CYLINDRICALLY ROTATABLE DESIGNS[1]

By Agnes M. Herzberg

University of Saskatchewan

1. Introduction. In what follows we use k-dimensional space to describe an experimental design for k factors. We refer to the combinations of levels of factors used in the design as points in k-dimensional space.

Box and Hunter (1957) gave conditions under which designs for the fitting of response surfaces would be rotatable. (Response surface designs are said to be rotatable if the variances of the estimated responses at all points equidistant from the origin of the design are equal.) These conditions for rotatability are restrictive. Some methods for forming rotatable designs are given in Bose and Draper (1959) and Draper (1960a, b). It is desirable to find designs which are both in some sense rotatable and also practical for the experimenter to employ.

Here we consider designs such that the variances of the estimated responses at points on the same $(k - 1)$-dimensional hyper-sphere centred on a specified axis are equal. We shall call such designs *cylindrically rotatable designs*. If the experimental design is rotated about the specified axis, the variances and covariances of the estimated coefficients of the response function remain unchanged. A cylindrically rotatable design is identical to a rotatable design of the same order except in the required levels of one factor.

2. Conditions for cylindrically rotatable designs. We assume that there are k factors whose standardized levels are denoted by $x_1, x_2, \cdots, x_k$. We also assume that the response surface may be represented in a given region by a polynomial of degree d, i.e.

$$\eta(\mathbf{x}) = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k + \beta_{11} x_1^2 + \cdots + \beta_{kk} x_k^2 + \beta_{12} x_1 x_2 + \cdots + \beta_{k-1,k} x_{k-1} x_k + \beta_{111} x_1^3 + \cdots, \qquad \text{of degree } d.$$

Let $\hat{y}(\mathbf{x})$ denote the estimated response at $\mathbf{x}$, where $\mathbf{x} = (x_1, x_2, \cdots, x_k)$. $\hat{y}(\mathbf{x})$ is the polynomial fitted by least squares to the response surface from the N observations made according to some particular design. Let $V(\hat{y}(\mathbf{x}))$ be the variance of the estimated value of the response at $\mathbf{x}$. We want to find conditions such that the variances of the estimated responses at all points on the same $(k - 1)$-dimensional hyper-sphere centered on the axis $x_1 = \cdots = x_{i-1} = x_{i+1} = \cdots = x_k = 0$ are equal.

Suppose

$$(1) \quad \hat{y}(\mathbf{x}) = b_0 + b_1 x_1 + \cdots + b_k x_k + b_{11} x_1^2 + \cdots + b_{kk} x_k^2 + b_{12} x_1 x_2 + \cdots + b_{k-1,k} x_{k-1} x_k + b_{111} x_1^3 + \cdots$$

Received 3 August 1964; revised 19 July 1965.

[1] This work was done while the author held a National Research Council of Canada Studentship at the University of Saskatchewan.

or, in matrix notation,

$$(2) \qquad \hat{y}(\mathbf{x}) = \mathbf{x}'^{[d]}\mathbf{b},$$

where $\mathbf{x}' = (1, x_1, x_2, \cdots, x_k)$, $\mathbf{x}'^{[d]}$ is such that $\mathbf{x}'^{[d]}\mathbf{x}^{[d]} = (\mathbf{x}'\mathbf{x})^d$ and $\mathbf{b}$ contains all the $b_{1^\alpha 2^\gamma \cdots k^\pi}$'s along with suitable multipliers, in order that (1) will equal (2).

Let

$$(3) \qquad \eta(\mathbf{x}) = \mathbf{x}'^{[d]}\boldsymbol{\beta},$$

where $\boldsymbol{\beta}$ is the vector of expected values of the elements of the vector $\mathbf{b}$.

From Box and Hunter (1957) (Equation 26), we know that

$$(4) \qquad V(\hat{y}(\mathbf{x})) = \mathbf{x}'^{[d]}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}^{[d]}\sigma^2,$$

where $\mathbf{X}$ is the $N \times L$ matrix of independent variables. (N is the number of design points and L is the number of terms in (1).)

We now want to consider the variance of $\hat{y}(\mathbf{z})$, where $\mathbf{z}$ is such that

$$(5) \qquad \sum_{j=1, j\neq i}^{k} x_j^2 = \sum_{j=1, j\neq i}^{k} z_j^2 \quad \text{and} \quad x_i = z_i .$$

Suppose $\mathbf{z} = \mathbf{M}\mathbf{x}$, where $\mathbf{x}' = (1, x_1, x_2, \cdots, x_k)$ and $\mathbf{M}$ is a matrix of the following form:

$$\mathbf{M} = \begin{array}{c} 0 \\ 1 \\ \vdots \\ i-1 \\ i \\ i+1 \\ \vdots \\ k \end{array}\begin{array}{c} \begin{array}{cccccccc} 0 & 1 & \cdots & i-1 & i & i+1 & \cdots & k \end{array} \\ \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & m_{11} & \cdots & m_{1,i-1} & 0 & m_{1,i+1} & \cdots & m_{1k} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ 0 & m_{i-1,1} & \cdots & m_{i-1,i-1} & 0 & m_{i-1,i+1} & \cdots & m_{i-1,k} \\ 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & m_{i+1,1} & \cdots & m_{i+1,i-1} & 0 & m_{i+1,i+1} & \cdots & m_{i+1,k} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ 0 & m_{k1} & \cdots & m_{k,i-1} & 0 & m_{k,i+1} & \cdots & m_{kk} \end{bmatrix} \end{array},$$

where

$$\begin{bmatrix} m_{11} & \cdots & m_{1,i-1} & m_{1,i+1} & \cdots & m_{1k} \\ \vdots & & \vdots & \vdots & & \vdots \\ m_{i-1,1} & \cdots & m_{i-1,i-1} & m_{i-1,i+1} & \cdots & m_{i-1,k} \\ m_{i+1,1} & \cdots & m_{i+1,i-1} & m_{i+1,i+1} & \cdots & m_{i+1,k} \\ \vdots & & \vdots & \vdots & & \vdots \\ m_{k1} & \cdots & m_{k,i-1} & m_{k,i+1} & \cdots & m_{kk} \end{bmatrix}$$

is an orthogonal $(k - 1) \times (k - 1)$ matrix. Then

$$(6) \qquad \begin{aligned} V(\hat{y}(\mathbf{z})) &= \mathbf{z}'^{[d]}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}^{[d]}\sigma^2 \\ &= \mathbf{x}'^{[d]}\mathbf{M}'^{[d]}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{M}^{[d]}\mathbf{x}^{[d]}\sigma^2, \end{aligned}$$

where $\mathbf{z}' = (1, z_1, z_2, \cdots, z_k)$. ($\mathbf{M}^{[d]}$ is defined in such a way that $\mathbf{z}^{[d]} = \mathbf{M}^{[d]}\mathbf{x}^{[d]}$.)

For the variance to be constant on $(k - 1)$-dimensional hyper-spheres with $x_i = z_i$ fixed we require that $V(\hat{y}(\mathbf{x})) = V(\hat{y}(\mathbf{z}))$. In order that $V(\hat{y}(\mathbf{x})) = V(\hat{y}(\mathbf{z}))$, we have, from (4) and (6),

$$(\mathbf{X}'\mathbf{X})^{-1} = \mathbf{M}'^{[d]}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{M}^{[d]} \tag{7}$$

for every matrix $\mathbf{M}$ of the form described above.

Box and Hunter (1957) show that

$$\begin{aligned} Q &= N^{-1}\mathbf{t}'^{[d]}\mathbf{X}'\mathbf{X}\mathbf{t}^{[d]}, \quad \text{where} \quad \mathbf{t}' = (1, t_1, t_2, \cdots, t_k), \\ &= N^{-1}\textstyle\sum_{u=1}^{N} (1 + t_1x_{1u} + t_2x_{2u} + \cdots + t_kx_{ku})^{2d} \end{aligned} \tag{8}$$

is the generating function of moments of order $2d$ and less of a design. If we let $[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}] = N^{-1}\sum_{u=1}^{N} x_{1u}^{\alpha_1}x_{2u}^{\alpha_2} \cdots x_{ku}^{\alpha_k}$, then the coefficient of $t_1^{\alpha_1}t_2^{\alpha_2} \cdots t_k^{\alpha_k}$ in Q is

$$[(2d)!/\textstyle\prod_{j=1}^{k} \alpha_j!(2d - \alpha)!][1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}], \tag{9}$$

where $\alpha = \sum_{j=1}^{k} \alpha_j =$ order of the moment and $0 \leqq \alpha \leqq 2d$.

From (7), we see that the design will be cylindrically rotatable if and only if

$$\begin{aligned} Q &= N^{-1}\mathbf{t}'^{[d]}\mathbf{X}'\mathbf{X}\mathbf{t}^{[d]} \\ &= N^{-1}\mathbf{t}'^{[d]}(\mathbf{M}'^{[d]}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{M}^{[d]})^{-1}\mathbf{t}^{[d]} \\ &= N^{-1}\mathbf{t}'^{[d]}(\mathbf{M}^{[d]})^{-1}\mathbf{X}'\mathbf{X}(\mathbf{M}'^{[d]})^{-1}\mathbf{t}^{[d]} \\ &= N^{-1}(\mathbf{t}'\mathbf{M}')^{[d]}\mathbf{X}'\mathbf{X}(\mathbf{M}\mathbf{t})^{[d]}. \end{aligned} \tag{10}$$

Therefore Q is a function of $\bar{\mathbf{t}}'\bar{\mathbf{t}}$ and t_i, where $\bar{\mathbf{t}}' = (1, t_1, t_2, \cdots, t_{i-1}, t_{i+1}, \cdots, t_k)$. Since Q is a polynomial in the t_j's, it must be of the form

$$Q = \textstyle\sum_{s=0}^{d} \sum_{r=0}^{2d} a_{2s,r}(\sum_{j=1, j\neq i}^{k} t_j^2)^s t_i^r, \tag{11}$$

where $2s + r \leqq 2d$. The coefficient of $t_1^{\alpha_1}t_2^{\alpha_2} \cdots t_k^{\alpha_k}$ in Q is zero if any one of the α_j's, $j = 1, \cdots, k; j \neq i$, is odd, and is

$$a_{\alpha-\alpha_i,\alpha_i}(\tfrac{1}{2}(\alpha - \alpha_i))!/\textstyle\prod_{j=1,j\neq i}^{k} (\tfrac{1}{2}\alpha_j)!, \tag{12}$$

if all the α_j's, $j = 1, \cdots, k; j \neq i$, are even integers.

Equating (9) and (12) we obtain

$$\begin{aligned} &[1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}] \\ &\quad = a_{\alpha-\alpha_i,\alpha_i}(\tfrac{1}{2}(\alpha - \alpha_i))!(2d - \alpha)!\textstyle\prod_{j=1}^{k} \alpha_j!/\prod_{j=1,j\neq i}^{k} (\tfrac{1}{2}\alpha_j)!(2d)!. \end{aligned} \tag{13}$$

Then letting

$$\lambda_{\alpha-\alpha_i,\alpha_i} = a_{\alpha-\alpha_i,\alpha_i}2^{\alpha/2}(\tfrac{1}{2}(\alpha - \alpha_i))!\,(2d - \alpha)!/(2d)!, \tag{14}$$

we see that

$$\begin{aligned} [1^{\alpha_1}, 2^{\alpha_2}, \cdots, k^{\alpha_k}] &= 0, \qquad \text{any } \alpha_j \text{ odd}, j \neq i, \\ &= \lambda_{\alpha-\alpha_i,\alpha_i} \textstyle\prod_{j=1}^{k} \alpha_j!/2^{\alpha/2} \prod_{j=1,j\neq i}^{k} (\tfrac{1}{2}\alpha_j)!, \\ &\qquad\qquad \text{all } \alpha_j \text{ even}, j \neq i. \end{aligned} \tag{15}$$

The design points for a cylindrically rotatable design are chosen in such a way that the moments are of the form given in (15). The design points must also be chosen so that the variance-covariance matrix, $\mathbf{X}'\mathbf{X}\,\sigma^2$, is non-singular.

In order to make the variance-covariance matrix as simple as possible, it is advisable to choose the design points so that $[1^{\alpha_1}, 2^{\alpha_2}, \cdots, i^{\alpha_i}, \cdots, k^{\alpha_k}] = 0$, where α_i is odd. (Note: this is not necessary for the design to be cylindrically rotatable.)

3. Interpretation. From the moment conditions, (15), for a cylindrically rotatable design, it can be seen that a k-dimensional cylindrically rotatable design is an extension of a $(k - 1)$-dimensional rotatable design of the same order. The variances of the estimated responses continue to be constant at points on $(k - 1)$-dimensional hyper-spheres. Therefore, by using a cylindrically rotatable design, it is possible to preserve this property of a $(k - 1)$-dimensional rotatable design with the added advantage of being able to estimate the coefficients of the terms of the polynomial involving the kth factor.

It is easily seen that since the moment conditions for a cylindrically rotatable design are not as restrictive as the moment conditions for a rotatable design of the same dimension and order, the number of points required for a cylindrically rotatable design is less than the number required for a rotatable design. The experimenter could start with a cylindrically rotatable design and then points could be added to form a rotatable design.

4. Examples. A set of points forms a second order rotatable design in k dimensions if

$$\text{(16)} \qquad \begin{aligned} &\sum x_{iu}^2 = N\lambda_2, \\ &\sum x_{iu}^4 = 3 \sum x_{iu}^2 x_{ju}^2 = 3N\lambda_4, \quad \lambda_4/\lambda_2^2 > k/(k+2), \end{aligned}$$

where $i \neq j$; $i, j = 1, 2, \cdots, k$ and all other sums of powers and products up to and including order four are zero and the summation is over all the N design points (Box and Hunter (1957)).

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

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

where

(i) $i, j, l, m = 1, 2, \cdots, k$ and are distinct,

(ii) at least one of $\alpha_i, \alpha_j, \alpha_l, \alpha_m$ is odd and $0 < \alpha_i + \alpha_j + \alpha_l + \alpha_m \leqq 4$,

(iii) the summation is taken over all the points of $U(x_1, x_2, \cdots, x_k)$.

I. Consider the following point sets in five dimensions:

$$\text{(17)} \qquad \begin{aligned} &(S(a, a, 0, 0), \pm b), \\ &(0, 0, 0, 0, \pm c), \\ &(0, 0, 0, 0, 0). \end{aligned}$$

For all values of a, b, c except zero these point sets will form a second order cylindrically rotatable design since the moments satisfy (15) with $i = 5$. The number of points involved is fifty-one. The moments of this design are

$$\begin{aligned} \sum x_{ju}^2 &= 24a^2, \\ \sum x_{ju}^4 &= 24a^4, \\ \sum x_{ju}^2 x_{lu}^2 &= 8a^4, \\ \sum x_{5u}^2 &= 48b^2 + 2c^2, \\ \sum x_{5u}^4 &= 48b^4 + 2c^4, \\ \sum x_{ju}^2 x_{5u}^2 &= 24a^2b^2, \end{aligned}$$

where $j \neq l$; $j, l = 1, \cdots, 4$ and all other sums of powers and products up to and including order four are zero. The summation is taken over all design points.

II. Consider the $(k - 1)$-dimensional point sets

$$\begin{aligned} &U(a, a, \cdots, a), \\ &S(c, 0, \cdots, 0). \end{aligned} \tag{18}$$

These point sets satisfy (16) when $c^2 = 2^{(k-p-1)/2}a^2$ and therefore form a second order rotatable design in $(k - 1)$ dimensions.

Now consider the following extension of these point sets in k dimensions:

$$\begin{aligned} &(U(a, a, \cdots, a), a), \\ &(S(c, 0, \cdots, 0), 0), \\ &(0, \cdots, 0, \pm c). \end{aligned} \tag{19}$$

When $c^2 = 2^{(k-p-1)/2}a^2$, these point sets, consisting of $2^{k-p-1} + 2k$ points, form a second order cylindrically rotatable design in k dimensions, since the moments of the design satisfy (15) with $i = k$. The moments of this design are

$$\begin{aligned} \sum x_{ju}^2 &= \sum x_{ku}^2 = 2^{k-p-1}a^2 + 2\cdot 2^{(k-p-1)/2}a^2, \\ \sum x_{ju}^4 &= 3\cdot 2^{k-p-1}a^4, \\ \sum x_{ju}^2 x_{lu}^2 &= 2^{k-p-1}a^4, \\ \sum x_{ku} &= 2^{k-p-1}a, \\ \sum x_{ku}^3 &= 2^{k-p-1}a^3, \\ \sum x_{ku}^4 &= 3\cdot 2^{k-p-1}a^4, \\ \sum x_{ju}^2 x_{ku}^2 &= 2^{k-p-1}a^4, \\ \sum x_{ju}^2 x_{ku} &= 2^{k-p-1}a^3, \end{aligned} \tag{20}$$

where $j \neq l; j, l = 1, 2, \cdots, k - 1$; and all other sums of powers and products up to and including order four are zero for all j, l and k. The summation is taken over all design points. (Note: When $k = 3$, points must be added at the centre in (19).)

If after performing an experiment using the above second order cylindrically rotatable design in k dimensions, the experimenter feels that it would have been better to have used a second order rotatable design, the following points in k dimensions can be added:

$$(U(a, a, \cdots, a), -a),$$
$$(S(c, 0, \cdots, 0), 0), \tag{21}$$
$$(0, 0, \cdots, 0, \pm c).$$

(19) and (21) will form a second order rotatable design in k dimensions of $2^{k-p} + 4k$ points.

When experiments using (19) and (21) are performed in blocks, the estimates of the block effects are uncorrelated with the estimates of all the polynomial coefficients, except the coefficient of x_k. This can be seen from Equations (4.2), (4.3) and (4.4) of Gardiner, Grandage, and Hader (1959).

5. Acknowledgment. The author is grateful for the help and guidance of Professor N. Shklov, who also suggested the problem, and for the comments of the referee.

REFERENCES

BOSE, R. C. and DRAPER, NORMAN R. (1959). Second order rotatable designs in three dimensions. *Ann. Math. Statist.* **30** 1097–1112.

BOX, G. E. P. and HUNTER, J. S. (1957). Multi-factor experimental designs for exploring response surfaces. *Ann. Math. Statist.* **28** 195–241.

DRAPER, NORMAN R. (1960a). Second order rotatable designs in four or more dimensions. *Ann. Math. Statist.* **31** 23–33.

DRAPER, NORMAN R. (1960b). Third order rotatable designs in three dimensions. *Ann. Math. Statist.* **31** 865–874.

GARDINER, D. A., GRANDAGE, A. H. E. and HADER, R. J. (1959). Third order rotatable designs for exploring response surfaces. *Ann. Math. Statist.* **30** 1082–1096.