SOME INFINITE SERIES OF SECOND ORDER ROTATABLE DESIGNS

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1. Introduction

In statistical designs of experiments in the field of industry (especially in the chemical industry), numerous problems have involved fitting of response surfaces in which yield depends on one or more controllable variables or factors. Box and Hunter (1957) introduced a new class of designs called "rotatable" designs which permit a response surface to be fitted easily and provide spherical information contours. A second order rotatable design aids the fitting of a quadratic surface.

Let k be the number of independent quantitative variables or factors and let $x_{1u}, x_{2u}, \ldots, x_{ku}$ be the coded levels of these factors for the u-th of the N experimental points in the k-dimensional factor space, $(u = 1, 2, \ldots, N)$. This set of N points is said to form a rotatable design of second order if the following relations hold:

(A) $\Sigma x_{1u}^2 = \Sigma x_{2u}^2 = \ldots\ldots\ldots\ldots = \Sigma x_{ku}^2 = \lambda_2 N,$

(B) $\Sigma x_{1u}^4 = \Sigma x_{2u}^4 = \ldots\ldots\ldots\ldots = \Sigma x_{ku}^4 = 3\,\Sigma x_{iu}^2 x_{ju}^2 = 3\lambda_4 N, (i \neq j = 1, 2, \ldots, k),$

(C) $\dfrac{\lambda_4}{\lambda_2^2} > \dfrac{k}{(k+2)};$

and all other sums of powers and products up to and including order four are zero. The summations are over all design points, $u = 1, 2, \ldots, N$. The relation (C) ensures the estimation of constants involved in the quadratic equation. This relation can always be satisfied merely by adding at least one point at the centre of the design.

Box and Hunter (1957) initiated the construction of rotatable designs and constructed many practically useful second order rotatable designs. Bose and Draper (1959) presented a new line of approach for the construction of rotatable designs and obtained second-order rotatable designs with three factors. Thereafter, Draper (1960) extended the method and derived second order designs with four and more factors. Recently, Box and Behnken (1960) derived simplex-sum designs through first order simplex designs. Das (1960) has suggested a further method using a modified form of factorial design for construction of rotatable designs. This paper makes use of cyclical group of elements for construction of second order rotatable designs.

2. Generation of Point Sets with k Factors

Let $(x_1, x_2, \ldots, x_k)$ be a point set and let C_k be the cyclical group of order k, that is, the group of cyclical permutations of k elements. Thus, we have k point sets, by operating upon $(x_1, x_2, \ldots, x_k)$, given by

$$
\begin{array}{l}
(x_1, x_2, \ldots\ldots\ldots\ldots, x_k),\\
(x_2, x_3, \ldots\ldots\ldots\ldots, x_1),\\
(x_3, x_4, \ldots\ldots\ldots\ldots, x_2),\\
\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
(x_k, x_1, \ldots\ldots\ldots\ldots, x_{k-1}).
\end{array}
$$

There will be $k2^k$ total number of points, since each point set will give 2^k permutations of the form $(\pm x_1, \pm x_2, \ldots, \pm x_k)$, if none of the elements is zero. When there are k factors, the number of constants to be estimated for a quadratic surface is $(k^2 + 3k + 2)/2$. For $4 \leqslant k \leqslant 7$, we have the following table:—

k	4	5	6	7
$(k^2 + 3k + 2)/2$	15	21	28	36

The desirable property for a practically useful design is that it should not contain excessively large number of points. To obtain a design consisting of number of points about twice the number of constants was regarded, by Draper (1960), as a very desirable achievement. The designs which possess this property are enumerated in addition to the illustrative designs from infinite series. Because of the large number of moments to be balanced for $k \geqslant 6$, this property is not assessable through the present method.

3. Designs with Four Factors

Let the point set (a, b, c, d) be generator of the cyclical group C_4. The 64 points of the resultant design are:

the 16 points of $(\pm a, \pm b, \pm c, \pm d)$,
the 16 points of $(\pm b, \pm c, \pm d, \pm a)$,
the 16 points of $(\pm c, \pm d, \pm a, \pm b)$,
the 16 points of $(\pm d, \pm a, \pm b, \pm c)$.

As there are two types of $\Sigma x_{iu}^2 x_{ju}^2$ $(i \neq j = 1, 2, \ldots, 4)$, the relation (B) gives

$$\begin{aligned} 16\,(a^4 + b^4 + c^4 + d^4) &= 3\,\{16\,(a^2b^2 + b^2c^2 + c^2d^2 + d^2a^2)\} \\ &= 3\,\{16\,(2a^2c^2 + 2b^2d^2)\}. \end{aligned} \tag{1}$$

Let $a^2 = sd^2$, $b^2 = td^2$, $c^2 = ud^2$, then equations (1) give

$$s^2 + t^2 + u^2 + 1 = 6\,(us + t), \tag{2}$$

$$st + ut + u + s = 2\,(us + t). \tag{3}$$

These two equations in three unknown variables will furnish infinite positive solutions for u, s and t. Putting $u + s = \alpha$, $t = \beta - 1$, in equations (2) and (3), the solutions for u, s, t can be shown to be

$$\left.\begin{aligned} u &= \frac{0\cdot268\beta \pm (-\,0\cdot464\beta^2 + 4\beta - 4)^{\frac{1}{2}}}{2}, \\ s &= \frac{0\cdot268\beta \mp (-\,0\cdot464\beta^2 + 4\beta - 4)^{\frac{1}{2}}}{2}, \\ t &= \beta - 1, \end{aligned}\right\} \tag{4}$$

where the limits of β are

$$\left.\begin{aligned} 6\cdot2745 \leqslant \beta \leqslant 7\cdot4655 \\ 1\cdot1551 \leqslant \beta \leqslant 1\cdot1898. \end{aligned}\right\} \tag{5}$$

When any one of u, s, t is zero, the resultant design will contain 32 non-central points since each point set of C_4 will give 8 points of the form $(0, \pm b, \pm c, \pm d)$. Draper (1960) obtained two designs in 32 points. The first design is derived by adding points of two octahedra to the points of a cube and the second design with the help of second-order rotatable design in three dimensions. Das (1960) has also got a design in 32 points. We are presenting two different designs in 32 non-central points with the solutions for u, s, t as:

Design 1		*Design* 2	
$t = 5\cdot2745$		$t = 0\cdot1898$	
$u = 0$, $s = 1\cdot3188$	or $u = 1\cdot3188$, $s = 0$	$u = 0$, $s = 0\cdot3188$	or $u = 0\cdot3188$, $s = 0$.

The designs presented in this paper will not satisfy the relation (C) because all the points are equidistant from the centre of the design. To obviate this difficulty, at least one centre point is to be added.

4. Designs with Five Factors

Let the point set (a, b, c, d, e) be the generator of the cyclical group C_5. To reduce the size of the experiment, a suitable fractional replicate can replace the full factorial. Since a second-order moment matrix identical with that of full factorial will be obtained with only that fractional replicate of the 2^k design in which neither main effects nor two factor interactions are confounded, we have to select that fractional replicate, for $k > 4$, in which no effects of second order or lower order are confounded.

With $k = 5$, if all the elements of C_5 are different from zero, then the resultant design will contain 80 non-central points by taking half-replicates of the point sets of C_5. But if one or more elements are zero then obviously a full factorial is to be taken. As there are two types of $\Sigma x_{iu}^2 x_{ju}^2 (i \neq j)$, the relation (B) gives

$$32(a^4+b^4+c^4+d^4+e^4) = 3\{32(a^2b^2+b^2c^2+c^2d^2+d^2e^2+e^2a^2)\}$$
$$= 3\{32(a^2c^2+b^2d^2+c^2e^2+d^2a^2+e^2b^2)\}. \quad (6)$$

Let

$$a^2 = ue^2,\ b^2 = ve^2,\ c^2 = se^2,\ d^2 = te^2,$$

then the equations (6) reduce to

$$u^2 + v^2 + s^2 + t^2 + 1 = 3(uv + vs + st + t + u), \quad (7)$$

$$uv + vs + st + t + u = us + vt + ut + s + v. \quad (8)$$

These two equations (7), (8) in four unknown variables u, v, s, t will furnish infinite real positive solutions for $u, v, s,$ and t which can be achieved by assigning any particular real positive value to one of the variables and then solve the two equations in three unknowns as indicated with $k = 4$. Draper (1960) obtained designs, with $k = 5$, in 52 and more number of points. We are presenting three different designs in 40 non-cental points.

Design 1	*Design* 2	*Design* 3
$u = 0,$	$u = 0,$	$u = 0,$
$v = 1 \cdot 422080,$	$v = 0 \cdot 296810,$	$v = 0 \cdot 703162,$
$s = 1 \cdot 369220,$	$s = 0,$	$s = 0,$
$t = 0.$	$t = 0 \cdot 422090.$	$t = 2 \cdot 368842.$

Das (1960) has also obtained a design in 40 points.

5. Designs with Six Factors

Let the point set (a, d, b, d, c, d) be generator of cyclical group C_6. By taking half replicates of the point sets of C_6, the resultant design will contain 196 non-central points. There being two types of $\Sigma x_{iu}^2 x_{ju}^2$ $(i \neq j)$, the relation (B) gives

$$32\,(a^4+b^4+c^4+3d^4) = 3\,\{32\,(a^2b^2 + b^2c^2 + c^2a^2 + 3d^4)\}$$
$$= 3\,\{32\,(2a^2d^2 + 2b^2d^2 + 2c^2d^2)\}. \qquad (9)$$

Putting $a^2 = sd^2$, $b^2 = td^2$, $c^2 = ud^2$, the equations (9) simplify to

$$u^2 + s^2 + t^2 + 3 = 6\,(u + s + t), \qquad (10)$$
$$us + ut + st + 3 = 2\,(u + s + t). \qquad (11)$$

These two equations (10), (11) in three unknowns u, s, t will furnish infinite real positive solutions for u, s, and t. It can easily be seen that to find the points of intersection of sphere and cone represented respectively by (10) and (11) is equivalent to find the points of intersection of plane and cone whose equations are:

$$\left.\begin{aligned} u + s + t &= 9 \\ us + ut + st &= 15 \end{aligned}\right\}, \qquad (12)$$

and

$$\left.\begin{aligned} u + s + t &= 1 \\ us + ut + st &= -1 \end{aligned}\right\}. \qquad (13)$$

The equations (13) will not yield positive solutions for u, s, and t since $us + ut + st = -1$. Thus infinite real positive solutions for u, s, t can be obtained by assigning any specified positive value to u and then getting positive solutions of s and t from (12). When either one of u, s, t is zero, the resultant design will have 96 non-central points with the solutions for u, s, t as:

Design 1	*Design* 2	*Design* 3
$u = 0$,	$u = \dfrac{(9 + \sqrt{21})}{2}$,	$u = \dfrac{(9 - \sqrt{21})}{2}$,
$s = \dfrac{(9 + \sqrt{21})}{2}$,	$s = \dfrac{(9 - \sqrt{21})}{2}$,	$s = 0$,
$t = \dfrac{(9 - \sqrt{21})}{2}$.	$t = 0$.	$t = \dfrac{(9 + \sqrt{21})}{2}$.

These three designs are identical because they give ultimately the same design points.

6. Designs with k-Factors

Let the point set $(x_1, x_2, \ldots, x_k)$ be generator of the cyclical group C_k. Note that all the elements are non-zero. Let $1/2^p$ be the appropriate fractional replicate of the full factorial so that no effects up to two factor interactions are confounded. The total number of points in the design is $k\,[1/2^p\,(2^k)]$, as there are k point sets and each supplying $1/2^p\,(2^k)$ points. When all the k elements in the point set $(x_1, x_2, \ldots, x_k)$ are different from each other then the total types of $\Sigma\, x_{iu}^2\, x_{ju}^2\,(i \neq j)$ will be $k/2$ or $(k-1)/2$ according as k is even or odd. Therefore, the relation (B) will give $k/2$ or $(k-1)/2$ equations in $(k-1)$ unknowns for even or odd k. The particular cases of this are the designs presented for $k = 4$ and 5.

It is interesting to note that the number of equations depends on the distinctness and spacing of the elements in the initial point set. That is, by a judicious selection of the initial point set, the total number of equations can be reduced considerably. Fortunately, we could investigate a point set for even number of factors which reduces considerably the total number of equations obtained through the relation (B).

7. Designs with Even Number of Factors

Let the point set $(x_1, x, x_2, x, \ldots, x_{k'}, x)$ be the generator of the cyclical group $C_{2k'}$ where the $(k'+1)$ elements $x, x_1, x_2, \ldots, x_{k'}$ are non-zero and different from each other. Note that the element x is placed alternatively at the even places. The total types of $\Sigma x_{iu}^2\, x_{ju}^2$ $(i \neq j)$ will be

$$\frac{2k'+4}{4}\left(=\frac{k'+2}{2}\right)$$

or

$$\frac{2k'+2}{4}\left(=\frac{k'+1}{2}\right)$$

according as k' is even or odd. This is evident since there will be only one type of $\Sigma x_{iu}^2 x_{ju}^2\,(i \neq j)$ at a jump of odd steps from x_1, which is of the form

$$\frac{1}{2^p}\,(2^{2k'})\,\{2\,(x_1^2\, x^2 + x_2^2 x^2 + \ldots\ldots\ldots + x_{k'}^2 x^2\}$$

while there will be $k'/2$ or $(k'-1)/2$ types of $\Sigma\, x_{iu}^2\, x_{ju}^2\,(i \neq j)$ at jumps of even steps, for even or odd k'. The $\Sigma\, x_{iu}^2\, x_{ju}^2\,(i \neq j)$ at a jump of step m from x_1 is defined as the sum of the squared products of the levels of the factors, which are at distance m, starting from x_1 and ending at $x_{2k'}$. For instance, with 8 factors, let (a, e, b, e, c, e, d, e) be the generator of the cyclical group C_8. Then, the $\Sigma x_{iu}^2 x_{ju}^2 (i \neq j)$ at jumps of steps 1, 3, 5, and 7 is

$$\frac{1}{2^p}(2^8)\{2a^2e^2 + 2b^2e^2 + 2c^2e^2 + 2d^2e^2\}$$

while the other two types of $\Sigma x_{iu}^2 x_{ju}^2 (i \neq j)$ at jumps of steps 2 and 4 are:

$$\frac{1}{2^p}(2^8)\{a^2b^2 + b^2c^2 + c^2d^2 + d^2a^2 + 4e^4\}$$

and

$$\frac{1}{2^p}(2^8)\{2a^2c^2 + 2b^2d^2 + 4e^4\}.$$

These three are the only types of $\Sigma x_{iu}^2 x_{ju}^2 (i \neq j)$ while the others will be identical with one of them.

Thus, the total types of $\Sigma x_{iu}^2 x_{ju}^2 (i \neq j)$ will be $(k' + 2)/2$ or $(k' + 1)/2$ for even or odd k'. Therefore the relation (B) will give $(k' + 2)/2$ or $(k' + 1)/2$ equations in k' unknowns, for even or odd k'. Thus, the reduction in the total number of equations as compared to the previous method is $(k' - 2)/2$ or $(k' - 1)/2$, for even or odd k'. The particular case of this approach is the designs presented for $k = 6$, $(k' = 3)$.

Another modified from of the above initial point set is $(x, x, \ldots, x, x_1, x, x, \ldots, x, x_2, \ldots; x, x, \ldots, x, x_{k''})$ where the elements $x_1, x_2, \ldots, x_{k''}$ succeed the element x only after the element x has run for $(k' - 1)$ times. The particular cases of this approach are the designs being presented in sections 8, 9, and 10 for $k = 3k'$, $4k'$, and $5k'$ factors respectively.

8. Designs with $k = 3k'$ Factors, $(k' = 2, 3, \ldots\ldots)$

Let the point set $(a, a, \ldots, a, b, a, a, \ldots, a, c, a, a, \ldots, a, d)$ be the generator of the cyclical group C_k. Note that the elements b, c, d succeed the element a only after the element a has run for $(k' - 1)$ times. Let $1/2^p$ be the appropriate fractional replicate of a full factorial, then the relation (B) gives

$$\left.\begin{aligned}&\frac{1}{2^p}(2^k)\{3(k'-1)a^4+b^4+c^4\}\\&\quad=3\left[\frac{1}{2^p}(2^k)\{3(k'-2)a^4+2a^2b^2+2a^2c^2+2a^2d^2\}\right]\\&\quad=3\left[\frac{1}{2^p}(2^k)\{3(k'-1)a^4+b^2c^2+c^2d^2+d^2b^2\}\right].\end{aligned}\right\} \tag{14}$$

Putting $b^2 = ua^2$, $c^2 = va^2$, $d^2 = sa^2$, the solutions for u, v, s can be obtained, as indicated earlier with $k = 6$, by solving the resulting two equations

$$u + v + s = 5 + \sqrt{4+6k'},$$

$$uv + us + vs = 7 + 2\sqrt{4+6k'}.$$

9. DESIGNS WITH $k = 4k'$ FACTORS, $(k' = 2, 3, \ldots\ldots)$

Let the point set

$$(a, a, \ldots, a, b, a, a, \ldots, a, c, a, a, \ldots, a, d, a, a, \ldots, a, e)$$

be a generator of the cyclical group C_k. The elements b, c, d, e succeed the element a only after the element a has run for $(k' - 1)$ times. Let $1/2^p$ be the appropriate fractional replicate of a full factorial, then the relation (B) gives

$$\left.\begin{aligned}&\frac{1}{2^p}(2^k)[4(k'-1)a^4+b^4+c^4+d^4+e^4]\\&\quad=3\left[\frac{1}{2^p}(2^k)\{4(k'-2)a^4+2(a^2b^2+a^2c^2+a^2d^2+a^2e^2)\}\right]\\&\quad=3\left[\frac{1}{2^p}(2^k)\{4(k'-1)a^4+b^2c^2+c^2d^2+d^2e^2+e^2b^2\}\right]\\&\quad=3\left[\frac{1}{2^p}(2^k)\{4(k'-1)a^4+2b^2d^2+2c^2e^2\}\right]\end{aligned}\right\} \tag{15}$$

Put

$$b^2 = ua^2 = (u'+1)a^2,\ c^2 = va^2 = (v'+1)a^2,\ d^2 = sa^2 = (s'+1)a^2,$$
$$e^2 = ta^2 = (t'+1)a^2$$

[*i.e.*, changing the origin of the variables u, v, s, t to $(1, 1, 1, 1)$] then the equations (15) simplify to

$$u'^2 + v'^2 + s'^2 + t'^2 = 4(u' + v' + s' + t') + 8k', \tag{16}$$

$$u'v' + v's' + s't' + u't' = 0, \tag{17}$$

$$u's' + v't' = 0. \tag{18}$$

From (17), either $u' + s' = 0$ or $v' + t' = 0$, therefore it can be seen that

$$\left.\begin{aligned} v' &= -t', \\ u's' &= -v'^2 = -t'^2, \\ u' + v' + s' + t' &= u' + s' = 2 \pm \sqrt{4 + 8k'}, \end{aligned}\right\} \quad (19)$$

in virtue of equations (17), (18), letting $v' + t' = 0$. The positive solutions for u, v, s, and t, after little use of algebra, are given by

$$\begin{aligned} v &= 2 - t, \\ u &= 2 + \sqrt{1 + 2k'} \pm [(t-1)^2 + 2 + 2k' + \sqrt{4 + 8k'}]^{\frac{1}{2}}, \\ v &= 2 + \sqrt{1 + 2k'} \mp [(t-1)^2 + 2 + 2k' + \sqrt{4 + 8k'}]^{\frac{1}{2}}, \\ & 0 \leqslant t \leqslant 2. \end{aligned}$$

10. Designs with $k = 5k'$ Factors, $(k' = 2, 3, \ldots\ldots.)$

Let the point set

$$(a, a, \ldots, a, b, a, a, \ldots, a, c, a, a, \ldots, a, d, a, a, \ldots, a, e, a, a, \ldots a, f)$$

be a generator of the cyclical group C_k where the elements b, c, d, e, f succeed the element a only after the element a has run for $(k' - 1)$ times. Let $1/2^p$ be the appropriate fractional replicate of the full factorial. The relation (B) gives

$$\left.\begin{aligned} & \frac{1}{2^p}(2^k)[5(k'-1)a^4 + b^4 + c^4 + d^4 + e^4 + f^4] \\ & = 3\left[\frac{1}{2^p}(2^k)\{5(k'-2)a^4 + 2(a^2b^2 + a^2c^2 + a^2d^2 + a^2e^2 + a^2f^2)\}\right] \\ & = 3\left[\frac{1}{2^p}(2^k)\{5(k'-1)a^4 + b^2c^2 + c^2d^2 + d^2e^2 + e^2f^2 + f^2b^2\}\right] \\ & = 3\left[\frac{1}{2^p}(2^k)\{5(k'-1)a^4 + b^2d^2 + c^2e^2 + d^2f^2 + e^2b^2 + f^2c^2\}\right] \end{aligned}\right\} \quad (20)$$

Put

$$b^2 = qa^2 = (q' + 1)a^2,\ c^2 = ua^2 = (u' + 1)a^2,\ e^2 = sa^2 = (s' + 1)a^2,\ f^2 = ta^2 = (t' + 1)a^2,$$

then the equations (20), in terms of q', u', s', t', simplify to

$$q'^2 + u'^2 + v'^2 + s'^2 + t'^2 = 4(q' + u' + v' + s' + t') + 10k', \quad (21)$$

$$q'u' + u'v' + v's' + s't' + t'q' = 0, \tag{22}$$

$$q'v' + q's' + u's' + u't' + v't' = 0. \tag{23}$$

It can be seen that $q' + u' + v' + s' + t' = 2 \pm \sqrt{4+10k'}$ in virtue of equations (22), (23). Substituting $u' = \alpha t'$, $v' = \beta t'$, $s' = \theta t'$, after putting $q' = 0$ (*i.e.*, $q = 1$) in equations (22) and (23), we finally get

$$\alpha = -\frac{\beta}{(1+\theta)},$$

$$\beta = \frac{[\theta(1+\theta) \pm \{\theta^2(1+\theta)^2 + 4\theta(1+\theta)\}^{\frac{1}{2}}]}{2},$$

and therefore the solutions for u', v', s' as

$$u' = -\frac{\theta(1+\theta) \pm \{\theta^2(1+\theta)^2 + 4\theta(1+\theta)\}^{\frac{1}{2}}}{2(1+\theta)} t',$$

$$v' = \frac{\theta(1+\theta) \pm \{\theta^2(1+\theta)^2 + 4\theta(1+\theta)\}^{\frac{1}{2}}}{2} t',$$

and

$$s' = \theta t'.$$

The values of u', v', s' are to be obtained by assigning a specified value to θ and then assess the value of t' through the attendant restriction

$$u'+v'+s'+t' = \frac{2(1+\theta)^2 + \theta[\theta(1+\theta) \pm \{\theta^2(1+\theta)^2 + 4\theta(1+\theta)\}^{\frac{1}{2}}]}{2(1+\theta)} t'$$

$$= 2 \pm \sqrt{4+10k'}, \quad (k' = 2, 3, \ldots).$$

Choose those values of θ which will bring real positive solutions for u, v, s, and t. For instance, when $k' = 6$, $\theta = 20$, the solutions for u, v, s, and t are

$$u = 0 \cdot 5248,$$

$$v = 10 \cdot 9776,$$

$$s = 1 \cdot 4740,$$

$$t = 1 \cdot 0236.$$

11. SUMMARY

It has been possible, through the present investigation, to obtain infinite series of second order rotatable designs with four, five and six factors. A general method for obtaining such designs for any number of factors has been indicated. A simplified method for even number of factors has also been discussed. Also presented are other infinite series of designs for $k = 3k'$, $4k'$, and $5k'$ factors, $(k' = 2, 3, \ldots)$,

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