SECOND ORDER ROTATABLE DESIGNS IN THREE DIMENSIONS[1]

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0. Summary. The technique of fitting a response surface is one widely used (especially in the chemical industry) to aid in the statistical analysis of experimental work in which the "yield" of a product depends, in some unknown fashion, on one or more controllable variables. Before the details of such an analysis can be carried out, experiments must be performed at predetermined levels of the controllable factors, i.e., an experimental design must be selected prior to experimentation. Box and Hunter [3] suggested designs of a certain type, which they called rotatable, as being suitable for such experimentation. Very few of these designs were then known. Since that time the work of R. L. Carter [6] has provided many new second order rotatable designs in two factors. However, additional methods were needed which would provide both second and third order designs in three and more factors. The present work represents an attempt to meet, in part, this need. New construction methods for obtaining rotatable designs of second order in three dimensions are here presented. By use of these methods various infinite classes of designs are obtained, and it may be shown that all the rotatable designs previously known can be derived as special cases of these infinite classes. Also derived is an infinite class of second order rotatable designs which contain only 16 points; only two particular designs contain fewer points.

1. Introduction. A great deal of information is now available about the theory of response surfaces and the use of rotatable designs. Such information may be found in papers by Box [1], [2], Box and Wilson [5], Box and Hunter [3], [4] and the Ph.D. dissertation of Carter [6]. The paper [3] by Box and Hunter provides the necessary background for the present work, and a discussion of polynomial approximation and of the desirability of rotatable designs will be found therein. We shall be concerned here with second order rotatable designs in three controllable factors and we shall assume that the measurements of the factors have been coded, permitting the use of Cartesian axes in three dimensional space to describe an experimental design.

Suppose, in an experimental investigation with k factors, N (not necessarily

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distinct) combinations of levels are employed. Thus the group of N experiments which arises can be described by the N points in k dimensions

$$(1.1) \qquad (x_{1u}, x_{2u}, \cdots, x_{ku}), \qquad u = 1, 2, \cdots, N;$$

where, in the uth experiment, factor t is at level x_{tu}.

The set of points (1.1) is said to form a *rotatable arrangement* of the second order in k factors if the following conditions are satisfied:

$$(1.2) \qquad \begin{aligned} &\sum_u x_{1u}^2 = \sum_u x_{2u}^2 = \cdots = \sum_u x_{ku}^2 = \lambda_2 N, \\ &\sum_u x_{1u}^4 = \sum_u x_{2u}^4 = \cdots = \sum_u x_{ku}^4 = 3\sum_u x_{iu}^2 x_{ju}^2 = 3\lambda_4 N, \qquad (i \neq j) \end{aligned}$$

and all other sums of powers and products up to and including order four are zero, where all summations are over $u = 1$ to $u = N$. The set (1.1) is said to form a *rotatable design* of second order if the conditions (1.2) are satisfied *and* a certain matrix used in a subsequent least squares estimation is non-singular. Box and Hunter [3] show that the necessary and sufficient condition for this to be so is

$$(1.3) \qquad \lambda_4/\lambda_2^2 > k/(k + 2),$$

a condition which may always be satisfied merely by theaddition of points at the center (0, 0, 0) of the design. Equality in (1.3) is attained when all the design points lie on a k-dimensional sphere, and it is impossible for the inequality in (1.3) to be reversed under any circumstances.

When presenting a rotatable design, it is customary to "scale" it. By this it is meant that the scale of the coded controllable variables is chosen in such a way that $\lambda_2 = 1$. The reason for this is as follows. Given a second order design which satisfies the conditions (1.2) with a *specified* value of λ_4/λ_2^2, there are an infinite number of values possible for $\lambda_2 > 0$. Since these designs can be derived one from the other merely by change of scale, we do not regard them as different. Thus the scaling condition $\lambda_2 = 1$ fixes a *particular* design and enables better comparison between two designs with different values of λ_4/λ_2^2.

2. A transformation group in three dimensions and its generated point sets. We shall define certain transformations applied to points in three dimensions. Let $W(x, y, z) = (y, z, x)$. Then $W^2(x, y, z) = (z, x, y)$ and $W^3(x, y, z) = (x, y, z)$. Thus W, W^2 and $W^3 = I$ form a cyclical group of order 3. Further let $R_1(x, y, z) = (-x, y, z)$, $R_2(x, y, z) = (x, -y, z)$, $R_3(x, y, z) = (x, y, -z)$.

The four transformations represented by W, R_1, and R_2 and R_3 generate a group G of transformations of order 24 with elements

$$(2.1) \qquad \begin{aligned} &W^j, W^jR_1, W^jR_2, W^jR_3, W^jR_2R_3, \\ &W^jR_3R_1, W^jR_1R_2, W^jR_1R_2R_3 \qquad (j = 1, 2, 3). \end{aligned}$$

It is easily seen that all the 24 elements in (2.1) are distinct. While R_1, R_2 and R_3 commute, W^j and R_i do not ($j = 1, 2; i = 1, 2, 3$).

A group table may be constructed, employing the identities

$$W^3 = R_1^2 = R_2^2 = R_3^2 = I \tag{2.2}$$

and identities of the type $WR_1 = R_3W$, to verify the statements above. Because of the size of the group the table will not be reproduced here.

Given a general point (x, y, z) in three dimensions, we may apply to it all the transformations of the group G. In this way we obtain a set of 24 points with coordinates

$$(\pm x, \pm y, \pm z), \quad (\pm y, \pm z, \pm x), \quad (\pm z, \pm x, \pm y). \tag{2.3}$$

We shall denote this set by

$$G(x, y, z). \tag{2.4}$$

Note that if (l, m, n) denotes any other point of the set, $G(x, y, z) = G(l, m, n)$, i.e., any point of the set, when operated on by G, will give rise to the same set. The set $G(x, y, z)$ satisfies all the moment conditions (1.2) except

$$\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 \qquad (i \neq j), \quad (i, j = 1, 2, 3). \tag{2.5}$$

We now define a function $K(x, y, z)$ of the point (x, y, z) as

$$K(x, y, z) = \tfrac{1}{3}(x^4 + y^4 + z^4 - 3y^2z^2 - 3z^2x^2 - 3x^2y^2). \tag{2.6}$$

This function is constant for all of the 24 points of $G(x, y, z)$. Furthermore, if it has the value zero, then $G(x, y, z)$ is a rotatable arrangement since the outstanding condition (2.5) becomes satisfied. Let

$$x^2 = sz^2, \qquad y^2 = tz^2. \tag{2.7}$$

Then, if $K(x, y, z)$ is zero and $z \neq 0$,

$$t^2 - 3t(s + 1) + (s^2 - 3s + 1) = 0. \tag{2.8}$$

This is the equation of a hyperbola. If the point (s, t) lies on the hyperbola and also in the first quadrant, $G(x, y, z)$ is a rotatable arrangement. Fig. 1 shows points (s, t) for which this is true. There is complete symmetry about the line $s = t$. The value of s at the points P_1 and P_2, where the hyperbola intersects the line $t = 0$, is $(3 - \sqrt{5})/2$ and $(3 + \sqrt{5})/2$, respectively. If we solve for t in terms of s, we obtain

$$t = \tfrac{1}{2}[3(s + 1) \pm \sqrt{5(s^2 + 6s + 1)}]. \tag{2.9}$$

This yields two non-negative solutions if $s^2 - 3s + 1 > 0$, which implies $s \geqq (3 + \sqrt{5})/2$ or $0 \leqq s \leqq (3 - \sqrt{5})/2$. Otherwise there is only one positive solution for each value of $s \geqq 0$. The reason for this is clear from Fig. 1.

The point set $G(x, y, z)$ is clearly spherical, and thus equality will be attained in the non-singularity condition (1.3) unless additional points are added at the center to form the design. If n_0 center points are added, $N = 24 + n_0$, and $\lambda_2 N = 8(x^2 + y^2 + z^2) = 8(s + t + 1)z^2$.

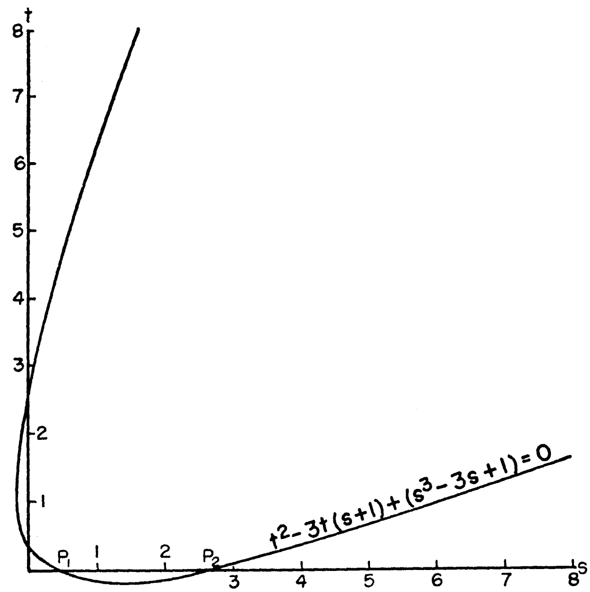

FIG. 1

Thus if we apply the scaling condition $\lambda_2 = 1$,

$$z^2 = N/8(s + t + 1), \tag{2.10}$$

and we have an infinite class of second order designs which depends on one parameter s. For if $s \geqq 0$ is specified,

$$\begin{aligned} t &= \tfrac{1}{2}[3(s + 1) \pm \sqrt{5(s^2 + 6s + 1)}], \qquad (t \geqq 0 \text{ only}), \\ z &= [N/8(s + t + 1)]^{\frac{1}{2}}, \qquad y = t^{\frac{1}{2}}z, \qquad x = s^{\frac{1}{2}}z, \end{aligned} \tag{2.11}$$

and all design points are fixed. Each non-negative s gives rise to one or two designs according as (2.9) yields one or two non-negative values of t. For this class, $\lambda_4/\lambda_2^2 = 8(x^2y^2 + y^2z^2 + z^2x^2)/N = 8(st + s + t)z^4/N$. Consider the special case $s = t = \sqrt{10} - 3$. We then have $x = y = (N - 8z^2)/16$, $z = [(5 + 2\sqrt{10})N/120]^{\frac{1}{2}}$. This is the design referred to as the truncated cube by Gardiner, Grandage and Hader ([9], Sec. 6, Par. 4).

Let us now suppose that $K(x, y, z) \neq 0$ for the points of the set $G(x, y, z)$. We shall define $\sum K(x, y, z)$ over a point set S to be the *excess* of that set and write it $\text{Ex}(S)$. Thus

$$\text{Ex}[G(x, y, z)] = 8(x^4 + y^4 + z^4 - 3y^2z^2 - 3z^2x^2 - 3x^2y^2). \tag{2.12}$$

This can take both positive and negative values according to the choice of x, y and z. Clearly, $\sum_j \text{Ex}(S_j) = \text{Ex}(\sum_j S_j)$, where the notation $\sum_j S_j$ means that points which belong to more than one set S_j contribute to the sum each time they occur. The notation thus does not denote the "union" of sets in the usual sense. Furthermore, if a number of sets S_1, S_2, $\cdots$, S_m (say) satisfy, either separately or together, the conditions for a second order rotatable arrangement except for the condition (2.5), then the condition

$$\text{(2.13)} \qquad \text{Ex}(S_1 + \cdots + S_m) = \text{Ex}(S_1) + \cdots + \text{Ex}(S_m) = 0$$

is a necessary and sufficient condition for the points of the whole set $S_1 + S_2 + \cdots + S_m$ to form a rotatable arrangement of second order. We shall make use of this important fact in Section 3.

For certain special choices of (x, y, z) in three dimensions, the 24 points of $G(x, y, z)$ will coincide in pairs or in triplets or in quadruplets. For example, $G(p, q, 0)$ consists of the twelve points

$$\text{(2.14)} \qquad (\pm p, \pm q, 0), \qquad (0, \pm p, \pm q), \qquad (\pm q, 0, \pm p),$$

each occurring twice. We may denote the 12 point set by $\frac{1}{2}G(p, q, 0)$. This set has excess

$$\text{(2.15)} \qquad \text{Ex}[\tfrac{1}{2}G(p, q, 0)] = 4(p^4 + q^4 - 3p^2q^2),$$

a quantity which may be made positive or negative according to the values of p and q.

The set $\frac{1}{2}G(p, q, 0)$ will itself form a rotatable arrangement if $p^4 - 3p^2q^2 + q^4 = 0$ or $p^2/q^2 = (3 \pm \sqrt{5})/2$. Thus $p/q = \theta$ or θ^{-1} where $\theta = (\sqrt{5} + 1)/2$, $\theta^{-1} = (\sqrt{5} - 1)/2$. Thus the set reduces to the 12 points $(\pm\theta, \pm 1, 0)$, $(\pm 1, 0, \pm\theta)$, $(0, \pm\theta, \pm 1)$, which as Coxeter [8] shows constitute the vertices of an icosahedron. Adding center points we get the icosahedron design given by Box and Hunter [3].

3. The formation of rotatable arrangements and rotatable designs by combination of several generated points sets. Consider the set $G(a, a, a)$; this consists of the eight points

$$\text{(3.1)} \qquad (\pm a, \quad \pm a, \quad \pm a)$$

each occurring three times. We may therefore denote this set of 8 points by $\frac{1}{3}G(a, a, a)$.

$$\text{(3.2)} \qquad \text{Ex}[\tfrac{1}{3}G(a, a, a)] = -16a^4,$$

which is always negative, hence this set alone cannot form a rotatable arrangement.

Consider the set $G(c, 0, 0)$; this consists of the six points

$$\text{(3.3)} \qquad (\pm c, 0, 0), \qquad (0, \pm c, 0), \qquad (0, 0, \pm c)$$

each occurring four times. The six points may be denoted by $\frac{1}{4}G(c, 0, 0)$.

$$\text{(3.4)} \qquad \text{Ex}[\tfrac{1}{4}G(c, 0, 0)] = 2c^4,$$

which is always positive, and so this set alone cannot form a rotatable arrangement.

For consistency of notation we may write the point $(0, 0, 0)$ as $(1/24)G(0, 0, 0)$. Hence n_0 center points may be denoted by

$$\frac{n_0}{24} G(0, 0, 0). \tag{3.5}$$

Consider the combination of sets $\frac{1}{3}G(a, a, a)$ and $\frac{1}{4}G(c, 0, 0)$. Then

$$\text{Ex}[\tfrac{1}{3}G(a, a, a) + \tfrac{1}{4}G(c, 0, 0)] = -16a^4 + 2c^4. \tag{3.6}$$

This is zero if $c^2 = 2\sqrt{2}a^2$, in which case the 14 points form a rotatable arrangement. The actual design points are obtained by applying the scaling condition $\lambda_2 = 1$. This gives $8a^2 + 2c^2 = N = 14 + n_0$, where n_0 is the number of center points added. Thus $4(2 + \sqrt{2})a^2 = N$, and both a and c are determined when N is given. We have obtained the well-known cube plus octahedron design first presented by Box and Hunter [3].

The method may now be extended. We have seen that the combination of generated sets leads to a single design when only two parameters are present, as in the example just given, since the two conditions $\text{Ex(set)} = 0$, $\lambda_2 = 1$, completely determine the design. The first condition alone completely determines the ratio of the two parameters and is sufficient to determine the design apart from scale. We now examine a combination of sets which contains three parameters. We shall see that we obtain a single infinity of designs which depend on a single parameter ratio. Consider the 20 points

$$\tfrac{1}{4}G(c_1, 0, 0), \qquad \tfrac{1}{4}G(c_2, 0, 0), \qquad \tfrac{1}{3}G(a, a, a).$$

The excess of this whole set is $2c_1^4 + 2c_2^4 - 16a^4$. Note that since $\text{Ex}[\frac{1}{3}G(a, a, a)] = -16a^4$ is negative, we must combine with it sets at least one of which has positive excess to compensate. Thus the set has zero excess if $c_1^4 + c_2^4 = 8a^4$. Set $c_1^2 = xa^2$, $c_2^2 = ya^2$. Then $x^2 + y^2 = 8$. Any positive values of x and y which satisfy this equation will give rise to a rotatable arrangement of second order. Thus if (x, y) is a point of the circle $x^2 + y^2 = 8$ and also lies in the first quadrant, then we shall have a rotatable arrangement. No additional center points are required to make the arrangement into a design since three radii of the parts of the arrangement: $x^{1/2}a$, $y^{1/2}a$ and $\sqrt{3}a$ are not all equal. Now $N\lambda_2 = 2c_1^2 + 2c_2^2 + 8a^2 = 2(x + y + 4)a^2$. Applying the scaling condition $\lambda_2 = 1$, we obtain

$$y = \sqrt{8 - x^2} \qquad a = [N/2(x + y + 4)]^{1/2}, \qquad c_1 = x^{1/2}a, \qquad c_2 = y^{1/2}a,$$

and the design becomes completely determined. For this class, $\lambda_4/\lambda_2^2 = 8a^4/N$. We now derive, as special cases of the infinite class just obtained, two designs which were previously known.

(1) $x = 0$. Then $y = 2\sqrt{2}$, $c_2 = c^{\frac{3}{4}}a$, $c_1 = 0$. We have obtained the cube plus octahedron design, with 6 center points which are vertices of the degenerate octahedron.

(2) $x = y = 2$. Then $c_1 = c_2 = a\sqrt{2}$. This gives rise to the design described by Gardiner, Grandage and Hader, which consists of the vertices of a cube plus those of a doubled octahedron ([9], Sec. 6, Par. 6, first stage).

The first summary table which occurs in Section 5 contains several other infinite classes of this type.

4. Classes of designs using sets with variable excess. In the previous section the sets we used in combination had a positive or a negative excess. Let us now consider the set of 12 points $\frac{1}{2}G(p, q, 0)$. The excess of this set is $4(p^4 + q^4 - 3p^2q^2)$, a quantity which may be made positive or negative according to the way p and q are chosen. Thus $\frac{1}{2}G(p, q, 0)$ may be combined with all of the sets $\frac{1}{3}G(a, a, a)$, $\frac{1}{4}G(c, 0, 0)$ and $\frac{1}{2}G(f, f, 0)$ to obtain rotatable arrangements and hence designs. For example, $\mathrm{Ex}[\frac{1}{2}G(p, q, 0) + \frac{1}{3}G(a, a, a)] = 0$ if $p^4 + q^4 = 3p^2q^2 + 4a^4$. Set $p^2 = xa^2$, $q^2 = ya^2$, and we have $x^2 - 3xy + y^2 = 4$. Any point of this hyperbola which lies in the first quadrant will give rise to a rotatable arrangement of second order. If we solve for y in terms of x, we obtain $y = [3x \pm \sqrt{5x^2 + 16}]/2$. This yields two positive solutions if $x > 2$; otherwise only one positive solution arises. This may easily be seen from Fig. 2. The radii of the separate point sets are $\sqrt{x + y}a$ and $\sqrt{3}a$ and these are equal when $x + y = 3$. Since the straight line $x + y = 3$ intersects the hyperbola in two points P and Q, equality in (1.3) occurs for two arrangements of the class. For these two arrangements, the addition of center points is necessary to satisfy the non-singularity condition. Applying the scaling condition $\lambda_2 = 1$, we obtain an infinite class of second order rotatable designs, each design consisting of 20 points plus any center points which may have been added. The class depends on one parameter x. Given $x \geqq 0$,

$$y = [3x \pm \sqrt{5x^2 + 16}]/2, \quad a = [N/4(x + y + 2)]^{1/2}, \quad p = x^{1/2}a, \quad q = y^{1/2}a,$$

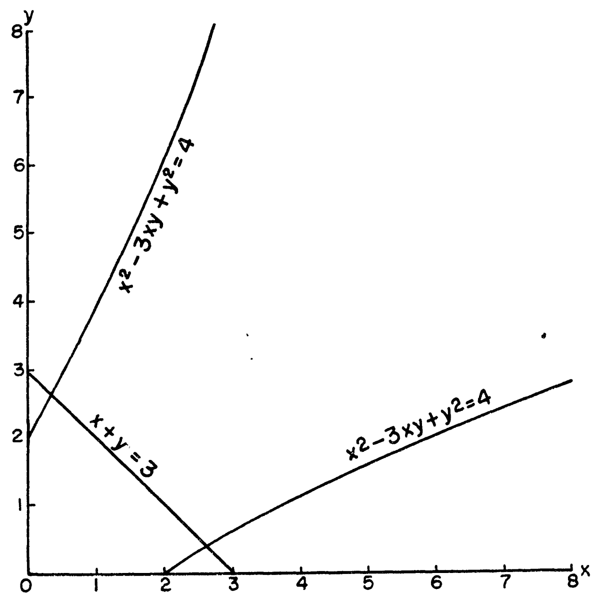

FIG. 2

where the lower sign in y is to be taken only when $x > 2$. For this class

$$\lambda_4/\lambda_2^2 = (8a^4 + 4p^2q^2)/N = 4(2 + xy)a^4/N.$$

This class has two well-known special cases.

(1) When $a = 0$, $x = \infty$, $y = \infty$. Ignoring the degenerate set $\frac{1}{3}G(a, a, a)$, we obtain the icosahedron design discussed at the end of Section 2.

(2) If we choose one of the two points on the hyperbola for which $x + y = 3$, then $x = y^{-1} = (3 \pm \sqrt{5})/2 = \theta^2, \theta^{-2}$, where $\theta = (\sqrt{5} + 1)/2$. Thus the 20 design points (other than the center points) consist of constant multiples of

$$(0, \pm\theta^{-1}, \pm\theta), \quad (\pm\theta, 0, \pm\theta^{-1}), \quad (\pm\theta^{-1}, \pm\theta, 0), \quad (\pm1, \pm1, \pm1).$$

As Coxeter [8] shows, these are the vertices of a dodecahedron, which form a well-known second order rotatable design, given in [3].

Several other classes of this type may be found in the summary table.

5. Summary table. Table I is a table of infinite classes of second order rotatable designs in three dimensions of the type derived in Sections 3 and 4. The table shows the generated sets used to form each class together with the design coordinate values in terms of a single parameter.

6. A second method of generating point sets suitable for building second order rotatable designs. Define

$$T_1 = \begin{bmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad T_2 = \begin{bmatrix} \cos\frac{\alpha}{2} & \sin\frac{\alpha}{2} & 0 \\ \sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

where $\alpha = 2\pi/s$. Consider the effect of applying T_1 and T_2 to points of the form $(r, 0, b)$, i.e., points on the plane $y = 0$, and to all other points obtained from repeated applications of T_1 and T_2. In this way we shall obtain $2s$ points with coordinates

$$(6.1) \quad (r\cos t\alpha, r\sin t\alpha, b), \qquad (r\cos(t + \tfrac{1}{2})\alpha, r\sin(t + \tfrac{1}{2})\alpha, -b),$$

where $t = 0, 1, 2, \cdots, (s - 1)$. We shall denote the set of these $2s$ points by $T_z(r, 0, b)$. Provided $s \geqq 5$, the set $T_z(r, 0, b)$ has the following sums of powers and products:

$$\sum_u x_u^2 = \sum_u y_u^2 = sr^2, \qquad \sum_u z_u^2 = 2sb^2,$$
$$\sum_u x_u^4 = \sum_u y_u^4 = 3sr^4/4, \qquad \sum_u z_u^4 = 2sb^4,$$
$$\sum_u x_u^2 y_u^2 = sr^4/4, \qquad \sum_u y_u^2 z_u^2 = \sum_u z_u^2 x_u^2 = sr^2b^2,$$

and all other sums of powers and products up to and including order four are zero. This is easily verified by using the fact that each of the two s-gons in the set of $2s$ points is a second order rotatable arrangement in two dimensions [3].

A rotation about the z axis of the complete point arrangement will not affect the properties held by the sums of powers and products. We now recall the cyclic group W, W^2, I, defined in Section 2, and apply this to $T_z(r, 0, b)$ to give set $T_x(b, r, 0)$ and $T_y(0, b, r)$. In all we now have $6s$ points, which we denote by $T(r, 0, b)$ with coordinates

$$(r \cos t\alpha, r \sin t\alpha, b), \qquad (r \cos (t + \tfrac{1}{2})\alpha, r \sin (t + \tfrac{1}{2})\alpha, -b),$$
$$(b, r \cos t\alpha, r \sin t\alpha), \qquad (-b, r \cos (t + \tfrac{1}{2})\alpha, r \sin (t + \tfrac{1}{2})\alpha),$$
$$(r \sin t\alpha, b, r \cos t\alpha), \qquad (r \sin (t + \tfrac{1}{2})\alpha, -b, r \cos (t + \tfrac{1}{2})\alpha),$$

where $\alpha = 2\pi/s$ ($s \geqq 5$) and $t = 0, 1, 2, \cdots, (s - 1)$.

The set $T(r, 0, b)$ has sums of powers and products

$$\sum_u x_u^2 = \sum_u y_u^2 = \sum_u z_u^2 = 2s(r^2 + b^2),$$
$$\sum_u x_u^4 = \sum_u y_u^4 = \sum_u z_u^4 = s(3r^4 + 4b^4)/2,$$
$$\sum_u x_u^2 y_u^2 = \sum_u y_u^2 z_u^2 = \sum_u z_u^2 x_u^2 = sr^2(r^2 + 8b^2)/4,$$

and all other sums of powers and products up to and including order four are zero.

The formulae for the sums of powers and products will extend to the case $s = 4$, provided we fix as the set $T_z(r, 0, b)$ the points

$$(\pm r, 0, b), \qquad (0, \pm r, b), \qquad (\pm r/\sqrt{2}, \pm r/\sqrt{2}, -b).$$

In the case $s = 4$, rotation of the s-gons about the z axis will affect the sums of powers and products and thus cannot be permitted. This point must be remembered whenever specific reference is made to the case $s = 4$. From the properties of sums of powers and products given above, it follows that the excess of the set, defined in the same way as before, is $s(3r^4 - 24r^2b^2 + 8b^4)/4$. Of course the excess of each single point varies in this case and it is necessary to consider the total effect over all the points. Since its excess can be made positive or negative according to the choice of r and b, it will be possible to combine the set $T(r, 0, b)$ with sets of both positive and negative excess. Because of the large number of points which would otherwise arise, we shall combine it only with $\frac{1}{3}G(a, a, a)$ and $\frac{1}{4}G(c, 0, 0)$. The designs thus obtained will be found in the second summary table below.

In the same way that special choices of x, y, and z made it possible to take fractions of $G(x, y, z)$, a special choice of b will enable us to use a smaller point set than $T(r, 0, b)$. Set $b = 0$; then by employing only the transformation T_1 and W we can produce a set of $3s$ points with suitable moment properties. We shall denote these $3s$ points by the notation $T_0(r, 0, 0)$. The points will have coordinates

$$(r \cos t\alpha, r \sin t\alpha, 0), \qquad (r \sin t\alpha, 0, r \cos t\alpha), \qquad (0, r \cos t\alpha, r \sin t\alpha),$$

TABLE I

Set	$G(p, q, r)$	$\frac{1}{2}G(p, q, 0)$	$\frac{1}{3}G(a,a,a)$	$\frac{1}{4}G(c,0,0)$	Number of points in design class	Range of first parameter ratio on which class depends	Second parameter ratio in terms of first	Design point coordinate values in terms of N and parameter ratios	Value of λ_4/λ_2^2
Points	$(\pm p, \pm q, \pm r)$ etc.	$(\pm p, \pm q, 0)$ etc.	$(\pm a, \pm a, \pm a)$	$(\pm c, 0, 0)$ etc.					
No. of points	24	12	8	6					
	Number of sets used for class								
	1				24	$0 \leqq t \leqq (3 - \sqrt{5})/2$ $t \geqq (3 + \sqrt{5})/2$	$s = \frac{1}{2}[3(t+1) \pm \sqrt{5(t^2 + 6t + 1)}]$	$r = [N/8(s + t + 1)]^{1/2}$ $p = s^{1/2}r, \quad q = t^{1/2}r$	$8(st + s + t)r^4/N$
			1	2	20	$0 \leqq x \leqq 2\sqrt{2}$	$y = \sqrt{8 - x^2}$	$a = [N/2(x + y + 4)]^{1/2}$ $c_1 = x^{1/2}a, \quad c_2 = y^{1/2}a$	$8a^4/N$
			2	1	22	$0 \leqq x \leqq \frac{1}{2\sqrt{2}}$	$y = \sqrt{\frac{1}{8} - x^2}$	$c = [N/2(4x + 4y + 1)]^{1/2}$ $a_1 = x^{1/2}c, \quad a_2 = y^{1/2}c$	c^4/N
		1 $p = q = f$		2	24	$0 \leqq x \leqq 1$	$y = \sqrt{2 - x^2}$	$f = [N/2(x + y + 4)]^{1/2}$ $c_1 = x^{1/2}f, c_2 = y^{1/2}f$	$4f^4/N$
		1 $p = q = f$	1	1	26	$0 \leqq x \leqq \frac{1}{2\sqrt{2}}$	$y = [(1 - 2x^2)/8]^{1/2}$	$c = [N/2(4x + 4y + 1)]^{1/2}$ $f = x^{1/2}c, a = y^{1/2}c$	$4(x^2 + 2y^2)c^4/N$
		1	1		20	$x \geqq 0$	$y = \frac{1}{2}[3x \pm \sqrt{5x^2 + 16}]$	$a = [N/4(x + y + 2)]^{1/2}$ $p = x^{1/2}a, q = y^{1/2}a$	$4(2 + xy)a^4/N$
		1		1	18	$x \geqq 0.63$	$y = \frac{1}{2}[3x \pm \sqrt{5x^2 - 2}]$	$c = [N/2(2x + 2y + 1)]^{1/2}$ $p = x^{1/2}c, q = y^{1/2}c$	$4xyc^4/N$

		2 (one $p = q = f$)			24	$x \geqq 0$	$y = \frac{1}{2}[3x \pm \sqrt{5x^2 + 4}]$	$f = [N/4(x + y + 2)]^{1/2}$ $p = x^{1/2}f,\ q = y^{1/2}f$	$4(xy + 1)f^4/N$
	1 $q = r$		1		32	$x \geqq \sqrt{2}$	$y = \sqrt{10x^2 - 2} - 3x$	$a = [N/8(x + 2y + 1)]^{1/2}$ $p = x^{1/2}a,\ q = y^{1/2}a$	$8(2xy + y^2 + 1)a^4/N$
	1 $q = r$			1	30	$x \geqq 0$	$y = \sqrt{10x^2 + \frac{1}{4}} - 3x$	$c = [N/2(4x + 8y + 1)]^{1/2}$ $p = x^{1/2}c,\ q = y^{1/2}c$	$2(8xy + 4y^2 + 1)c^4/N$

where $t = 0, 1, 2, \cdots, (s-1)$ and $s \geqq 5$. The sums of powers and products of the set are

$$\sum_u x_u^2 = \sum_u y_u^2 = \sum_u z_u^2 = sr^2,$$

$$\sum_u x_u^4 = \sum_u y_u^4 = \sum_u z_u^4 = 3sr^4/4,$$

$$\sum_u x_u^2 y_u^2 = \sum_u y_u^2 z_u^2 = \sum_u z_u^2 x_u^2 = sr^4/8,$$

and all other sums of powers and products up to and including order four are zero.

Clearly any rotation of the 3 s-gons about their axes will also give rise to the same moments, but we shall restrict attention here to the set $T_0(r, 0, 0)$. From the sums of powers and products it follows that the excess of this set is $3sr^4/8$ which is a positive excess. Thus to form an infinite class of second order designs we must combine $T_0(r, 0, 0)$ with sets at least one of which has negative excess Two examples of this will be found in Table II.

7. An extension of the method: a 16 point design class. Consider the set of 12 points

$$\begin{array}{cccc} (x, y, z), & (x, -y, -z), & (-x, y, -z), & (-x, -y, z), \\ (y, z, x), & (-y, -z, x), & (y, -z, -x), & (-y, z, -x), \\ (z, x, y), & (-z, x, -y), & (-z, -x, y), & (z, -x, -y). \end{array} \tag{7.1}$$

This set consists of all points of $G(x, y, z)$ for which the product of the coordinates is xyz. It can be described as a $\frac{1}{2}$ replicate of $G(x, y, z)$ and we shall write it

$$G^{(+\frac{1}{2})}(x, y, z). \tag{7.2}$$

The complementary set, where the product of the coordinates is $-xyz$, we shall denote by

$$G^{(-\frac{1}{2})}(x, y, z). \tag{7.3}$$

The set (7.2) satisfies all the conditions for a second order rotatable arrangement except two. These are

$$\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2, \qquad (i, j = 1, 2, 3), \qquad (i \neq j) \tag{7.4}$$

and

$$\sum_{u=1}^{N} x_{1u} x_{2u} x_{3u} = 0. \tag{7.5}$$

We recall that

$$\begin{aligned} \text{Ex[Point set}(x_{1u}, x_{2u}, x_{3u}), \quad u = 1, 2, \cdots, N] &= \sum_{u=1}^{N} x_{iu}^4 - \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2, \\ (i, j = 1, 2, 3), &\qquad (i \neq j) \end{aligned} \tag{7.6}$$

TABLE II

Set......	$T(r,0,b)$	$T_0(r,0,0)$	$\frac{1}{3}G(a,a,a)$	$\frac{1}{4}G(0,0,c)$	Number of points in design class	Range of first parameter ratio on which class depends	Second parameter ratio in terms of first	Design point coordinate values in terms of N and parameter ratios	Value of λ_4/λ_2^2
Points....	(r cos $t\alpha$, r sin $t\alpha$, b etc.)	(r cos $t\alpha$, r sin $t\alpha$, 0) etc.	$(\pm a, \pm a, \pm a)$	$(\pm c,0,0)$ $(0,\pm c,0)$ $(0,0,\pm c)$					
No. of points .	s≧4 6s	s≧5 3s	8	6					
	Number of sets used for class								
	1		1		$6s + 8$ $s \geqq 4$	$x \geqq 0$	$y = \frac{1}{4}[6x \pm \sqrt{30x^2 + 128/s}$	$a = [N/2(s(x+y) + 4)]^{1/2}$ $r = x^{1/2}a,\ b = y^{1/2}a$	$\frac{[sx(x + 8y) + 32]a^4}{4N}$
	1			1	$6s + 6$ $s \geqq 4$	$x \geqq \sqrt{8/15s}$	$y = \frac{1}{4}[6x \pm \sqrt{30x^2 - 16/s}$	$c = [N/2(s(x+y) + 1)]^{1/2}$ $r = x^{1/2}c,\ b = y^{1/2}c$	$\frac{[sx(x + 8y) + 8]c^4}{4N}$
		1	2		$3s + 16$ $s \geqq 5$	$0 \leqq x \leqq \sqrt{3s/256}$	$y = \sqrt{3s/128 - x^2}$	$r = [N/(8x + 8y + s)]^{1/2}$ $a_1 = x^{1/2}r,\ a_2 = y^{1/2}r$	$5sr^4/16N$
		1	1	1	$3s + 14$ $s \geqq 5$	$0 \leqq x \leqq \sqrt{128/3s}$	$y = \frac{1}{4}\sqrt{128 - 3sx^2}$	$a = [N/(sx + 2y + 8)]^{1/2}$ $r = x^{1/2}a,\ c = y^{1/2}a$	$(64 + sx^2)a^4/8N$

Let us define a second excess function which relates to the left member of (7.5) as

$$\text{(7.7)} \quad \text{Fx[Point set } (x_{1u}, x_{2u}, x_{3u}), \quad u = 1, 2, \cdots, N] = \sum_{u=1}^{N} x_{1u}x_{2u}x_{3u} .$$

Then if S is a point set or a combination of points sets which satisfies all of conditions (1.2) except (7.4) and (7.5), and if

$$\text{(7.8)} \qquad \text{Ex}(S) = 0, \qquad Fx(S) = 0,$$

then S is a rotatable arrangement of the second order. Now

$$\text{(7.9)} \qquad \text{Ex}[G^{(\pm\frac{1}{2})}(x, y, z)] = 4(x^4 + y^4 + z^4 - 3y^2z^2 - 3z^2x^2 - 3x^2y^2)$$

$$\text{(7.10)} \qquad \text{Fx}[G^{(\pm\frac{1}{2})}(x, y, z)] = \pm 12\, xyz.$$

The set $G^{(+\frac{1}{2})}(a, a, a)$ consists of the four points

$$\text{(7.11)} \quad (a, a, a), \quad (a, -a, -a), \quad (-a, a - a), \quad (-a, -a, a),$$

each repeated three times. Thus we may denote the four points (7.11) which form a half replicate of the 2^3 factorial design, by $\frac{1}{3}G^{(\frac{1}{2})}(a, a, a)$. Similarly the set $\frac{1}{3}G^{(-\frac{1}{2})}(a, a, a)$ consists of the four point

$$(-a, -a, -a), \qquad (-a, a, a), \qquad (a, -a, a), \qquad (a, a, -a).$$

It is easily seen that

$$\text{Ex}[\tfrac{1}{3}G^{(\pm\frac{1}{2})}(a, a, a)] = -8a^4, \qquad \text{Fx}[\tfrac{1}{3}G^{(\pm\frac{1}{2})}(a, a, a)] = \pm 4a^3.$$

Let S be the set of 16 points defined by

$$S = G^{(+\frac{1}{2})}(x, y, z) + \tfrac{1}{3}G^{(-\frac{1}{2})}(a, a, a),$$

$$\text{Ex}(S) = -8a^4 + 4(x^4 + y^4 + z^4 - 3y^2z^2 - 3z^2x^2 - 3x^2y^2),$$

$$\text{Fx}(S) = 12\, xyz - 4a^3.$$

Thus S is a rotatable arrangement if

$$\text{(7.12)} \qquad x^4 + y^4 + z^4 - 3(y^2z^2 + z^2x^2 + x^2y^2) = 2a^4, \qquad 3\, xyz = a^3.$$

If we set

$$\text{(7.13)} \qquad x^2 = ua^2, \qquad y^2 = va^2, \qquad z^2 = wa^2,$$

it follows from (7.12) that we can write

$$u + v + w = \beta, \qquad uv + vw + wu = (\beta^2 - 2)/5, \qquad uvw = 1/9.$$

These equations imply that u, v and w are the roots of the cubic

$$\text{(7.14)} \qquad t^3 - \beta t^2 + (\beta^2 - 2)t/5 - 1/9 = 0.$$

If for a given β this cubic has three positive roots u, v and w, we shall be able to use these values to obtain a rotatable arrangement of the second order which contains only 16 points, using the relations (7.13). A sufficient condition for

$$Ax^3 + Bx^2 + Cx + D = 0 \tag{7.15}$$

to have three positive roots (provided all roots are real) is $A > 0$, $B < 0$, $C > 0$, $D < 0$. Thus if $\beta > \sqrt{2}$ and all three roots of (7.14) are real, they are all positive. The necessary and sufficient condition for (7.15) to have three real roots is $\Delta = B^2C^2 + 18ABCD - 4AC^3 - 27A^2D^2 - 4B^3D > 0$ (see Conkwright [7]). For the equation (7.14) we find

$$\Delta(\beta) = 3645(9\beta^6 + 36\beta^4 - 50\beta^3 - 252\beta^2 - 900\beta - 87). \tag{7.16}$$

It may be shown that $\Delta(2.691376)/3645 = .0031$, $\Delta(2.691375)/3645 = -.04$, so that a root of $\Delta = 0$ lies near $\beta = 2.691376$. Furthermore

$$\Delta(2.691376 + s)/3645 = .0031 + \Delta_1(s),$$

where $\Delta_1(s)$ is the following sixth degree polynomial in s with all coefficients positive:

$$\Delta_1(s) = 9s^6 + 145.3s^5 + 1013.9s^4 + 3846.7s^3 + 7992.1s^2 + 7089.8s$$

Hence $s > 0 \Rightarrow \Delta_1(s) > 0 \Rightarrow \Delta(2.691376 + s) > 0$, and

$$\Delta(\sqrt{2})/3645 = -1789, \quad \Delta''(\beta)/7290 = 135\beta^4 + 216\beta^2 - 150\beta - 250 > 0 \quad \text{for } \beta > \sqrt{2}.$$

TABLE III

A Selection of Designs from the 16 Point Series (when $n_0 = 0$)

β	a	x	y	z	λ_4/λ_2^2
2.691376	1.04096	.49090	.49090	1.56026	.60140
2.7	1.03975	.45968	.52238	1.56036	.60131
3	1.00000	.31645	.67348	1.56405	.60000
4	.89443	.18375	.82366	1.57775	.60800
5	.81650	.12862	.88669	1.59078	.62222
6	.75593	.09737	.92330	1.60206	.63673
7	.70711	.07722	.94697	1.61160	.65000
8	.66667	.06328	.96348	1.61965	.66173
9	.63246	.05321	.97559	1.62647	.67200
11	.57735	.03951	.99212	1.63732	.68889
14	.51640	.02767	1.00687	1.64887	.70756
19	.44721	.01759	1.02001	1.66110	.72800
49	.28284	.00430	1.04018	1.68464	.76928
99	.20000	.00151	1.04601	1.69288	.78432
∞	0	0	1.05146	1.70130	.80000

When $n_0 = 0$, multiply a, x, y and z by α and multiply λ_4/λ_2^2 by α^2, where $\alpha^2 = 1 + (n_0/16)$.

The variation in the values of a x, y and z is so well controlled that it is possible to use a graph to find their values for values of β other than those in the table.

This means that the function Δ is convex for $\beta > \sqrt{2}$ and thus has only one root in that range which must be at approximately $\beta = 2.691376$. Thus if $\beta > 2.7$ the equation (7.14) gives rise to three real positive roots u, v and w and the 16 points of S form a second order rotatable arrangement. The radii of the two sets of points which comprise the arrangement are $\sqrt{\beta}\, a$ and $\sqrt{3}\, a$. Thus, when $\beta = 3$ it will be necessary to add center points to the arrangement in order to satisfy the non-singularity condition. It is desirable to add center points to arrangements which arise from values of β near the singular value 3 in order that the variances of the estimates of the model coefficients will not be large. When $a = 0$, we shall retain the degenerate points as center points. If $N = 16 + n_0$ where n_0 is the number of center points added, it is easy to verify that the scaling condition $\lambda_2 = 1$ leads to $a^2 = N/4(\beta + 1)$. Thus we have found an infinite class of second order rotatable designs depending on a parameter β; each design contains 16 points excluding any center points which may have been added. Given a value of $\beta > 2.691376$, we can find u, v and w, the positive roots of (7.14). Then

$$a = [N/4(\beta + 1)]^{\frac{1}{2}}, \qquad x = u^{\frac{1}{2}}a, \qquad y = v^{\frac{1}{2}}a, \qquad z = w^{\frac{1}{2}}a,$$

and the design is completely determined. An easy calculation shows that

$$\lambda_4/\lambda_2^2 = (\beta^2 + 3)N/20(\beta + 1)^2. \tag{7.17}$$

Table III contains some of the designs of this series. The table was obtained by substituting for β in (7.14) a specific value and solving the cubic equation. Only the range $\beta > 2.691376$ need be considered. The values given for x, y, z and a are those to be used when $n_0 = 0$, i.e., when no center points are added; for n_0 center points these values must be multiplied by the factor $\alpha = [1 + (n_0/16)]^{\frac{1}{2}}$. The design points are obtained from (7.1) and (7.11) with appropriate values for x, y, z and a from the table. The value of λ_4/λ_2^2 in the table is calculated from (7.17) when $N = 16$. For n_0 center points these values must be multiplied by $\alpha^2 = 1 + (n_0/16)$.

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