. 1097–8, Section 1) and we shall follow the notation and definitions of that section. In Section 7 of the same paper (p. 1108) a 16 point second order design class was obtained by combining a set consisting of the 12 points of the form $(\pm x, \pm y, \pm z)$ and cyclic permutations for which $x_{1u}x_{2u}x_{3u} = -xyz$, with the four points of a half replicate of the 2^3 factorial $(\pm a, \pm a, \pm a)$, where $x_{1u}x_{2u}x_{3u} = a^3$. In Section 2, this method will be extended to obtain further rotatable designs.

Choosing the number of center points. The variance function for a second order rotatable design takes the form $V(r) = P + Tr^2 + Rr^4$, where $r^2 = x_1^2 + x_2^2 +$

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$\cdots + x_k^2$,

$$P = 2(k+2)\lambda_4^2/a, \qquad T = 2\lambda_4(k+2)(\lambda_4 - \lambda_2^2)/a\lambda_2,$$

$$R = \{(k+1)\lambda_4 - (k-1)\lambda_2^2\}/a, \qquad a = 2N\lambda_4\{(k+2)\lambda_4 - k\lambda_2^2\}.$$

If, following Box and Hunter (1957), we choose the number of center points so that $V(0) = V(1)$ when $\lambda_2 = 1$, we obtain, for the total number of points in the design,

$$(1.1) \qquad N = \{k + 3 + (9k^2 + 14k - 7)^{\frac{1}{2}}\}/\{4\alpha(k+2)\},$$

where α is such that $N\alpha$ is the value of λ_4/λ_2^2 for the design (with $\lambda_2 = 1$). This formula can be used to determine the number of center points to be added. Once this number is determined, the condition $\lambda_2 = 1$ can be relaxed, and the design can be used with any desired scaling.

2. Rotatable designs.

Fractional 'cubes' plus 'star' type. Useful designs which are really variations of the basic cube plus star design can be constructed by extending the technique mentioned above. Let us denote the full 2^k factorial design or 'cube' $(\pm a, \pm a, \cdots, \pm a)$ by $S(a, a, \cdots, a)$ and the $2k$-point 'star' $(\pm p, 0, \cdots, 0), \cdots, (0, 0, \cdots, \pm p)$ by $S(p, 0, \cdots, 0)$. We shall also use the notation of Box and Hunter (1961) so that, for example, "$\frac{1}{2}S(a, a, a)$ with $I = 123$" will denote the half fraction of a 2^3 design such that $\sum x_{1u}x_{2u}x_{3u} = 4a^3$. (All summations are over $u = 1, 2, \cdots, n$.) Rotatable designs can be formed as follows.

$k = 3$: Consider the point sets:

$$(2.1) \qquad \tfrac{1}{2}S(a, a, a), \quad \text{with} \quad I = -123 \text{ (4 points)},$$

$$(2.2) \qquad \tfrac{1}{2}S(c, c, c), \quad \text{with} \quad I = 123 \quad \text{(4 points)},$$

$$(2.3) \qquad S(p, 0, 0), \qquad \text{(6 points)}.$$

If we attempt to combine these three sets to form a second order rotatable design we see that, to make $\sum x_{1u}x_{2u}x_{3u} = 0$, we must have $c = a$ and thus we obtain the standard 'cube' plus 'star' design. However, if we combine *two* set (2.1)'s with one each of sets (2.2) and (2.3), then we obtain a rotatable design of second order with 18 points where

$$c^3 = 2a^3, \qquad p^4 = 8(1 + 2^{\frac{1}{3}})a^4.$$

A design of this type can be valuable when a sequential design is required, i.e., one which can be performed in two parts. After the first part is performed, a first order surface is fitted and, if this is not satisfactory, additional runs are made and a second order surface is fitted. The design can be performed as follows:

Reference	Point sets used in	
	Part 1	Part 2
A	(2.1), (2.1)-8 points	(2.2), (2.3)-10 points
B	(2.1)-4 points	(2.1), (2.2), (2.3)-14 points
C	(2.1), (2.2)-8 points	(2.1), (2.3)-10 points

In A, the replicated points in part 1 allow an internal estimate of error to be made and this can be used to check both first and second order surfaces. In this case it must be assumed that no block effects occur between parts 1 and 2. In both B and C the replicated points occur in each part thus enabling a direct check on block effects to be made. The observations in one part can then be adjusted for any block effects which exist and the second order fitting carried out. These rotatable designs thus provide an alternative, with four more points, to the orthogonally blocked design (Cochran and Cox, (1957)) which is not rotatable. Now for our design, $\lambda_4/\lambda_2^2 = N(0.034616)$, which equals 0.623088 when $N = 18$. Since $k/(k + 2) = 0.6$, the addition of a few center points would be sensible; equation (1.1) suggests six center points.

$k = 4$: Consider the point sets

(2.4) $\frac{1}{2}S(a, a, a, a)$, with $I = -1234$ (8 points),

(2.5) $\frac{1}{2}S(c, c, c, c)$, with $I = 1234$ (8 points),

(2.6) $S(p, 0, 0, 0)$, (8 points).

Combining two set (2.4)'s with (2.5) ($c^4 = 2a^4$) and (2.6) ($p^4 = 32a^4$), we obtain a second order rotatable design, with similar properties to the $k = 3$ case design above, containing 32 points. Since $\lambda_4/\lambda_2^2 = N(0.021447)$ which equals 0.686304 when $N = 32$, and since $k/(k + 2) = \frac{2}{3}$, the addition of a few center points would be sensible; equation (1.1) suggests nine center points.

$k = 5$: Although the method used above for $k = 2, 3$ still applies when $k \geqq 5$, there is no point using it since half-fractions ($5 \leqq k \leqq 7$) and quarter fractions ($k \geqq 8$) are usable alone with $S(p, 0, \cdots, 0)$ (Box and Hunter, (1957)). In fact for $k = 5$, no simple design of the above type (with reasonably few points) appears possible.

$k = 6$: When $k = 6$, however, the additional factor gives us the possibility of an extension of the method above, employing greater fractionation. Consider the point sets

(2.7) $\frac{1}{4}S(a, a, \cdots, a)$ with $I = -123 = -456 (= 123456)$ (16 points),

(2.8) $\frac{1}{4}S(c, c, \cdots, c)$ with $I = 123 = 456 (= 123456)$ (16 points),

(2.9) $S(p, 0, \cdots, 0)$ (12 points).

We can now combine two set (2.7)'s with one set (2.8) ($c^3 = 2a^3$) and one set

(2.9) ($p^4 = 32(1 + 2^{\frac{1}{2}})a^4$) to obtain a second order rotatable design containing 60 points. The design can be blocked as before. For this design, $\lambda_4/\lambda_2^2 = N(0.0130624)$ which equals 0.783744 when $N = 60$. Since $k/(k + 2) = 0.75$, the addition of a few center points would be sensible; equation (1.1) suggests nine center points.

$k = 7$: A design similar to the $k = 6$ case can be obtained, using $I = -123 = -4567$, etc.

$k = 8$: At this point, the quarter fraction is, together with $S(p, 0, \cdots, 0)$, adequate for a design, and so further fractionation must be sought. Designs *can* be formed in this manner but they contain a fairly large number of points. For $k = 8$, no simple design of the above type (with reasonably few points) appears possible.

$k = 9$: Again the extra factor helps further fractionation.
Consider

(2.10) $\frac{1}{8}S(a, a, \cdots, a)$ with $I = -123 = -456 = -789$ (64 points),

(2.11) $\frac{1}{8}S(c, c, \cdots, c)$ with $I = 123 = 456 = 789$ (64 points),

(2.12) $S(p, 0, \cdots, 0)$ (18 points).

Two (2.10)'s, a (2.11) with $c^3 = 2a^3$, and a (2.12) with $p^4 = 128(1 + 2^{\frac{1}{3}})a^4$ give a 210 point rotatable design. Here $\lambda_4/\lambda_2^2 = N(0.00416275)$ which equals 0.874178 when $N = 210$. Since $k/(k + 2) = 0.818182$, the addition of a few center points might be sensible; equation (1.1) suggests fifteen center points.

Designs of similar type can also be constructed for larger k.

Fractionation applied to cyclical group point sets. The following example is for $k = 5$. One of the cyclical point sets used by Thaker (1962), p. 113, consists of the 40 points $(0, \pm b, \pm c, 0, \pm e)$ plus cyclic permutations. Suppose we select only half of these in such a way that the product of the non-zero elements is $+bce$ and then add points of the form $(0, \pm f, \pm f, 0, \pm f)$ plus cyclic permutations, such that the product of the non-zero elements is $-f^3$. The question is whether b, c, e, and f can be chosen to give a 40 point second order rotatable design. Write $b^2 = uf^2$, $c^2 = vf^2$, $e^2 = wf^2$. There are two types of sums of products $\sum_u x_{iu}^2 x_{ju}^2$. They are equal if $uv = vw + uw + 1$. If all third order sums of products are to be zero, then we must have $bce = f^3$, or $(uvw)^{\frac{1}{2}} = uvw = 1$. Furthermore the condition $\sum x_{iu}^4 = 3 \sum x_{iu}^2 x_{ju}^2$ $(i \neq j)$ leads to the equation $u^2 + v^2 + w^2 = 3uv$. It follows that u, v, and w are the solutions of the cubic equation $x^3 - Ax^2 + Bx - 1 = 0$, where $A = (7/w - 2)^{\frac{1}{2}}$, $B = (2/w - 1)$. But since $x = w$ is a solution, we must have $w^6 - 5w^3 + w^2 - 2w + 1 = 0$ which has two real positive solutions. Only one of these leads to $u \geqq 0$, $v \geqq 0$, and so the single solution is $u = 2.479977$, $v = 0.978087$, $w = 0.412264$. Center points would be strictly required only if the two point sets have the same radii, i.e. if $w = 7/11$ which is not the case. In fact $\lambda_4/\lambda_2^2 = N(0.018144)$. When $n = 40$, this equals 0.725760. Since $k/(k + 2) = 0.714$, the addition of some center points would probably be sensible; equation (1.1) suggests nine center points.

(We note in passing that "Design 1" given by Thaker (1962), p. 113, contains a misprint. The correct value of s appears to be $s = 3.369220$.)

For a second example consider the $k = 4$ case and the point sets (i) $(\pm a, \pm b, 0, \pm d)$ plus cyclic permutations and such that all non-zero triple products $= abd$; (ii) $(\pm f, \pm f, 0, \pm f)$ plus cyclic permutations and such that all non-zero triple products $= -f^3$. If we let $a^2 = tf^2$, $b^2 = uf^2$, $d^2 = vf^2$, the conditions for obtaining a second order rotatable arrangement imply that $tu + tv = 2uv$, $tuv = 1$, and $t^2 + u^2 + w^2 = 6uv + 3$. It follows that t, u, v, are the roots of $x^3 - Ax^2 + Bx - 1 = 0$, where $A = (3 + 12/t)^{\frac{1}{2}}$ and $B = 3/t$. Since t is a solution, $t^6 - 3t^4 - 8t^3 + 4 = 0$ which yields two real positive solutions, only one of which provides $u \geqq 0$, $v \geqq 0$. The single solution is $t = 0.741366$, $u = 3.219947$, $v = 0.418908$. Here $\lambda_4/\lambda_2^2 = N(0.0215620)$; when $N = 32$, this equals 0.689984. Since $k/(k + 2) = \frac{2}{3}$, the addition of some center points might be sensible; equation (1.1) suggests eight center points.

Further designs of this type can be constructed. For example, infinite classes of 4 factor, 40 point second order rotatable designs have been constructed by Draper and McGregor (1967) using the following point sets

1. $(\pm x, \pm y, \pm z, \pm w)$ plus cyclic permutations, such that

$$\sum x_{1u}x_{2u}x_{3u}x_{4u} = 32xyzw,$$

2. $\frac{1}{2}S(b, b, b, b)$ such that

$$\sum x_{1u}x_{2u}x_{3u}x_{4u} = -8b^4.$$

The equations which arose were solved by using a nonlinear estimation program

Further extensions. It is possible to extend this method further by using deeper fractionation and/or interlocked compensations as was done by Draper and Stoneman (1968) for a slightly different purpose. The difficulty in further extensions is the usual one, that of keeping the number of points reasonable, say about twice the number of coefficients to be estimated or fewer. While we have been able to construct second order rotatable designs in this manner we have, so far, found none we would consider to have a reasonable number of points.

Other second order rotatable designs in the literature. Many other methods of constructing second order rotatable designs have been given since the paper of Box and Hunter (1957) which contained the basic 'cube' plus 'star' method of construction, already mentioned. Box and Behnken (1960a) built up second order rotatable designs from first order rotatable designs with $k + 1$ points. The number of points in such designs is less than or equal to $2^{k+1} - 2 + n_0$, where n_0 denotes the number of center points. Thaker (1962), as discussed earlier, made use of a cyclic group of points. His designs require $2^{k-p}\, k + n_0$ points, where p denotes the largest fraction so that all the second order moment conditions hold except for $\sum x_{iu}^4 = 3 \sum x_{iu}^2 x_{ju}^2$, $i \neq j$, the summations being over u. Several authors (for example Box and Behnken, (1960b); Das, (1961) and Das and Narasimham, (1962)) have constructed rotatable designs through balanced and doubly balanced incomplete block designs.

Table 1 shows, for comparison purposes, the *minimum* number of points so

TABLE 1

A comparison with second order rotatable designs containing a minimum number of points

No. of factors	No. of coefficients to be estimated	No. of points in our designs	Minimum no. of design points	References for previous column
3	10	18	14	CS
4	15	32	$24 + n_0$	CS or S$(a, a, 0, 0)$
5	21	40	26	CS
6	28	60	44	CS
7	36	108	$56 + n_0$	Box and Behnken (1960b)
8	45	—	80	CS
9	55	210	$120 + n_0$	Box and Behnken (1960b)

n_0 denotes that points *must* be added at the center.
CS is the smallest 'cube' + 'star' type design.

far found to be needed for second order rotatable designs for up to 9 factors. The designs given here require more points than the minimum, but possess the properties mentioned earlier. Many designs in the literature require considerably more points, however.

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