A METHOD FOR THE CONSTRUCTION OF SECOND ORDER ROTATABLE DESIGNS IN k DIMENSIONS[1]

By Agnes M. Herzberg[2]

University of Saskatchewan

1. Introduction. Box and Hunter (1957) gave conditions under which designs for the exploration of response surfaces would be rotatable. Since the appearance of their paper, many methods have been developed for constructing rotatable designs. In particular, Draper (1960) presented the following method of constructing a second order rotatable design in k dimensions from a second order rotatable design in $(k - 1)$ dimensions.

If the N' points

$$(x_{1u}, x_{2u}, \cdots, x_{(k-1)u}), \qquad u = 1, 2, \cdots, N', \tag{1}$$

form a second order rotatable arrangement in $(k - 1)$ dimensions, that is, the points of (1) are such that

$$\textstyle\sum_{u=1}^{N} x_{iu}^2 = A \neq N', \qquad \sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = 3C, \tag{2}$$

where $(i \neq j)$ $i, j = 1, 2, \cdots, (k - 1)$ and all other sums of powers and products up to and including order four are zero, then the point sets

$$\begin{array}{llllll} (x_{1u}, & x_{2u}, & \cdots, & x_{(k-1)u}, & \pm b), & \qquad u = 1, 2, \cdots, N', \\ (\ 0, & 0, & \cdots, & 0, & \pm p), & \\ (\ 0, & 0, & \cdots, & 0, & \pm q), & \end{array} \tag{3}$$

where

$$b^2 = C/A,$$

$$p^2, q^2 = \{(A^2 - N'C) \pm [2C(3A^2 - N'C) - (A^2 - N'C)^2]^{\frac{1}{2}}\}/2A,$$

form a second order rotatable arrangement in k dimensions. The number of points in the derived design will be $N = 2N' + 4 + n_0$, where n_0 denotes the number of center points needed to make the arrangement into a design. Since p^2 and q^2 must be real and non-negative, it is required that

$$1 \leqq \phi \leqq 2, \qquad \text{where} \qquad \phi = (A^2 - N'C)^2/C(3A^2 - N'C). \tag{4}$$

Therefore, it is possible to form second order rotatable designs in k dimensions

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[2] Now at Imperial College, University of London.

from only those second order rotatable arrangements in $(k-1)$ dimensions which satisfy (4).

In what follows, we demonstrate another method for constructing second order rotatable designs in k dimensions from second order rotatable designs in $(k-1)$ dimensions.

2. Method of construction. Let $S(x_1, x_2, \cdots, x_k)$ be the set of all permutations of $(\pm x_1, \pm x_2, \cdots, \pm x_k)$, and $U(x_1, x_2, \cdots, x_k)$ be any one of the smallest 2^{-p} fractions of a 2^k factorial design such that

$$\sum_u x_{iu}^{\alpha_i} x_{ju}^{\alpha_j} x_{lu}^{\alpha_l} x_{mu}^{\alpha_m} = 0,$$

where

(i) $i, j, l, m = 1, 2, \cdots, k$ and are distinct,
(ii) at least one of $\alpha_i, \alpha_j, \alpha_l, \alpha_m$ is odd and $0 < \alpha_i + \alpha_j + \alpha_l + \alpha_m \leqq 4$, and
(iii) the summation is taken over all the points of $U(x_1, x_2, \cdots, x_k)$.

We consider the N' points of (1) and use the notation of (2). To each of the points of (1) is added a kth coordinate $x_{ku} = 0$, forming the N' points

$$(5) \qquad (x_{1u}, x_{2u}, \cdots, x_{(k-1)u}, 0), \qquad u = 1, 2, \cdots, N'.$$

To these points are added the k dimensional point sets

$$(6) \qquad \begin{array}{ll} (0, 0, \cdots, 0, \pm a), & (0, 0, \cdots, 0, \pm b), \\ (S(v, 0, \cdots, 0), 0), & U(r, r, \cdots, r, s). \end{array}$$

The values of a, b, r, s and v are then determined so that (5) and (6) will form a second order rotatable arrangement in k dimensions. The number of points in the derived design will be $N = N' + 2^{k-p} + 2k + 2 + n_0$, where n_0 denotes the number of center points needed to make the arrangement into a design. For the new set of points, the following relations hold:

$$(7) \qquad \begin{aligned} \sum_{u=1}^N x_{iu}^2 &= A + 2^{k-p}r^2 + 2v^2, & 1 \leqq i \leqq k-1, \\ \sum_{u=1}^N x_{iu}^4 &= 3C + 2^{k-p}r^4 + 2v^4, & 1 \leqq i \leqq k-1, \\ \sum_{u=1}^N x_{iu}^2 x_{ju}^2 &= C + 2^{k-p}r^4, & 1 \leqq i \neq j \leqq k-1, \\ \sum_{u=1}^N x_{ku}^2 &= 2^{k-p}s^2 + 2a^2 + 2b^2, & \\ \sum_{u=1}^N x_{ku}^4 &= 2^{k-p}s^4 + 2a^4 + 2b^4, & \\ \sum_{u=1}^N x_{iu}^2 x_{ku}^2 &= 2^{k-p}r^2 s^2, & 1 \leqq i \leqq k-1, \end{aligned}$$

and all other sums of powers and products up to and including order four are zero. In order to satisfy the requirements for a second order rotatable arrangement

$$(8) \qquad 2a^2 + 2b^2 + 2^{k-p}s^2 - 2v^2 - 2^{k-p}r^2 = A,$$

$$(9) \qquad 2a^4 + 2b^4 + 2^{k-p}s^4 - 2v^4 - 2^{k-p}r^4 = 3C,$$

$$2^{k-p}r^2s^2 - 2^{k-p}r^4 = C, \tag{10}$$

$$2a^4 + 2b^4 + 2^{k-p}s^4 = 3\cdot 2^{k-p}r^2s^2. \tag{11}$$

Let

$$a^2 = tr^2, \quad b^2 = wr^2, \quad s^2 = ur^2, \quad v^2 = qr^2, \tag{12}$$
$$A = A'r^2, \quad C = C'r^4.$$

Then (8), (9), (10) and (11) become

$$2t + 2w + 2^{k-p}u - 2q - 2^{k-p} = A', \tag{13}$$

$$2t^2 + 2w^2 + 2^{k-p}u^2 - 2q^2 - 2^{k-p} = 3C', \tag{14}$$

$$2^{k-p}u - 2^{k-p} = C', \tag{15}$$

$$2t^2 + 2w^2 + 2^{k-p}u^2 = 3\cdot 2^{k-p}u. \tag{16}$$

Solving (13), (14), (15) and (16), we obtain

$$u = (C' + 2^{k-p})/2^{k-p}, \tag{17}$$

$$q = 2^{(k-p)/2}, \tag{18}$$

$$\begin{aligned} t, w = \{(A' - C' + 2^{(k-p+2)/2}) \\ \pm [4(3C' + 3\cdot 2^{k-p} - 2^{p-k}(C' + 2^{k-p})^2) \\ - (A' - C' + 2^{(k-p+2)/2})^2]^{\frac{1}{2}}\}/4. \end{aligned} \tag{19}$$

For t and w to be real, it is required that

$$\begin{aligned} 2^{2k-2p+2}r^8 - 2^{(3k-3p+4)/2}Ar^6 + \{(2^{k-p+2} + 2^{(3k-3p+4)/2})C - 2^{k-p}A^2\}r^4 \\ + 2^{k-p+1}ACr^2 - (2^2 + 2^{k-p})C^2 \geqq 0. \end{aligned} \tag{20}$$

For t and w to be positive, it is required that

$$\begin{aligned} 2^{(3k-3p+4)/2}Ar^6 + \{2^{k-p}A^2 - (2^{k-p+1} + 2^{(3k-3p+4)/2})C\}r^4 - 2^{k-p+1}ACr^2 \\ + (2 + 2^{k-p})C^2 \geqq 0. \end{aligned} \tag{21}$$

Equations (20) and (21) can always be satisfied for a sufficiently large r. Once r has been selected, A' and C' are determined; and therefore, u, t and w can be found. Then a, b, s and v can be obtained.

3. Interpretation. Both of the methods described above for constructing a second order rotatable design in k dimensions from a second order rotatable design in $(k - 1)$ dimensions have their advantages. Draper's method has the advantage that the number of points required is usually fewer than the number required in the author's method. However, Draper's method fails when (4) is not satisfied, whereas the author's method works in all cases. Therefore, when both methods are applicable, that method should be used which requires the least number of points. These methods are useful not only in the construction of second order rotatable designs, but also in the performance of experiments. If, after performing a second order rotatable design in $(k - 1)$ dimensions, the experimenter feels that another factor should have been included in the analysis, he can then proceed by the methods described above without discarding the original results.

4. Example. Consider the following second order rotatable design in five dimensions:

$$S(2^{3/4}d,\ 2^{3/4}d,\ 0,\ 0,\ 0),\quad U(d,\ d,\ d,\ d,\ d). \tag{22}$$

Here $A = 16(2\cdot 2^{\frac{1}{2}} + 1)\, d^2$, $C = 48d^4$, $N' = 56$ and $\phi = 2.7$. Since $\phi > 2$, Draper's method cannot be used. 102 points are required for the author's method. In order to satisfy (20) and (21), we let $r = 4d$. Then $A' = 2\cdot 2^{\frac{1}{2}} + 1$ and $C' = \frac{3}{16}$. From (17), (18) and (19), $u = 1.0057$, $q = 5.6568$, $t = 2.2733$ and $w = 5.1890$. Substituting these values into (12), we find that $a^2 = 36.3724d^2b^2 = 83.0236d^2$, $s^2 = 16.0912d^2$ and $v^2 = 90.5088d^2$. Therefore, $a = 6.04d, b = 9.11d$, $s = 4.01d$ and $v = 9.51d$. Therefore, we have a second order rotatable design in six dimensions given by

$$\begin{array}{l} (S(2^{3/4}d,\ 2^{3/4}d,\ 0,\ 0,\ 0),\ 0), \\ (U(\ \ d,\ \ \ d,\ d,\ d,\ d),\ 0), \\ (\ \ \ \ 0,\ \ \ \ 0,\ 0,\ 0,\ 0,\ \pm 6.04d), \\ (\ \ \ \ 0,\ \ \ \ 0,\ 0,\ 0,\ 0,\ \pm 9.11d), \\ (S(9.51d,\ 0,\ 0,\ 0,\ 0),\ 0), \\ U(\ \ 4d,\ 4d,\ 4d,\ 4d,\ 4d,\ 4.01d). \end{array} \tag{23}$$

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