THIRD ORDER ROTATABLE DESIGNS IN THREE DIMENSIONS[1]

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0. Summary. Two recent papers by Bose and Draper [1] and Draper [3] showed how it was possible, by combining certain sets of points, to construct infinite classes of second order rotatable designs in three and more dimensions. In this paper, *third order* rotatable designs in three dimensions are discussed. First, a general theorem is proved that provides the conditions under which a third order rotatable arrangement of points in k dimensions is non-singular. The four previously known third order designs in three dimensions are stated; it is then shown how some of the second order design classes constructed earlier [1] may be combined in pairs to give infinite classes of sequential third order rotatable designs in three dimensions. One example of such a combination is worked out in full and it is shown that two of the four known designs are special cases of this class. A summary of further third order rotatable design classes that have been shown to exist, and that have been tabulated by the author, concludes the paper.

1. Introduction. 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 [2] suggested designs of a certain type, which they called rotatable, as being suitable for such experimentation. Such designs permit a response surface to be fitted easily and provide spherical information contours. A second order rotatable design aids the fitting of a second order (i.e., a quadratic) surface, and a third order rotatable design aids the fitting of a third order (i.e., a cubic) surface.

Let us assume that the measurements of the k factors have been coded, permitting the use of cartesian axes in k-dimensional space to describe an experimental design for k factors. Suppose that, in an experimental investigation with k factors, N (not necessarily distinct) combinations of levels are employed. Thus

Received December 9, 1959.

[1] The early stages of this work, at the University of North Carolina, were supported in part by the United States Air Force through the Air Force Office of Scientific Research of the Air Research and Development Command under contract No. AF 18(600)-83 and in part by a Bell Telephone Graduate Fellowship Award to the author, who acknowledges gratefully his indebtedness. Sponsorship was also provided by the United States Army under Contract No. DA-11-022-ORD-2059 at the Mathematics Research Center. Reproduction in whole or part is permitted for any purpose of the United States Government.

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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}. This set of points is said to form a *rotatable arrangement* of the third order in k factors if

$$(1.2) \qquad \begin{aligned} \sum_u x_{1u}^2 &= \cdots = \sum_u x_{ku}^2 = \lambda_2 N, \quad \text{(say)}, \\ \sum_u x_{iu}^4 &= 3\sum_u x_{iu}^2 x_{ju}^2 = 3\lambda_4 N, \quad \text{(say)} \\ \sum_u x_{iu}^6 &= 5\sum_u x_{iu}^4 x_{ju}^2 = 15\sum_u x_{iu}^2 x_{ju}^2 x_{lu}^2 = 15\lambda_6 N, \quad \text{(say)}, \end{aligned}$$

where $i, j, l = 1, 2, \cdots, k, i \neq j \neq l \neq i, u = 1, 2, \cdots, N$, and all other similar sums of powers and products up to and including order six are zero. Conditions (1.2) and the condition variance $\hat{y}(\mathbf{x}) = f(\mathbf{x}'\mathbf{x})$ are equivalent. The N points of the arrangement are said to form a *rotatable design* of third order if they give rise to a non-singular $\mathbf{X}'\mathbf{X}$ matrix. By convention, the scale of the design is normally adjusted so that $\lambda_2 = 1$. (This adjustment is a convenience [1] and not an essential. In this paper designs are presented in terms of a parameter and scaling, which merely fixes this parameter, has not been performed.) The conditions for non-singularity of the $\mathbf{X}'\mathbf{X}$ matrix for the third order arrangement are

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

(this, alone, is the condition that the matrix for a second order design should be non-singular) and

$$(1.4) \qquad \lambda_6\lambda_2/\lambda_4^2 > (k + 2)/(k + 4).$$

These conditions are derived by Gardiner, Grandage and Hader [4]. Note that the left members of (1.3) and (1.4) are independent of the scale of the design.

For a third order design, the determinant of $\mathbf{X}'\mathbf{X}$ is proportional to $[(k + 2)\lambda_4 - k\lambda_2^2][(k + 4)\lambda_6\lambda_2 - (k + 2)\lambda_4^2]$. Thus, if either of these factors is zero, $\mathbf{X}'\mathbf{X}$ is singular and some of the coefficients in the third order polynomial to be fitted by least squares to the experimental results are not estimable. (These coefficients are given by $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$, in the usual notation, when $\mathbf{X}'\mathbf{X}$ is non-singular.) If either factor is very near to zero, some of the variances of the estimates are large and the design is said to be almost singular. It is impossible for either factor to be less than zero, i.e., for either of the inequalities (1.3) and (1.4) to be reversed, as will be shown.

Since the left member of (1.3) is of order N, this first inequality may always be satisfied merely by an increase in N which leaves the original points unaltered and which adds nothing to the sums of powers and products, namely by the addition of center points. However, the left member of (1.4) is of order zero in N and depends only on the points $(x_{1u}, \cdots, x_{ku})$, $u = 1, 2, \cdots, N$. Thus, if a third order arrangement is singular (i.e., gives rise to a singular matrix) because equality is attained in (1.4), the situation cannot be altered by the addition of center points. The question now arises: under what conditions is a third order arrangement singular? An exact answer to the question may be given as follows.

THEOREM: *A third order rotatable design in k dimensions is singular if and only if all of its points, excluding center points, lie on a k dimensional sphere centered at the origin.*

PROOF: Let

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

Then, if the points (1.1) satisfy the conditions (1.2),

$$S_4^{(i)} = \sum_{u=1}^{N} x_{iu}^4 = 3 \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2,$$

$$S_6^{(i)} = \sum_{u=1}^{N} x_{iu}^6 = 5 \sum_{u=1}^{N} x_{iu}^4 x_{ju}^2 = 15 \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 x_{lu}^2,$$

$i, j, l = 1, 2, \cdots, k, i \neq j \neq l \neq i$, and $S_j^{(i)}$ may be denoted by S_j since it is independent of i if conditions (1.2) hold. It follows that

$$\begin{aligned} kS_6 = \sum_{i=1}^{k} S_6^{(i)} &= \sum_{u=1}^{N} \sum_{i=1}^{k} x_{iu}^6 = \sum_{u=1}^{N} (x_{1u}^6 + x_{2u}^6 + \cdots + x_{ku}^6) \\ &= \sum_{u=1}^{N} \left[(x_{1u}^2 + \cdots + x_{ku}^2)^3 - 3 \sum_{i \neq j} x_{iu}^4 x_{ju}^2 - \sum_{i \neq j \neq l} x_{iu}^2 x_{ju}^2 x_{lu}^2 \right] \\ &= \sum_{u=1}^{N} r_u^6 - 3k(k-1) \sum_{u=1}^{N} x_{1u}^4 x_{2u}^2 - k(k-1)(k-2) \sum_{u=1}^{N} x_{1u}^2 x_{2u}^2 x_{3u}^2 \\ &= \sum_{u=1}^{N} r_u^6 - 3k(k-1)S_6/5 - k(k-1)(k-2)S_6/15 \end{aligned}$$

where $r_u^2 = x_{1u}^2 + x_{2u}^2 + \cdots + x_{ku}^2$. Solving for S_6 and referring to (1.2), we obtain

$$15\lambda_6 N = S_6 = 15 \sum_{u=1}^{N} r_u^6 / k(k+2)(k+4).$$

Similarly

$$3\lambda_4 N = S_4 = 3 \sum_{u=1}^{N} r_u^4 / k(k+2), \qquad \lambda_2 N = S_2 = \sum_{u=1}^{N} r_u^2 / k.$$

Hence

$$\frac{\lambda_4}{\lambda_2^2} = N \frac{\sum_{u=1}^{N} r_u^4}{\left\{ \sum_{u=1}^{N} r_u^2 \right\}^2} \frac{k}{k+2}.$$

(This expression is equal to $k/(k + 2)$ if and only if all points lie on a sphere and it can be increased merely by an increase in N, i.e., by an addition of center points.) Also

$$\frac{\lambda_6 \lambda_2}{\lambda_4^2} = \frac{\left\{\sum_{u=1}^{N} r_u^6\right\}\left\{\sum_{u=1}^{N} r_u^2\right\}}{\left\{\sum_{u=1}^{N} r_u^4\right\}^2} \frac{k+2}{k+4} = F\frac{k+2}{k+4}, \quad \text{say.}$$

Now, by the Cauchy-Schwartz inequality [5], the factor F is greater than unity unless all the non-zero r_u are equal, when unity is attained and the right hand side reduces to $(k + 2)/(k + 4)$. Thus the arrangement is singular if and only if all its points (excluding center points) lie on a sphere in k dimensions.

Hence in order to get usable third order designs, we must combine at least two spherical sets of points with different positive radii.

2. The known third order rotatable designs in three dimensions. We may divide third order designs into two groups, sequential and non-sequential. A sequential design can be performed in two parts. One part is a second order rotatable design which may be run first; then, if the second order polynomial approximation is found to be inadequate, the trials of the second part may be run and a third order surface fitted. Such designs are more useful in practice than the non-sequential type, of which all the trials must be run at one time in order to make a rotatable least squares fitting possible.

Only four third order designs are known in three dimensions [4]; these contain points which are the vertices of

(2.1)
(a) icosahedron plus dodecahedron (32 points),
(b) cube plus two octahedra plus cuboctahedron (32 points),
(c) (cube plus octahedron) plus (truncated cube plus octahedron) (44 points),
(d) (cube plus doubled octahedron) plus (truncated cube plus octahedron) (50 points).

Bose and Draper introduced [1] a point set notation in which the 24 points $(\pm p, \pm q, \pm r)$, $(\pm q, \pm r, \pm p)$, $(\pm r, \pm p, \pm q)$ were denoted by $G(p, q, r)$. The eight points $(\pm a, \pm a, \pm a)$ were then denoted by $\frac{1}{3}G(a, a, a)$, since $G(a, a, a)$ consists of the eight points $(\pm a, \pm a, \pm a)$ three times over. Other sets of points, derivable from $G(p, q, r)$ by setting some of p, q and r zero or equal to one another, were similarly described. If we translate the designs (2.1) into this notation, they become

(2.2)
(a) $\frac{1}{2}G(p_1, q_1, 0) + \frac{1}{2}G(p_2, q_2, 0) + \frac{1}{3}G(a, a, a)$,
(b) $\frac{1}{3}G(a, a, a) + \frac{1}{4}G(c_1, 0, 0) + \frac{1}{4}G(c_2, 0, 0) + \frac{1}{2}G(f, f, 0)$,
(c) $[\frac{1}{3}G(a, a, a) + \frac{1}{4}G(c_1, 0, 0)] + [G(p, q, q) + \frac{1}{4}G(c_2, 0, 0)]$,
(d) $[\frac{1}{3}G(a, a, a) + \frac{1}{2}G(c_1, 0, 0)] + [G(p, q, q) + \frac{1}{4}G(c_2, 0, 0)]$,

where in each case the values of the parameters are determined by the rotatability conditions, and will not be quoted here.

Design (a) is such that the radii of the two spheres on which all its points lie are very nearly equal. In fact, $\lambda_2\lambda_6/\lambda_4^2 = (1.00028)5/7$, which means that the design is almost singular. Thus the variances of the linear and cubic coefficients are very large. This design is of the sequential type. Design (b) is a combination of our basic generated sets and is non-sequential. Designs (c) and (d) are both sequential; (c) is almost singular, as was noted in the original presentation.

3. The construction of infinite classes of third order rotatable designs in three dimensions. We shall now show how to obtain infinite classes of third order designs of the sequential type by making use of the previously derived [1] second order classes. In order to do this, we shall find it necessary to construct additional functions similar to the excess function previously introduced in [1].

We recall that

$$Ex[G(p, q, r)] = 8(p^4 + q^4 + r^4 - 3p^2q^2 - 3q^2r^2 - 3r^2p^2). \tag{3.1}$$

Additionally we define

$$\begin{aligned} Ax[G(p, q, r)] &= 8(p^2 + q^2 + r^2), \\ Gx[G(p, q, r)] &= 8(p^4q^2 + q^4r^2 + r^4p^2 - p^2q^4 - q^2r^4 - r^2p^4), \\ Hx[G(p, q, r)] &= 8(p^6 + q^6 + r^6 - 45p^2q^2r^2), \\ Ix[G(p, q, r)] & \\ &= 4(p^4q^2 + q^4r^2 + r^4p^2 + p^2q^4 + q^2r^4 + r^2p^4 - 18p^2q^2r^2). \end{aligned} \tag{3.2}$$

Note that, for the point set $G(p, q, r)$,

$$\begin{aligned} &\sum_u x_{iu}^2 = Ax(G), \qquad \sum_u x_{iu}^4 = 8(p^4 + q^4 + r^4), \\ &\qquad\qquad \sum_u x_{iu}^2x_{ju}^2 = 3(p^2q^2 + q^2r^2 + r^2p^2), \\ &\sum_{\substack{u \\ i>j}} x_{iu}^4\, x_{ju}^2 = 8(p^4q^2 + q^4r^2 + r^4p^2), \\ &\qquad\qquad \sum_{\substack{u \\ i>j}} x_{iu}^2\, x_{ju}^4 = 8(p^2q^4 + q^2r^4 + r^2p^4), \\ &\sum_u x_{iu}^6 = 8(p^6 + q^6 + r^6), \qquad \sum_u x_{iu}^2x_{ju}^2x_{lu}^2 = 24p^2q^2r^2, \end{aligned} \tag{3.3}$$

where $i \neq j \neq l \neq i$, $i, j, l = 1, 2, 3$ and $u = 1, 2, \cdots, N$; the notation $i > j$ here denotes that i is before j in *cyclic* order, i.e., $1 > 2$, $2 > 3$, $3 > 1$. Consideration of (3.2) and (3.3) together with (1.2) shows that if

$$Ex(G) = Gx(G) = Hx(G) = Ix(G) = 0, \tag{3.4}$$

then the points of $G(p, q, r)$ form a rotatable arrangement of the third order. All of the excess functions we have defined operate linearly on sets of points of the form $G(p, q, r)$ and fractions of $G(p, q, r)$, that is to say $Qx(\sum_i S_i) = \sum_i Qx(S_i)$, where Q represents any of E, G, H or I. Thus if the four functions of (3.4) are zero for any aggregate of points, then this aggregate forms a third order rotatable arrangement. The arrangement will be a design provided that the non-singularity conditions are satisfied.

Listed in Table I are the generated sets of the form $G(p, q, r)$ or fractions thereof which were used previously [1], together with the values of the excess functions for each set.

It is, of course, possible to form non-sequential third order designs and classes of designs by a skillful combination of these sets. We have already said that design (2.1)(b) is of this type. We shall leave aside this possibility and instead form some infinite classes of designs that may be performed sequentially. Since, for sequential performance, each of the two parts of the design must be itself a second order design, we shall employ some of the infinite classes of second order designs already obtained. Table II contains a number of unscaled second order design classes which may be used, and the values of the various excess functions for each class are shown. Since each class satisfies the second order conditions, $Ex(\text{class}) = 0$, as is indicated in the table. The classes we shall consider, which are obtainable from the basic generated point sets, have $Gx(\text{class}) = 0$. Each class contains three parameters which give rise to two ratios connected by one equation ($Ex = 0$). If we combine two such classes and apply the other conditions of (3.4), we shall have a set of points with six parameters giving five ratios connected by four equations. Thus we shall obtain

Table I: Generated Point Sets.

Point Set	* $G(p,q,r)$	* $\frac{1}{2}G(p,q,0)$	$\frac{1}{2}G(p,q,0) + \frac{1}{2}G(q,p,0)$	$G(p,q,q)$	$\frac{1}{2}G(f,f,0)$	$\frac{1}{3}G(a,a,a)$	$\frac{1}{4}G(c,0,0)$
No. of points	24	12	24	24	12	8	6
Ax	$8(p^2+q^2+r^2)$	$4(p^2+q^2)$	$8(p^2+q^2)$	$8(p^2+2q^2)$	$8f^2$	$8a^2$	$2c^2$
Ex	$8(p^4+q^4+r^4 -3p^2q^2-3q^2r^2-3r^2p^2)$	$4(p^4+q^4-3p^2q^2)$	$8(p^4+q^4-3p^2q^2)$	$8(p^4-q^4-6p^2q^2)$	$-4f^4$	$-16a^4$	$2c^4$
Gx	$8(p^4q^2+q^4r^2+r^4p^2 -p^2q^4-q^2r^4-r^2p^4)$	$4(p^4q^2-p^2q^4)$	0	0	0	0	0
Hx	$8(p^6+q^6+r^6 -45p^2q^2r^2)$	$4(p^6+q^6)$	$8(p^6+q^6)$	$8(p^6+2q^6-45p^2q^4)$	$8f^6$	$-112a^6$	$2c^6$
Ix	$8(p^4q^2+q^4r^2+r^4p^2-9p^2q^2r^2)$ or $8(p^2q^4+q^2r^4+r^2p^4-9p^2q^2r^2)$	$4p^4q^2$ or $4p^2q^4$	$4(p^4q^2+p^2q^4)$	$8(p^4q^2+q^6-8p^2q^4)$	$4f^6$	$-16a^6$	0

* For these two sets a unique expression for Ix does not exist since there is a lack of symmetry. The two possible values of the expression Ix are shown; they are equal when p = q.

Table II: Second Order Rotatable Design Classes.

Reference	D_1	D_2	D_3	D_4	D_5	D_6
Set composition of class	$\frac{1}{3}G(a,a,a)$ $+\frac{1}{4}G(c_1,0,0)$ $+\frac{1}{4}G(c_2,0,0)$	$\frac{1}{3}G(a_1,a_1,a_1)$ $+\frac{1}{3}G(a_2,a_2,a_2)$ $+\frac{1}{4}G(c,0,0)$	$\frac{1}{2}G(f,f,0)$ $+\frac{1}{4}G(c_1,0,0)$ $+\frac{1}{4}G(c_2,0,0)$	$\frac{1}{2}G(f,f,0)$ $+\frac{1}{3}G(a,a,a)$ $+\frac{1}{4}G(c,0,0)$	$G(p,q,q)$ $+\frac{1}{3}G(a,a,a)$	$G(p,q,q)$ $+\frac{1}{4}G(c,0,0)$
No. of points	20	22	24	26	32	30
Ax	$8a^2+2(c_1^2+c_2^2)$	$8(a_1^2+a_2^2)+2c^2$	$8f^2+2(c_1^2+c_2^2)$	$8f^2+8a^2+2c^2$	$8(p^2+2q^2+a^2)$	$8(p^2+2q^2)+2c^2$
Ex (zero)	$2(c_1^4+c_2^4-8a^4)$	$2(c^4-8(a_1^4+a_2^4))$	$2(c_1^4+c_2^4-2f^4)$	$2(c^4-2f^4-8a^4)$	$8(p^4-q^4-6p^2q^2)$ $-16a^4$	$8(p^4-q^4-6p^2q^2)$ $+2c^4$
Gx	0	0	0	0	0	0
Hx	$2(c_1^6+c_2^6)-112a^6$	$2c^6-112(a_1^6+a_2^6)$	$2(c_1^6+c_2^6)+8f^6$	$2c^6+8f^6-112a^6$	$8(p^6+2q^6-45p^2q^4)$ $-112a^6$	$8(p^6+2q^6-45p^2q^4)$ $+2c^6$
Ix	$-16a^6$	$-16(a_1^6+a_2^6)$	$4f^6$	$4f^6-16a^6$	$8(p^4q^2+q^6-8p^2q^4)$ $-16a^6$	$8(p^4q^2+q^6-8p^2q^4)$

a single infinity of third order rotatable arrangements dependent on one parameter ratio.

We shall now illustrate by an example the formation of infinite classes of third order rotatable arrangements by the combination, in pairs, of certain of D_1, D_2, $\cdots$, D_6 and the application of conditions (3.4).

Consider the combination $D_1 + D_6$, containing 50 points. These points form a sequential rotatable arrangement in three dimensions if all the excess functions are zero, namely if

$$Ex(D_1) = Ex(D_6) = Gx(D_1 + D_6) = Hx(D_1 + D_6) = Ix(D_1 + D_6) = 0. \tag{3.5}$$

In full, these equations are

$$\begin{aligned} c_1^4 + c_2^4 - 8a^4 &= 0, \\ 4(p^4 - q^4 - 6p^2q^2) + c^4 &= 0, \\ c_1^6 + c_2^6 - 56a^6 + 4(p^6 + 2q^6 - 45p^2q^4) + c^6 &= 0, \\ -2a^6 + p^4q^2 + q^6 - 8p^2q^4 &= 0. \end{aligned} \tag{3.6}$$

Make the substitutions

$$c_1^2 = xa^2, \quad c_2^2 = ya^2, \quad p^2 = uc^2, \quad q^2 = vc^2, \quad c^6 = ta^6. \tag{3.7}$$

Since equations (3.6) are homogeneous, they may be put in the form

$$\begin{aligned} x^2 + y^2 &= 8, \\ u^2 - 6uv - v^2 + \tfrac{1}{4} &= 0, \\ x^3 + y^3 - 56 + (4u^3 + 8v^3 - 18uv^2 + 1)t &= 0, \\ -2 + (u^2v + v^3 - 8uv^2)t &= 0, \end{aligned} \tag{3.8}$$

a system of four equations in five unknowns; thus if one variable is specified, the values of the other variables are determined. However, we are interested only in solutions for which x, y, u, v and t are all real and positive. Only in such a case will a rotatable arrangement exist. Simple algebraic solution of the equations (3.8) is not possible. We proceed by selecting one variable and obtaining the others successively, applying the conditions for positive solutions as we go. Select $v \geqq 0$. Then from the second equation, $u = 3v \pm \frac{1}{2}(40v^2 - 1)^{\frac{1}{2}}$. From the fourth equation, $2t^{-1} = \mp v^2(40v^2 - 1)^{\frac{1}{2}} - 4v^3 - v/4$. Now $t \geqq 0$. Thus the top root alternative is impossible, which means that

$$u = 3v - \tfrac{1}{2}(40v^2 - 1)^{\frac{1}{2}} \tag{3.9}$$

and

$$2t^{-1} = v^2(40v^2 - 1)^{\frac{1}{2}} - 4v^3 - v/4. \tag{3.10}$$

Now $u \geqq 0$ implies that $0.025 \leqq v^2 \leqq 0.25$ and $t \geqq 0$ implies that $0.143187 \leqq v^2$. Thus we shall require

$$0.143187 \leqq v^2 \leqq 0.25 \tag{3.11}$$

in order that all of t, u, and v shall be real and positive. By substituting for u and t in the third equation we find that $x^3 + y^3 = f(v)$, where

$$f(v) = 24 - \frac{4[2(16v^2 - 7v + 1) + (1 + 8v - 24v^2)(40v^2 - 1)^{\frac{1}{2}}]}{v(384v^4 - 48v^2 - 1)}.$$

But since $x^2 + y^2 = 8$, real, non-negative solutions exist for x and y only when $16 \leqq f(v) \leqq 16(2)^{\frac{1}{2}} = 22.627424$. The range of v for this to be true is more difficult to find and involves considerable computation. We find, considering only points in the range (3.11), that $f(0.419894) = 16$, $f(0.466316) = 16(2)^{\frac{1}{2}}$, and $f(v)$ increases monotonically from its lower value (16) to its upper value $[16(2)^{\frac{1}{2}}]$ for v in the indicated range. This may be observed from the summary table of solutions to be presented later. Thus we see that whenever

$$0.419894 \leqq v \leqq 0.466316, \quad \text{i.e.,} \quad 0.176311 \leqq v^2 \leqq 0.217451, \tag{3.12}$$

then equations (3.8) have a solution that gives rise to a third order rotatable arrangement. We have already obtained both t and u in terms of v. It remains only to express x and y in terms of v. We recall that

$$x^2 + y^2 = 8, \qquad x^3 + y^3 = f(v). \tag{3.13}$$

Set

$$x + y = 2\theta, \qquad xy = \phi; \tag{3.14}$$

then, substituting in (3.13), we find $4\theta(6 - \theta^2) = f(v)$, a cubic which, given v, may be solved for $\theta = \theta(v)$, either iteratively or by the trigonometric method for solution of cubics. From (3.13) and (3.14), $x, y = \theta \pm (4 - \theta^2)^{\frac{1}{2}}$, which are functions of v only. These calculations were carried out for 12 values of v

TABLE III

A Third Order Rotatable Design Class

v	u	t	x	y	$\lambda_2 Na^{-2}$	$\lambda_4 Na^{-4}$	$\lambda_6 Na^{-6}$	$\lambda_4/\lambda_2^2 N$	$\lambda_6\lambda_2/\lambda_4^2$
0.419894	0.029596	61.248478	2	2	51.299493	33.005920	15.670698	0.012542	0.737934
0.420	0.029553	61.069211	2.073576	1.923612	51.264057	32.963451	15.640735	0.012543	0.737912
0.425	0.027503	53.553302	2.438052	1.433843	49.742964	31.187123	14.384946	0.012604	0.735680
0.430	0.025484	47.517331	2.563986	1.194143	48.418222	29.705827	13.373640	0.012671	0.733796
0.435	0.023497	42.568299	2.640568	1.013607	47.249791	28.449362	12.542421	0.012743	0.732211
0.440	0.021539	38.440873	2.695576	0.856661	46.195292	27.368099	11.847274	0.012825	0.730679
0.445	0.019610	34.949405	2.735256	0.719982	45.242534	26.428609	11.257215	0.012912	0.729171
0.450	0.017709	31.960134	2.765977	0.590668	44.359086	25.599301	10.750681	0.013010	0.727717
0.455	0.015834	29.374247	2.790168	0.463593	43.531524	24.864635	10.310955	0.013121	0.726003
0.460	0.013984	27.117168	2.809441	0.327169	42.726269	24.208077	9.925752	0.013261	0.723665
0.465	0.012159	25.131560	2.824930	0.140614	41.867093	23.617604	9.585751	0.013474	0.719494
0.466316	0.011682	24.648331	2.828428	0	41.462397	23.471355	9.502710	0.013653	0.715197

in the range (3.12), including the end points of the range, and the results are shown in the first five columns of Table III. Any line of the table gives five ratios which may be employed in (3.7) to give five of the parameters c_1, c_2, a, p, q and c in terms of the sixth. (After the addition of any center points to be used, the sixth parameter can be fixed by applying the scaling condition $\lambda_2 = 1$.) Thus we obtain a rotatable arrangement which is a design if the non-singularity conditions are satisfied. Since the first of these can be satisfied by the addition of center points, it need not be considered further. We require, then, that $\lambda_6\lambda_2/\lambda_4^2 > 5/7 = 0.714286$. By our theorem, this will be so unless all the points lie on one sphere. Now each design consists of five separate point sets of squared radii $3a^2$, c_1^2, c_2^2, $p^2 + 2q^2$ and c^2 or $3a^2$, xa^2, ya^2, $(u + 2v)c^2$ and c^2. It is easy to see from the table that the various radii are different. The actual values of the parameters are given by:

$$\lambda_2 N = a^2(8 + 2x + 2y) + (8(u + 2v) + 2)c^2,$$
$$\lambda_4 N = 8a^4 + (16uv + 8v^2)c^4,$$
$$\lambda_6 N = 8a^6 + 24uv^2c^6.$$

Since $c^6 = ta^6$, these values may be found in terms of a, as shown in Table III.

We now examine further the extreme cases of the table. The bottom line gives a design consisting of

$$[\tfrac{1}{3}G(a, a, a) + \tfrac{1}{4}G(c_1, 0, 0) + \tfrac{1}{4}G(0, 0, 0)] + [G(p, q, q) + \tfrac{1}{4}G(c, 0, 0)]$$

with values of the parameter ratios as derived above. Reference to (2.2) will show that this is known design (c) with six center points (represented by $\tfrac{1}{4}G(0, 0, 0)$). The top line gives a design consisting of

$$[\tfrac{1}{3}G(a, a, a) + \tfrac{1}{4}G(c_1, 0, 0) + \tfrac{1}{4}G(c_1, 0, 0)] + [G(p, q, q) + \tfrac{1}{4}G(c, 0, 0)]$$

with the values of the parameter ratios as derived above. Reference to (2.2) will show that this is known design (d). The details of the verifications will not be reproduced here. Thus the infinite class of third order rotatable designs obtained has, as its two extreme cases, two of the designs already known, and the passage from one extreme to the other is by a continuous infinite sequence of new third order designs for which the second non-singularity condition becomes successively stronger.

The class of designs just obtained was chosen for a detailed presentation because of its link with the only sequential type designs known previously (ignoring the claims of design (2.2) (a) which is almost singular).

4. Further classes of third order rotatable designs in three dimensions. Several other combinations of $D_1, D_2, \cdots, D_6$ also give rise to infinite classes of third order designs. Of the 15 possible pairs, $D_1 + D_4$, $D_1 + D_6$, $D_2 + D_3$, $D_2 + D_4$, $D_2 + D_6$, $D_3 + D_4$, $D_3 + D_5$ and $D_3 + D_6$ all provide third order designs and these have been tabulated in the same way as the example of the previous section. The combinations $D_1 + D_2$, $D_1 + D_3$, $D_1 + D_5$ and $D_2 + D_5$ do not give third order designs. The remaining three combinations, $D_4 + D_5$, $D_4 + D_6$ and $D_5 + D_6$ have not yet been investigated.

The intention of this paper is to show *how* the design classes can be constructed and to indicate which classes are known to exist. It is hoped to present, in a future report, some specific single designs (selected from the infinite classes mentioned above) in a form in which they can be used conveniently by experimenters.

5. Acknowledgment. I am grateful to Dr. R. C. Bose for his guidance and encouragement during the preparation of this paper.

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