# THIRD ORDER ROTATABLE DESIGNS FOR EXPLORING RESPONSE SURFACES[1, 2]

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**1. Introduction.** This paper considers a problem arising in the design of experiments for empirically investigating the relationship between a dependent and several independent variables, all variables being continuous. It is assumed that the form of the functional relationship is unknown but that within the range of interest, the function may be represented by a Taylor series expansion of moderately low order. Specifically, the problem considered herein is that choice of combinations of levels of the independent variables which, a) will enable an experimenter to approximate a functional relationship by fitting a Taylor series expansion through terms of order 3, by the method of least squares, and b) will have the property of rotatability. Such a choice of combinations of levels of the independent variables will be called a third order rotatable design.

For the sake of brevity, the abbreviation $d$th ORD will be used to denote $d$th order rotatable design.

**2. Rotatability.** The property of rotatability as a desirable quality of an experimental design was first advanced by Box and Hunter in [1]. This property is that the variances of estimates of the response made from the least squares estimates of the Taylor series are constant on circles, spheres or hyper-spheres about the center of the design. Thus, a rotatable design, that is, a design which achieves this property, could be rotated through any angle around its center and the variances of responses estimated from it would be unchanged.

Box and Hunter proved that a necessary and sufficient condition for a design of order $d$ ($d = 1, 2, 3, \cdots$) to be rotatable is that the moments of the independent variables be the same, through order $2d$, as those of a spherical distribution, or that these moments be invariant under a rotation of the design around its center.

Let $k$ be the number of independent variables, or factors, and let $x_{1u}, x_{2u}, \cdots, x_{ku}$ be the levels of these variables for the $u$th experimental point in the factor space, ($u = 1, 2, \cdots, N$). Then a $p$th order moment is defined as

$$N^{-1} \sum_{u=1}^{N} x_{1u}^{q} x_{2u}^{r} \cdots x_{ku}^{t},$$

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where $0 \leqq q$, $0 \leqq r$, $\cdots$, $0 \leqq t$, and $q + r \cdots + t = p$. Further, let the independent variables be standardized so that

$$\sum_{u=1}^{N} x_{iu}^2 = N \qquad (i = 1, 2, \cdots, k). \tag{2.1}$$

Let $\eta_u$ be the expectation of the response at the $u$th experimental point. For a polynomial equation of third order this may be written

$$\eta_u = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i \leqq j=1}^{k} \beta_{ij} x_{iu} x_{ju} + \sum_{i \leqq j \leqq l=1}^{k} \beta_{ijl} x_{iu} x_{ju} x_{lu} \tag{2.2}$$

or in vector notation as

$$\eta_u = \underline{x}_u \underline{\beta}. \tag{2.3}$$

(For what is to follow, the order of the terms in (2.3) is different from that in (2.2).) If the $(N \times L)$ matrix $\underline{X}$ is defined as

$$\underline{X} = \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \vdots \\ \underline{x}_N \end{bmatrix}, \tag{2.4}$$

where $L = \binom{k+3}{3}$, the number of terms in (2.2), and if $\underline{X}'$ is the transpose of $\underline{X}$, then $N^{-1}(\underline{X}'\underline{X})$ is the moment matrix of a configuration of $N$ points in the $k$-dimensional factor space.

For the configuration of $N$ points, or the design, to be rotatable, $N^{-1}(\underline{X}'\underline{X})$ must satisfy

$$N^{-1}(\underline{X}'\underline{X}) = \begin{bmatrix} \underline{G} & \underline{0} & \underline{0} & \underline{0} & \cdots & \underline{0} & \underline{0} \\ & \lambda_4 I & \underline{0} & \underline{0} & \cdots & \underline{0} & \underline{0} \\ & & \underline{K}_1 & \underline{0} & \cdots & \underline{0} & \underline{0} \\ & & & \underline{K}_2 & \cdots & \underline{0} & \underline{0} \\ & & & & \ddots & \vdots & \vdots \\ & \text{(symmetric)} & & & & \underline{K}_k & \underline{0} \\ & & & & & & \lambda_6 I \end{bmatrix} \tag{2.5}$$

in which the submatrices are defined as follows:

$$\underline{G} = \begin{array}{c} \begin{array}{ccccc} \underline{x_0} & \underline{x_1^2} & \underline{x_2^2} & \cdots & \underline{x_k^2} \end{array} \\ \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ & 3\lambda_4 & \lambda_4 & \cdots & \lambda_4 \\ & & 3\lambda_4 & \cdots & \lambda_4 \\ & & & \ddots & \vdots \\ & & & & 3\lambda_4 \end{bmatrix} \end{array} \tag{2.6}$$

$$
(2.7) \qquad \underline{K}_i \begin{array}{c} \begin{array}{cccccc} \underline{x_i} & \underline{x_i^3} & \underline{x_i x_1^2} & \underline{x_i x_2^2} & & \underline{x_i x_k^2} \end{array} \\ \left[ \begin{array}{cccccc} 1 & 3\lambda_4 & \lambda_4 & \lambda_4 & \cdots & \lambda_4 \\ & 15\lambda_6 & 3\lambda_6 & 3\lambda_6 & \cdots & 3\lambda_6 \\ & & 3\lambda_6 & \lambda_6 & \cdots & \lambda_6 \\ & & & 3\lambda_6 & \cdots & \lambda_6 \\ & & & & \ddots & \vdots \\ & & & & & 3\lambda_6 \end{array} \right] \end{array}, \qquad (i = 1, 2, \cdots, k)
$$

$$
(2.8) \qquad \lambda_4 I = \begin{array}{c} \begin{array}{cccc} \underline{x_1 x_2} & \underline{x_1 x_3} & & \underline{x_{k-1} x_k} \end{array} \\ \left[ \begin{array}{cccc} \lambda_4 & 0 & \cdots & 0 \\ & \lambda_4 & \cdots & 0 \\ & & \ddots & \vdots \\ & & & \lambda_4 \end{array} \right] \end{array},
$$

$$
(2.9) \qquad \lambda_6 I = \begin{array}{c} \begin{array}{cccc} \underline{x_1 x_2 x_3} & \underline{x_1 x_2 x_4} & \cdots & \underline{x_{k-2} x_{k-1} x_k} \end{array} \\ \left[ \begin{array}{cccc} \lambda_6 & 0 & \cdots & 0 \\ & \lambda_6 & \cdots & 0 \\ & & \ddots & \vdots \\ & & & \lambda_6 \end{array} \right] \end{array}
$$

The headings at the top of the matrices in (2.6) through (2.9) are intended to indicate the form of the elements in the matrices; they are not the vectors of (2.4). The reader will note that the arrangement of the moment matrix (2.5) is different from the arrangement of the second order moment matrix in [1]. (2.5) is written in this form to point out the amount of orthogonality present and to facilitate the calculation of the inverse.

In (2.5), $\underline{0}$ denotes a null matrix of appropriate size and in (2.7) the column and row corresponding to $x_i^3$ appears only once and always in the second position.

The constants, $\lambda_4$ and $\lambda_6$, must satisfy the restrictions

$$
(2.10) \qquad \lambda_4 > \frac{k}{k+2}
$$

$$
(2.11) \qquad \lambda_6 > \frac{\lambda_4^2(k+2)}{k+4}
$$

if (2.5) is to be positive definite.

The criterion of rotatability for a third order design is characterized mathematically by equation (2.5) with its attendant restrictions, equations (2.10) and (2.11). To find a 3rd ORD in $k$ factors, one must discover a set of combinations of factor levels whose moments are those of equation (2.5).

The inverses of the submatrices in (2.5) are

$$\underset{\sim}{G}^{-1} = A \begin{bmatrix} b & c & c & \cdots & c \\ & d & e & \cdots & e \\ & & d & \cdots & e \\ & & & \ddots & \vdots \\ & & & & d \end{bmatrix}$$

$$\underset{\sim}{K}_i^{-1} = B \begin{bmatrix} f & g & g & g & \cdots & g \\ & h & m & m & \cdots & m \\ & & w & m & \cdots & m \\ & & & w & \cdots & m \\ & & & & \ddots & \vdots \\ & & & & & w \end{bmatrix}.$$

$$(\lambda_4 I)^{-1} = I/\lambda_4 \qquad (\lambda_6 I)^{-1} = I/\lambda_6$$

in which

$$b = 2(k+2)\lambda_4^2 \qquad c = -2\lambda_4 \qquad d = (k+1)\lambda_4 - k + 1$$

$$e = 1 - \lambda_4 \qquad f = 6(k+r)\lambda_6$$

$$g = -6\lambda_4 \qquad h = k + 1 - (k-1)\lambda_4^2/\lambda_6 \qquad m = 3\left(\frac{\lambda_4^2}{\lambda_6} - 1\right)$$

$$w = 3[k + 3 - (k+1)\lambda_4^2/\lambda_6]$$

and where $A$ and $B$ are given by

$$1/A = 2\lambda_4[(k+2)\lambda_4 - k] \tag{2.12}$$

$$1/B = 6[(k+4)\lambda_6 - (k+2)\lambda_4^2]. \tag{2.13}$$

**3. Third order rotatable designs in two factors.** Consider an arrangement of $n$ points equally spaced on a circle in a two dimensional factor space. In reference [1], Box and Hunter prove that $n > 2d$ is a sufficient condition for all moments through order $2d$ of the coordinates of these points to be invariant under rotation. That is, $n > 2d$ is sufficient for the arrangement to be rotatable of order $d$. We shall prove the necessity of this condition as well.

We shall use a theorem given by Bose and Carter in reference [3], an earlier version of which was stated by Carter in [4]. Let $(x_{1u}, x_{2u})$ $(u = 1, 2, \cdots, n)$ be the $n$ points of any arrangement $A$ (which may be a design) in the space of $x_1$ and $x_2$. Denote by $\alpha(x_{1u})$, $\alpha(x_{2u})$ the coordinates of the point $(x_{1u}, x_{2u})$

after a rotation about the origin through a fixed angle $\alpha$. From Section 2, it is clear that the arrangement $A$ is rotatable of order $d$ if and only if, for any rotation $\alpha$ performed on all $n$ points of $A$,

$$(3.1)\quad \sum_{u=1}^{n} \alpha^q(x_{1u})\alpha^r(x_{2u}) = \sum_{u=1}^{n} x_{1u}^q x_{2u}^r \quad \text{for} \quad 0 \leqq q, 0 \leqq r, 0 < q + r \leqq 2d.$$

The Bose-Carter theorem proceeds as follows: Let $z_u = x_{1u} + ix_{2u}$ and $\alpha(z_u) = z_u e^{i\alpha}$. Also let $\bar{z}_u$ be the complex conjugate of $z_u$, and $\bar{z}_u e^{-i\alpha}$ the complex conjugate of $\alpha(z_u)$. Put $q + r = p$. Then we may write

$$(3.2)\quad \sum_{u=1}^{n} x_{1u}^q x_{2u}^r = 2^{-p} i^{-r} \sum_{u=1}^{n} (z_u + \bar{z}_u)^q (z_u - \bar{z}_u)^r = 2^{-p} i^{-r} \sum_{s+t=p} m_{st} \sum_{u=1}^{n} z_u^s \bar{z}_u^t,$$

where the $m_{st}$ are sums of combinatorial constants, some of which may be zero. Similarly

$$(3.3)\quad \sum_{u=1}^{n} \alpha^q(x_{1u})\alpha^r(x_{2u}) = 2^{-p} i^{-r} \sum_{s+t=p} m_{st}\, e^{i\alpha(s-t)} \sum_{u=1}^{n} z_u^s \bar{z}_u^t .$$

From (3.2) and (3.3) we see that to satisfy (3.1) it is sufficient that

$$(3.4)\quad \sum_{u=1}^{n} z_u^s \bar{z}_u^t = 0 \text{ for } 0 \leqq s,\ 0 \leqq t,\ 0 < s + t \leqq 2d \text{ unless } s = t.$$

Since

$$z^s \bar{z}^t = (x_1 + ix_2)^s (x_1 - ix_2)^t = \sum_{q+r=s+t} n_{qr} x_1^q x_2^r ,$$

then

$$e^{i\alpha(s-t)} \sum_{u=1}^{n} z_u^s \bar{z}_u^t = \sum_{q+r=s+t} n_{qr} \sum_{u=1}^{n} \alpha^q(x_{1u})\alpha^r(x_{2u}).$$

Hence, if the arrangement $A$ is rotatable of order $d$ (i.e., if (3.1) holds), then

$$e^{i\alpha(s-t)} \sum_{u=1}^{n} z_u^s \bar{z}_u^t = \sum_{q+r=s+t} n_{qr} \sum_{u=1}^{n} x_{1u}^q x_{2u}^r$$

is independent of $\alpha$, from which it follows that (3.4) must hold. Thus (3.4) is necessary and sufficient in order that $A$ be rotatable of order $d$. This is a statement of the theorem of Bose and Carter.

Now let the $n$ points $(x_{1u}, x_{2u})$ be points equally spaced on a circle of radius $\rho$. Then we may put

$$x_{1u} = \rho \cos (2\pi v/n),$$
$$x_{2u} = \rho \sin (2\pi v/n)$$

whence

$$z_u = \rho e^{2\pi i v/n},$$
$$\bar{z}_u = \rho e^{-2\pi i v/n}, \qquad v = 0, 1, \cdots, n - 1.$$

The arrangement consisting of these $n$ points is rotatable of order $d$ if and only if

$$(3.5)\quad \sum_{u=1}^{n} z_u^s \bar{z}_u^t = \rho^{s+t} \sum_{v=0}^{n-1} e^{2\pi i v(s-t)/n}$$

$$= 0 \quad \text{for } 0 \leqq s,\ 0 \leqq t,\ 0 < s + t \leqq 2d,\ s \neq t$$

which is a corollary of (3.4). By a well known theorem on the roots of unity $\sum_{v=0}^{n-1} e^{2\pi i v(s-t)/n} = 0$ if and only if $s - t$ is not an integer multiple of $n$. One sees immediately that $s - t$ cannot be an integer multiple of $n$ if $s + t < n$ and that $s - t$ will be such a multiple for some $s$ and $t$ if $s + t \geqq n$. Since (3.5) should be satisfied for any non-negative $s$, $t$ with $0 < s + t \leqq 2d$, then $n > 2d$ is necessary and sufficient for equally spaced points on a circle to be rotatable of order $d$.

Equation (2.5), then, if satisfied by $n > 6$ points equally spaced on a circle. But it may be verified that for this arrangement

$$\lambda_4 = \frac{n \sum_u x_{1u}^2 x_{2u}^2}{\left[\sum_u x_{iu}^2\right]^2} = \frac{n\rho^4 n/8}{(\rho^2 n/2)^2} = \frac{1}{2}, \qquad i = 1, 2,$$

which does not satisfy (2.10). Therefore, these points do not constitute a rotatable design. If $n_1$ is the number of points on the circle and $n_2$ points are added at the center, $\lambda_4$ becomes

$$\lambda_4 = \frac{(n_1 + n_2)\rho^4 n_1/8}{(\rho^2 n_1/2)^2} = \frac{1}{2}\left[1 + \frac{n_2}{n_1}\right] > \frac{1}{2}$$

which satisfies (2.10), but then

$$\lambda_6 = \frac{(n_1 + n_2)^2 \rho^6 n_1/16}{3(\rho^2 n_1/2)^3} = \frac{1}{6}\left[1 + \frac{n_2}{n_1}\right]^2 = \frac{2}{3}\lambda_4^2$$

and (2.11) is not satisfied. Equally spaced points on a circle with additional points at the center, then, do not constitute a 3rd ORD.

Now consider an arrangement of $N$ points on two concentric circles with $n_1$ points equally spaced on a circle of radius $\rho_1$ and $n_2$ points equally spaced on a circle of radius $\rho_2$, where $n_1 + n_2 = N$, $\rho_1 \neq \rho_2$, $\rho_1 > 0$, $\rho_2 > 0$. We shall prove that the arrangement consisting of these $n_1 + n_2$ points is rotatable of order $d$ if and only if both $n_1 > 2d$ and $n_2 > 2d$.

In the same manner as before take the first $n_1$ points as

$$\rho_1 e^{2\pi i v/n_1} \ (v = 0, 1, \cdots, n_1 - 1).$$

To allow the second $n_2$ points to take any orientation with respect to the $n_1$ points, take them as $e^{i\beta}\rho_2 e^{2\pi i v/n_2}$ $(v = 0, 1, \cdots, n_2 - 1)$. The arrangement is rotatable of order $d$ if and only if

$$(3.6)\qquad \rho_1^{s+t} \sum_{v=0}^{n_1-1} e^{2\pi i v(s-t)/n_1} + e^{i(s-t)\beta} \rho_2^{s+t} \sum_{v=0}^{n_2-1} e^{2\pi i v(s-t)/n_2} = 0$$

for $0 \leqq s$, $0 \leqq t$, with $0 < s + t \leqq 2d$ unless $s = t$. But the sums in (3.6) are 0 or $n_1$ and 0 or $n_2$ respectively. Hence (3.6) holds if and only if both sums are zero. In order that this be true we know that $n_1 > 2d$ and $n_2 > 2d$ is necessary and sufficient.

It is easily shown that this type of arrangement provides a 3rd ORD if $n_1$, $n_2 > 6$. For then

$$\lambda_4 = \frac{N(n_1 \rho_1^4 + n_2 \rho_2^4)/8}{[n_1 \rho_1^2 + n_2 \rho_2^2]^2/4} = \frac{1}{2} \frac{n_1^2 \rho_1^4 + n_2^2 \rho_2^4 + n_1 n_2(\rho_1^4 + \rho_2^4)}{n_1^2 \rho_1^4 + n_2^2 \rho_2^4 + 2n_1 n_2 \rho_1^2 \rho_2^2},$$

and since $\rho_1^4 + \rho_2^4 > 2\rho_1^2\rho_2^2$, for $\rho_1 \neq \rho_2$, $\lambda_4 > \frac{1}{2}$. Therefore, (2.10) is satisfied. Similarly

$$\lambda_6 = \frac{N^2}{3} \frac{(n_1 \rho_1^6 + n_2 \rho_2^6)/16}{[n_1 \rho_1^2 + n_2 \rho_2^2]^3/8} > \frac{2}{3} \lambda_4^2$$

since

$$\frac{\lambda_6}{\lambda_4^2} = \frac{2}{3} \frac{n_1^2 \rho_1^8 + n_2^2 \rho_2^8 + n_1 n_2 \rho_1^2 \rho_2^2(\rho_1^4 + \rho_2^4)}{n_1^2 \rho_1^8 + n_2^2 \rho_2^8 + n_1 n_2 \rho_1^2 \rho_2^2(2\rho_1^2 \rho_2^2)}$$

which is greater than $\frac{2}{3}$ for $\rho_1 \neq \rho_2$ and so (2.11) is satisfied, also.

Thus, it has been shown that a simple class of 3rd ORDs in two factors exists. This class consists of designs which have seven or more points equally spaced on each of two concentric circles. Each of the circles may be rotated independently of the other and therefore there are an infinite number of configurations possible for designs with a given $n_1$ and $n_2$. Since points located at the center of the circles do not disturb the moment properties of the configuration, these may be added at will to achieve variations in the parameters $\lambda_4$ and $\lambda_6$.

**4. Sequential third order rotatable designs in two factors.** A 3rd ORD of the type described in the previous section may be performed in two "blocks." By judicious selection of $\rho_1$ and $\rho_2$, the radii of the two circles, the coefficients in the Taylor series expansion may be estimated independently of the block effects. If one block of points is a complete 2nd ORD and the second block consists of additional points necessary to make the whole a 3rd ORD, the design may be called sequential, in that an experimenter need not perform the second block of points if he feels the first block has given him an adequate approximation to the phenomenon.

Suppose the first block consists of seven or more points equally spaced on a circle with some points at the center. This allows the estimation of polynomial coefficients up to and including the second order. Now add a second block consisting of seven or more points equally spaced on a circle of different radius from the first. Let $n_1$ be the number of points in the first block and $n_2$ the number of points in the second block. Let $\delta_1$ be the effect of the first block, $\delta_2$ the effect of the second block, and let $Z_{wu} = 1$ if the $u$th observation occurs in the $w$th block, $w = 1, 2$, and $Z_{wu} = 0$ otherwise. Then, the expectation of the $u$th observation can be written

$$\eta_u = \beta_0 + \sum_i \beta_i x_{iu} + \sum_i \sum_j \beta_{ij} x_{iu} x_{ju} + \sum_i \sum_j \sum_l \beta_{ijl} x_{iu} x_{ju} x_{lu} + \sum_w \delta_w (Z_{wu} - \bar{Z}_{wu}) \tag{4.1}$$

in which $\bar{Z}_w = \sum_u Z_{wu}/N$, and $N = n_1 + n_2$.

If the estimates of the block effects are to be independent of the estimates of the polynomial coefficients, it is required that

$$\sum_u (Z_{wu} - \bar{Z}_w) = 0 \tag{4.2}$$

$$\sum_u (Z_{wu} - \bar{Z}_w) x_{iu} = 0 \tag{4.3}$$

$$\sum_u (Z_{wu} - \bar{Z}_w) x_{iu} x_{ju} = 0 \tag{4.4}$$

$$\sum_u (Z_{wu} - \bar{Z}_w) x_{iu} x_{ju} x_{lu} = 0 \tag{4.5}$$

for $w = 1, 2$ and $i, j, l = 1, 2$. (4.2) is satisfied by the definition of $\bar{Z}_w$, while (4.3), (4.4) and (4.5) are satisfied with one exception, by the fact that $Z_{wu} - \bar{Z}_w$ is constant within blocks and each block contains a rotatable arrangement of points. The exception is in (4.4) when $i = j$. For this case, if $n_{01}$ = the number of points at the center in the first block, and $n_{02}$ = the number of points at the center in the second block, (4.4) becomes

$$\left[1 - \frac{n_1}{N}\right] [n_1 - n_{01}] \frac{\rho_1^2}{2} + \left[\frac{-n_1}{N}\right] [n_2 - n_{02}] \frac{\rho_2^2}{2} = 0$$

or

$$\frac{\rho_2^2}{\rho_1^2} = \frac{n_2(n_1 - n_{01})}{n_1(n_2 - n_{02})}. \tag{4.6}$$

Therefore, by selecting $\rho_2$, the radius of the circle in the second block, in accordance with (4.6) the experiment may be performed sequentially and estimates of polynomial coefficients will be free of block effects. It is interesting to note that (4.6) is independent of the number of points in the second block, if $n_{02} = 0$, it being required only that $n_2 > 6$. A 3rd ORD with these blocking properties is not possible, however, if $n_2 n_{01} = n_1 n_{02}$.

The 3rd ORD may be sequentialized in three stages with a total of either three or four blocks. Block I would consist of $n_1/2$ points of which $n_{01}/2$ are central points and such that $(n_1 - n_{01})/2$ is an integer greater than or equal to 4. The $(n_1 - n_{01})/2$ points would be equally spaced on a circle of radius $\rho_1$, and the $(n_1 - n_{01})/2$ points would constitute a 1st ORD. Block II would be identical with Block I with the points superposed so that Blocks I and II jointly would have $n_1 - n_{01}$ points equally spaced on a circle of radius $\rho_1$ and $n_{01}$ points at the center and thus would form a complete 2nd ORD.

The third stage, Block III, would consist of $n_2 - n_{02}$ points, greater than 6, equally spaced on a circle of radius $\rho_2$ (where $\rho_2$ is determined from (4.6)) and $n_{02}$ points at the center, in a three block design. Blocks I, II, and III would make up a complete 3rd ORD.

If the experiment were to be sequentialized in three stages and four blocks, the third stage would be constructed of two blocks similar to Blocks I and II, but with radius $\rho_2$, and with the possibility of no central points.

**5. Third order rotatable designs in three factors (non-sequential).** A 3rd ORD in three factors may be formed from the points at the vertices of a cube, two octahedra of different radii, and a cuboctahedron, all oriented symmetrically to one another. The coordinates of the points of the cube can be represented by all possible permutations of the elements of the vector, $(\pm a, \pm a, \pm a)$; of one octahedron by the permutations of the elements of $(\pm 1.82969a, 0, 0)$; of the other octahedron by the permutations of the elements of $(\pm 1.16343a, 0, 0)$; and of the cuboctahedron by the 12 permutations of the elements of $(\pm a2^{\frac{1}{3}}, \pm a2^{\frac{1}{3}}, 0)$. The value of $a$ is the scaling factor chosen so that $\sum_{u=1}^{N} x_{iu}^2 = N$, the total number of points. The constants, 1.82969, 1.16343, and $2^{\frac{1}{3}}$ are those which will satisfy the moment requirements inherent in equations (2.6) and (2.7) for this composite configuration. The parameters for this design are given below for various numbers of points added at the center of the design. Also given are the values $(5/7)\lambda_4^2$, which, in accordance with (2.11), must always be exceeded by $\lambda_6$.

| $N$ | No. of Center Points | $\lambda_4$ | $\lambda_6$ | $5\lambda_4^2/7$ |
|---|---|---|---|---|
| 32 | 0 | .638 | .300 | .291 |
| 33 | 1 | .658 | .319 | .309 |
| 34 | 2 | .678 | .339 | .328 |
| 35 | 3 | .698 | .359 | .348 |
| 36 | 4 | .718 | .380 | .368 |
| 37 | 5 | .738 | .402 | .389 |
| 38 | 6 | .758 | .423 | .410 |
| 39 | 7 | .778 | .446 | .432 |
| 40 | 8 | .798 | .469 | .455 |

Another 3rd ORD of the non-sequential type can be formed by orienting an icosahedron of radius $a$ symmetrically with respect to a dodecahedron of radius $1.11236224a$, with or without central points. But with 0 to 8 central points $\lambda_6 - (5/7)\lambda_4^2$ is never greater than 0.000061, so that this design could not be recommended.

**6. Third order rotatable designs in three factors (sequential).** Of greater interest than a 3rd ORD *per se* is the 3rd ORD which can be performed sequentially, and particularly those sequential designs in three factors which may be extended to higher dimensions.

Consider the sequential design as being performed in two parts: the first part to be a 2nd ORD and the second part a set of points which, when added to the first part, makes a 3rd ORD. If the second order moment properties are to be preserved after the addition of the second set of points, it is obvious than both parts of the design must be complete 2nd ORDs in themselves.

For the first of these 3 dimensional sequential designs consider the design whose initial portion is the cube + octahedron configuration with points at the center. By adding to this, the points of a truncated cube and of another octahedron, a 3rd ORD results. This design would not be recommended in practice because, like the icosahedron-dodecahedron design of the previous section, the resultant matrix of normal equations is poorly conditioned. That is, although the inequalities (2.10) and (2.11) are satisfied, (2.11) is very close to an equality. Consequently, the linear and cubic coefficients are very poorly estimated. The design is presented here because it provides a basis for a more useful design which follows.

The coordinates of a truncated cube in 3 dimensions can be written as all 24 permutations of the elements of the vector, $(\pm c, \pm d, \pm d)$, where the radius of the figure is given by $\rho^2 = c^2 + 2d^2$ and where $c$ is a measure of the amount of truncation. For example, if $c = d$ the figure is not truncated at all and the 24 points make up a triply replicated cube. If $c = 0$, the truncation is extreme and the figure becomes a doubly replicated cuboctahedron. It can be shown that if

$$c = \frac{5 + 2\sqrt{10}}{15} \rho^2$$

the 24 points constitute a 2nd ORD, but this value of $c$ is not helpful in constructing a 3rd ORD.

For the first portion of this sequential design let the cube have radius $\rho_1$ and an octahedron have radius

$$\rho_2 = \frac{2^{3/4}}{\sqrt{3}} \rho_1 .$$

Box and Hunter [1] show that this arrangement of 14 points comprises a 2nd ORD. To this, as the second portion of the sequential design, add a truncated cube of radius $\rho_3$ and coordinates, $(\pm c, \pm d, \pm d)$ and another octahedron with coordinates $(\pm \rho_4, 0, 0)$. Then it can be shown that if $\rho_1 = \sqrt{3}$, $\rho_2 = 2^{3/4}$, $\rho_3 = 1.657765$, $\rho_4 = 1.705945$, $c = 0.184388$, $d = 1.164944$, a 3rd ORD results. But for 0 to 10 central points $\lambda_6 - 5\lambda_4^2/7$ is never larger than .0005.

However, the difficulty of the ill-conditioned matrix may be avoided by modifying the design slightly. This is accomplished by using a cube and "doubled octahedron," instead of a cube and octahedron in the first stage of experimentation. By doubled octahedron is meant *two* experimental points at each vertex of an octahedron. Let $\rho_1$, $\rho_2$, $\rho_3$ and $\rho_4$ designate the radii of a cube, doubled octahedron, truncated cube and octahedron respectively. If the first portion, consisting of the cube and doubled octahedron is to be second order rotatable, then

$\rho_2 = \rho_1\sqrt{2/3}$. The second portion of the design consisting of the truncated cube and the other octahedron must have dimensions satisfying the equations

$$\rho_4^4 = \rho_3^4 + 10c^2\rho_3^2 - 15c^4 \tag{6.1}$$

$$2\rho_4^6 = -21c^6 + 9c^4\rho_3^2 + c^2\rho_3^4 + 3\rho_3^6 \tag{6.2}$$

$$\tfrac{16}{27}\rho_1^6 = \rho_3^6 - 19c^2\rho_3^4 + 39c^4\rho_3^2 - 21c^6 \tag{6.3}$$

which, in turn, will satisfy equation (2.5). If $\rho_1$ again equals $\sqrt{3}$ and hence $\rho_2 = \sqrt{2}$, then an admissable solution of (6.1), (6.2) and (6.3) is $\rho_3 = 1.851208$, $\rho_4 = 1.985406$, $c = 0.341564$. The coordinates of the resultant design are

(for the first stage of experimentation)
- the 8 permutations of $(\pm a, \pm a, \pm a)$,
- the 6 permutations of $(\pm a\sqrt{2}, 0, 0)$,
- the 6 permutations of $(\pm a\sqrt{2}, 0, 0)$ again,
- and, if desired, points with coordinates $(0, 0, 0)$;

(for the second stage of experimentation)
- the 24 permutations of $(\pm .341564a, \pm 1.286527a, \pm 1.286527a)$,
- the 6 permutations of $(\pm 1.985406a, 0, 0)$,
- and, if desired, points with coordinates $(0, 0, 0)$,

where, again, $a$ is chosen so that $\sum_{u=1}^{N} x_{iu}^2 = N$.

The values of the parameters for number of central points to 10 are:

| $N$ | Number of Central Points | $\lambda_4$ | $\lambda_6$ | $5\lambda_4^2/7$ |
|---|---|---|---|---|
| 50 | 0 | .6271 | .2902 | .2809 |
| 51 | 1 | .6396 | .3019 | .2922 |
| 52 | 2 | .6522 | .3139 | .3038 |
| 53 | 3 | .6647 | .3261 | .3156 |
| 54 | 4 | .6773 | .3385 | .3277 |
| 55 | 5 | .6898 | .3511 | .3399 |
| 56 | 6 | .7023 | .3640 | .3523 |
| 57 | 7 | .7149 | .3771 | .3651 |
| 58 | 8 | .7274 | .3905 | .3779 |
| 59 | 9 | .7400 | .4041 | .3911 |
| 60 | 10 | .7525 | .4179 | .4045 |

Block coefficients may be introduced into the model with this design also. Following Section 4, $n_1 - n_{01} = 20$ and $n_2 - n_{02} = 30$, so the equation which expresses the condition for orthogonal blocking is

$$(30 + n_{02}) \sum_{u=1}^{n_1} x_{iu}^2 = (20 + n_{01}) \sum_{u=n_1+1}^{N} x_{iu}^2$$

or

$$n_{02} = 2.206n_{01} + 14.124 \tag{6.4}$$

Applying equation (6.4), the following table of design numbers for approximately orthogonal blocking results.

| $n_{01}$ | $n_{02}$ | $n_1$ | $n_2$ | $N$ |
|---|---|---|---|---|
| 0 | 14 | 20 | 44 | 64 |
| 1 | 16 | 21 | 46 | 67 |
| 2 | 19 | 22 | 49 | 71 |
| 3 | 21 | 23 | 51 | 74 |
| 4 | 23 | 24 | 53 | 77 |
| 5 | 25 | 25 | 55 | 80 |
| 6 | 27 | 26 | 57 | 83 |
| 7 | 30 | 27 | 60 | 87 |

**7. Third order rotatable designs in more than three factors.** As is well known, only the analogues of the tetrahedron, the octahedron and the cube exist, as regular figures in more than four dimensions. The latter two were used successfully by Box and Hunter [1] in their development of 2nd ORDs in the higher dimensional factor spaces. In Sections 5 and 6 some semi-regular figures were described which provided 3rd ORDs for three dimensions. Of these semi-regular figures, the truncated cube was of particular interest in that it provided a basis for the construction of three dimensional sequential 3rd ORDs.

The higher dimensional analogue of the truncated cube is not easy to identify. The obvious extension from three dimensions to $k$ dimensions would be the figure whose coordinates are the permutations of the elements of $(\pm c, \pm d, \cdots, \pm d)$, there being $k - 1$ elements $\pm d$. Call this "truncated cube (1)." A less obvious, but nevertheless reasonable extension to $k$ dimensions is the figure whose coordinates are the permutations of $(\pm c, \pm c, \cdots, \pm c, \pm d, \pm d, \cdots, \pm d)$ with, say, $r$ elements $\pm c$ and $k - r$ elements $\pm d$, and with $1 < r < (k + 1)/2$. Let this figure be called "truncated cube $(r)$."

From the point of view of economy in the number of experiments, "truncated cube (1)" would be preferred as a part of a design since it contains fewer points. The number of points in "truncated cube (1)" is $k2^k$. The number of points in "truncated cube $(r)$" is $\binom{k}{r} 2^k$, which is always larger for $1 < r < k - 1$. Unfortunately "truncated cube (1)" cannot be used with the "cube" and "octahedra" to form sequential 3rd ORDs for $k > 3$. This can be shown as follows.

Consider the configuration made up of the $k$-dimensional "truncated cube (1)" and a $k$-dimensional "octahedron" of radius $\rho$. For a sequential design of the type described in Section 6, this composite configuration would comprise the second stage of experimentation and therefore the coordinates must satisfy the requirement (in addition to the requirements satisfied by the symmetry of the configuration),

$$(7.1) \qquad \sum_u x_{iu}^4 = 3 \sum_u x_{iu}^2 x_{ju}^2 \qquad (i \neq j = 1, 2, \cdots, k).$$

For this configuration

$$\sum_u x_{iu}^4 = 2^k[c^4 + (k - 1)\, d^4] + 2\rho^4$$

$$\sum_u x_{iu}^2 x_{ju}^2 = 2^k d^2[2c^2 + (k - 2)\, d^2].$$

Substitution of the above into (7.1), requires

(7.2) $$c^2 = 3\, d^2 \pm [(4 + 2k)\, d^4 - 2^{1-k}\rho^4]^{\frac{1}{2}}.$$

The configuration for the second stage when combined with the first stage configuration consisting of a $k$-dimensional "cube" of radius $(k)^{\frac{1}{2}}$ and $k$-dimensional "octahedron" of radius $(2)^{k/4}$ must satisfy the condition

(7.3) $$\sum_u x_{iu}^4 x_{ju}^2 = 3 \sum_u x_{iu}^2 x_{ju}^2 x_{lu}^2\,, \quad (i \neq j \neq l = 1, 2, \cdots, k).$$

For the combined configurations (7.3) requires

(7.4) $$c^2 = \frac{4d^4 \pm [(9 + 2k)d^8 + 2d^2]^{\frac{1}{2}}}{d^2}$$

The minus sign in (7.4) will give a negative $c^2$ (with $k > 3$) and therefore must be disregarded. Equating (7.2) to (7.4) (with the plus sign) and simplifying gives

(7.5) $$3d^6 + d^2[2^{-k}\rho^4 + \sqrt{(9 + 2k)\, d^8 + 2d^2}] + 1 = 0,$$

which is impossible since each term on the left of (7.5) must be a positive quantity. Therefore, "truncated cube (1)" cannot be used in a 3rd ORD of this form if $k$ is greater than 3.

With $k = 4$ a sequential 3rd ORD was discovered. The first stage of the design consists of a four dimensional "cube" of radius 2 and a 4-dimensional "octahedron," also of radius 2. (Actually, this is a 4-dimensional regular figure of 24 points.) The second stage is comprised of a 4-dimensional "truncated cube (2)" with coordinates $(\pm c, \pm c, \pm d, \pm d)$ and another 4-dimensional "octahedron" of radius $\rho$. To satisfy equation (2.5), we must have $c = 1.200919$, $d = .256303$, $\rho = 1.736604$. This design contains 16 points on the "cube," 8 points on the first "octahedron," 96 points on the "truncated cube" and 8 points on the second "octahedron" for a total of 128 points without center points. The design parameters are $\lambda_4 = .676$ and $\lambda_6 = .349$. The coordinates of experimental points for this design are

(for the first stage)

the 16 permutations of $(\pm a, \pm a, \pm a, \pm a)$,

the 8 permutations of $(\pm 2a, 0, 0, 0)$,

and, if desired, central points $(0, 0, 0, 0)$;

(for the second stage)

the 96 permutations of $(\pm 1.200919a, \pm 1.200919a, \pm .256303, \pm .256303a)$,

the 8 permutations of $(\pm 1.736604a, 0, 0, 0)$,

and, if desired, central points $(0, 0, 0, 0)$,

with $a$ such that $\sum_{u=1}^{N} x_{iu}^2 = N$.

For approximately orthogonal blocking of the two stages of experimentation, the number of center points in each block, $n_{01}$ and $n_{02}$, is shown in the following table. The total number of points and the design parameters are also given.

| $n_{01}$ | $n_{02}$ | $n_1$ | $n_2$ | $N$ | $\lambda_4$ | $\lambda_6$ | $6\lambda_4^2/8$ |
|---|---|---|---|---|---|---|---|
| 8 | 0 | 32 | 104 | 136 | .719 | .394 | .388 |
| 9 | 4 | 33 | 108 | 141 | .745 | .423 | .416 |
| 10 | 7 | 34 | 111 | 145 | .766 | .447 | .440 |
| 11 | 10 | 35 | 114 | 149 | .787 | .472 | .465 |

The relationship, $\lambda_6 > 6\lambda_4^2/8$, appears to be sufficiently well satisfied so that no investigation of the design utilizing a doubled octahedron (and 8 additional points) was made.

No attempt was made to extend the concept of 3rd ORDs to more than four dimensions, chiefly because the approach pursued in this paper required the use of an excessive number of experimental points. Investigations were made, following this approach, only of the sequential type of rotatable design because this is the type which seems likely to be most useful to an experimenter.

Considerable savings were demonstrated by Box and Hunter in the case of 2nd ORDs by the use of fractional replication for $k > 4$. With $k$ equal to five or more the second order coefficients are confounded only with third and higher order effects when fractional replication is used. But for third order coefficients to be confounded only with fourth and higher effects, the dimensionality must be at least seven in order to make use of fractional replication. If a half replicate of a 7-dimensional design of the type described in the preceding section were possible it would require at least 1,436 experimental points.

If a full replicate, 5-dimensional design of this type were possible, 372 points would be required. The same design in six factors would require 1,048. Third order rotatable designs derived from figures which are symmetrical in all $k$-dimensions would appear to be impractical for $k > 4$.

**8. Summary and conclusions.** This paper is concerned with extending the criterion of rotatability, as advanced by Box and Hunter [1], to experimental designs for estimating response surfaces by third order polynomial equations. The method of attack has been to examine combinations of regular and semi-regular geometrical figures and find those combinations whose coordinate points satisfy the moment properties, to order six, of spherical distributions. Designs with these properties and the attendant restrictions were shown by Box and Hunter to have spherical variance contours when the polynomial coefficients were estimated by the method of least squares.

It was found that 3rd ORDs in two factors could be attained by locating seven or more experimental points equally spaced on each of two concentric circles of different non-zero radii. Also it was shown that certain rotatable designs in two factors can be performed in two stages, so that second order polynomial coefficients can be estimated after the first stage and third order polynomial coefficients after the second stage. By choosing the radii of the two circles in the proper ratio it is possible to obtain estimates of the polynomial coefficients which are independent of "block" effects due to running the experiments in two stages. Such designs were termed sequential 3rd ORDs.

In three factors, 3rd ORDs were presented which consisted of composites of cubes, truncated cubes, octahedra, cuboctahedra, icosahedra and dodecahedra. Two of these designs in three factors were constructed so that they might be performed sequentially.

One sequential 3rd ORD in four factors was also presented. This design has as its experimental points the vertices of the 4-dimensional analogues of a cube, a truncated cube and two octahedra of different dimensions.

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