SECOND - ORDER ROTATABLE DESIGNS

by

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1. INTRODUCTION

It frequently happens that an experimenter is interested in studying a system for which it is assumed that a mathematical equation relates the expected value of a response or yield $\psi = E(y)$ to the controllable experimental variables $\xi_1, \xi_2, \ldots, \xi_k$. Thus, let

$$\psi = \psi(\xi_1, \xi_2, \ldots, \xi_k; \theta_1, \theta_2, \ldots, \theta_p) = \psi(\xi', \theta), \tag{1}$$

where $\theta = (\theta_1, \theta_2, \ldots, \theta_p)$ is a vector of parameters of the system, and $\xi' = (\xi_1, \xi_2, \ldots, \xi_k)$ is a vector of observed values of the experimental variables.

Before the details of an analysis can be carried out, experiments must be performed at predetermined levels of the controllable factors; that is, an experimental design must be selected prior to experimentation. Box and Hunter [4] suggested designs of rotatability where the standard error is the same for all points that are at the same distance from the center of the region in which the relation between ψ and ξ_i's $(i = 1, 2, \ldots, k)$ is under investigation.

It is the purpose of this paper to concentrate on some general application of the second-order rotatable design. Suppose the functional relationship exists, and can be closely approximated by a quadratic (second degree) polynomial of the form.

$$\psi_u = \theta_0 + \sum_{i=1}^{k} \theta_i \xi_{iu} + \sum_{i=1}^{k} \theta_{ii} \xi_{iu}^2 + \sum_{i \neq j}^{k} \theta_{ij} \xi_{iu} \xi_{ju} \tag{2}$$

In order to elucidate certain aspects of this relationship, measurements of ψ are to be made for each of N combinations of levels of the variables

$$\xi_u' = (\xi_{1u}, \xi_{2u}, \ldots, \xi_{ku}), \quad (u = 1, 2, \ldots, N) \tag{3}$$

2. BASIS FOR THE SELECTION OF SECOND-ORDER ROTATABLE DESIGN

The general problem of selecting a response surface design is to choose a design such that:

(i) the polynomial $f(\xi') = f(\xi_1, \xi_2, \ldots, \xi_k)$ in the k-variables $\xi' = (\xi_1, \xi_2, \ldots, \xi_k)$ fitted by the method of least squares most closely represents the true function $\psi(\xi_1, \xi_2, \ldots, \xi_k)$ over some region of interest $\underline{R}$ in the $\underline{\xi}$ space, no restrictions being introduced that the experimental points should necessarily lie inside $\underline{R}$; and

(ii) subject to satisfaction of (i) there is a high chance that inadequacy of $f(\underline{\xi})$ to represent $\psi(\underline{\xi})$ will be detected.

When the observations are subject to error, discrepancies between the fitted polynomial and the true function occur

(i) due to sampling error (called here variance error), and

(ii) due to the inadequacy of the polynomial $f(\xi')$ exactly to represent $\psi(\underline{\xi})$ (called here bias error).

2.1 Choice of Region of Interest

Call the region in the $\underline{\xi}$ space, in which experiments can actually be performed, the operability region $\underline{O}$. This region is usually bounded although its limits are often known only vaguely. Usually a particular group of experiments is used to explore a rather limited region of interest $\underline{R}$, entirely contained within the operability region $\underline{O}$.

2.2 Choice of Measure of Closeness

Let $\hat{y}(\xi)$ denote the response estimated by the graduating function at the point ξ, then it is desirable to choose a design, so that the difference $\hat{y}(\xi) - \psi(\xi)$ will be small over the region of interest $\underline{R}$. The measure of closeness which is used at a particular point ξ will be $E[\hat{y}(\xi) - \psi(\xi)]^2$. Over the region $\underline{R}$, the average is

$$\Omega \int_R E[\hat{y}(\xi) - \psi(\xi)]^2 \, d\xi \ , \qquad (4)$$

where $\Omega^{-1} = \int_R d\xi$. Let $W(\xi)$ be a weighted function such that

$$\int_o W(\xi) \, d\xi = 1.$$

Then the measure of closeness is

$$\int_o W(\xi) \, E[\hat{y}(\xi) - \psi(\xi)]^2 \, d\xi \ ,$$

where $W(\xi) = \begin{cases} \Omega & \text{in } \underline{R} \\ 0 & \text{elsewhere} \end{cases}$.

It is desirable to be able to compare designs which do not contain the same number of points and in which the criterion of closeness is independent of the variance σ^2 of the observations which are assumed to be constant. The measure of closeness will be

$$J = \int_o w(\xi) \, E[\hat{y}(\xi) - \psi(\xi)]^2 \, d\xi \ , \qquad (5)$$

where $w(\xi) = NW(\xi)/\sigma^2$.

Let $\hat{y}(\xi) - \psi(\xi) = \{\hat{y}(\xi) - E[\hat{y}(\xi)]\} + \{E[\hat{y}(\xi) - \psi(\xi)\}$.

Then $J = \int_{O} w(\xi)\, E\{[\hat{y}(\xi) - E\,\hat{y}(\xi)] + [E\hat{y}(\xi) - \psi(\xi)]\}^2\, d\xi$

$$= \int_{O} w(\xi)[\hat{y}(\xi) - E\hat{y}(\xi)]^2\, d\xi + \int_{O} w(\xi)[E\hat{y}(\xi) - \psi(\xi)]^2\, d\xi$$

$$= V + B,$$

where V is the average weighted variance

$$V = \int_{O} w(\xi)\ [\hat{y}(\xi) - E\hat{y}(\xi)]^2\ d\xi \quad , \tag{6}$$

and B is the average squared bias

$$B = \int_{O} w(\xi)\ [E\hat{y}(\xi) - \psi(\xi)]^2\ d\xi \quad . \tag{7}$$

A reasonable criterion would be to choose a design such that

$$J = B + V \tag{8}$$

is minimum.

2.3 Detection of Inadequacy of Model

Let $\hat{y}_u$ be the estimated response and y_u be the actual observation, $u = 1, 2, \ldots, N$. The quantity $S_R = \sum_{u=1}^{N} (\hat{y}_u - y_u)^2$ is the residual sum of squares and is compared either with a prior value σ^2 of the experimental error variance, supposed to be known exactly, or with some independent estimate s^2.

In either case, a parameter which determines the power of the test for goodness of fit will be the quantity $\sum_{u=1}^{N} [E(\hat{y}_u) - \psi_u]^2 = E(S_R) - \omega\,\sigma^2$, where ω is the number of degrees of freedom on which the residual sum of squares is based. While the ultimate objective should be to make the power of the test as large as possible, in any particular instance in which ω is assumed fixed this will be equivalent to making the expectation of S_R large. Therefore the design should be chosed so as to make $E(S_R)$ large.

3. SECOND-ORDER ROTATABLE DESIGN IN A PLANE

It is likely, especially in complex situations, that the exact form of the response function ψ in equation (1) will be unknown. But a flexible graduating function f (for example, a polynomial) will often be satisfactory to express the relationship between the response ψ and the k important variables $\xi_1, \xi_2, \ldots, \xi_k$.

Suppose the graduating function is a polynomial of degree d_1, in $\underline{\xi}$

$$f(\underline{\xi}) = \underline{\xi}_1' \underline{\beta}_1 . \tag{9}$$

Where the vector $\underline{\xi}_1$ contains p_1 elements, all of which are powers and products of $\xi_1, \xi_2, \ldots, \xi_k$ of order d_2 or less but greater than d_1.

As in Box and Hunter [4], for a rotatable design of order d all moments of order 2d+1 are zero. Therefore if one considers designs which are second-order rotatable, then the fifth moments will be zero.

3.1 Design Obtained From Consideration of Closeness

Assume $\psi(\xi)$ is a cubic polynomial and $f(\xi)$ is a quadratic polynomial in $\xi_1, \xi_2, \ldots, \xi_k$. Also assume the points $(\xi_1, \xi_2, \ldots, \xi_k)$ have been linearly transformed to points $(x_1, x_2, \ldots, x_k)$ in such a way that the centre of the design is at the origin $(0, 0, \ldots, 0)$ and that the region $\underline{R}$ is the k-dimensional sphere. Then d_1=2, d_2=3 and the graduating function $f(x)$, where $x = (x_1, x_2, \ldots, x_k)$, is

$$y = b_0 + b_1x_1 + b_2x_2 + \ldots + b_kx_k + b_{11}x_1^2 + \ldots + b_{kk}x_k^2 + b_{12}x_1x_2 + \\ + \ldots + b_{k-1,k}x_{k-1}x_k \tag{11}$$

or in matrix notation $y = \underline{x}_1'\underline{b}_1$,

where

$$\underline{b}_1' = (b_0; b_1, \ldots, b_k; b_{11}, \ldots, b_{kk}; b_{12}, \ldots, b_{k-1,k}), \tag{12}$$

$$\underline{x}_1' = (1; x_1, \ldots, x_k; x_1^2, \ldots, x_k^2; x_1x_2, \ldots, x_{k-1}x_k). \tag{13}$$

The true relationship which applies over the whole region $\underline{O}$ is assumed to be the cubic polynomial

$$\psi = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2 \tag{14}$$

where x_1' is as above, $\underline{\beta}_1$ is defined like $\underline{b}_1$,

and

$$\underline{\beta}_2' = (\beta_{111}, \beta_{122}, \ldots, \beta_{1kk}; \beta_{222}, \beta_{211}, \ldots, \beta_{2kk}; \ldots, \beta_{kk,k-1}; \\ \beta_{123}, \beta_{124}, \ldots, \beta_{k-2,k-1,k}) \tag{15}$$

$$\underline{x}_2' = (x_1^3, x_1x_2^2, \ldots, x_1x_k^2; x_2^3, x_2x_1^2, \ldots, x_2x_k^2; \ldots, x_{k-1}x_k^2; \\ x_1x_2x_3, x_1x_2x_4, \ldots, x_{k-2}x_{k-1}x_k). \tag{16}$$

Exactly as in [2], one has $J = V + B$,

where
$$V = N\,\Omega \int_R \underline{x}_1' \,(\underline{X}_1'\underline{X}_1)^{-1}\, \underline{x}_1 \, dx \tag{17}$$

$$B = N\,\sigma^{-2}\,\Omega \int_R \underline{\beta}'_2\, [A'\underline{x}_1 - x_2][\underline{x}_1'A - \underline{x}_2]\, \underline{\beta}_2 \, dx . \tag{18}$$

And
$$\underline{X}_1' = [\underline{x}_{11}, \ldots, \underline{x}_{1u}, \ldots, \underline{x}_{1N}] \tag{19}$$

is a $(1/2)(k+1)(k+2)$ by N matrix with

$$\underline{x}_{1u}' = (1;\ x_{1u}, \ldots, x_{ku};\ x_{1u}^2, \ldots, x_{ku}^2; \\ x_{1u}x_{2u}, \ldots, x_{k-1,u}x_{ku}). \tag{20}$$

$$\underline{X}_2' = [\underline{x}_{21}, \ldots, \underline{x}_{2u}, \ldots, \underline{x}_{2N}] \tag{21}$$

is a $k(k+1)(k+2)/6$ by N matrix with

$$\underline{x}_{2u}' = (x_{1u}^3,\ x_{1u}x_{2u}^2, \ldots, x_{1u}x_{ku}^2;\ x_{2u}^3, \ldots, x_{2u}x_{ku}^2; \\ x_{1u}x_{2u}x_{3u}, \ldots, x_{k-2,u}x_{k-1,u}x_{ku}). \tag{22}$$

$A = (\underline{X}_1'\underline{X}_1)^{-1}\,\underline{X}_1'\underline{X}_2$ is an $(1/2)(k+1)(k+2)$ by $(k+2)(k+1)k/6$ matrix of bias coefficients which has been called the <u>alias</u> matrix. This last matrix has, for its elements, quantities which measure the extent to which the estimates $\underline{b}_1$ are biased by higher order coefficients in accordance with the equation:

$$E(\underline{b}_1) = \underline{\beta}_1 + A\underline{\beta}_2 .$$

Let $\alpha_2 = \underline{\beta}_2 N^{1/2}/6$ be substituted into (18). Then

$$\Omega^{-1} B = \alpha_2' A' \left(\int_R \underline{x}_1\underline{x}_1'\, dx \right) A\alpha_2 - 2\alpha_2' \left(\int_R \underline{x}_2\underline{x}_1'\, dx \right) A\alpha_2 + \alpha_2' \left(\int_R \underline{x}_2\underline{x}_2'\, dx \right) \alpha_2 \tag{23}$$

Since the design is second order rotatable with fifth-order moments zero,

$$A = \lambda_4/\lambda_2 \left(\begin{array}{c|c|c|c|c} 0 & 0 & & 0 & 0 \\ \hline 311\cdots1 & & & & \\ & 311\cdots1 & & & 0 \\ & & \cdots & & \\ & & & 311\cdots1 & \\ \hline 0 & 0 & & 0 & 0 \end{array} \right),$$

where $$3\lambda_4 N = \sum_{u=1}^{N} x_{iu}^4 = 3 \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 \quad \text{and} \quad \lambda_2 N = \sum_{u=1}^{N} x_{iu}^2 \tag{24}$$

are the parameters of the design. The columns of A correspond to the elements of $\underline{x}_2'$ (16) and the rows of A correspond to the elements of $\underline{x}_1'$ (13).

Denote this fact by saying that A is $(\underline{x}_1)(\underline{x}_2')$. Only k^2 elements of A are non-zero, and these are shown. They occupy the second, third, $\cdots$, $(k+1)^{th}$ rows. In the second row they are in the first k columns, $\cdots$, in the $(k+1)^{th}$ row they are in the columns numbered $(k^2 - k+1)$ to k^2. The divisions in both rows and columns of A correspond to the semicolons in the x-vectors. Furthermore,

$$\Omega \int_R \underline{x}_1 \underline{x}_1' \, dx = \left(\begin{array}{c|c|c|c} 1 & 0 & \underline{j}_k' & 0 \\ \hline 0 & \underline{I}_k & 0 & 0 \\ \hline \underline{j}_k & 0 & v(2\underline{I}_k + \underline{j}_k \underline{j}_k') & 0 \\ \hline 0 & 0 & 0 & v\underline{I}_p \end{array} \right),$$

where $(k+2) = v(k+2)(k+4) = 1$.

$\underline{I}_k$ denotes the k by k unit matrix and $\underline{j}_k$ is a column vector of ones. This matrix is of shape $(\underline{x}_1)(\underline{x}_1')$, the divisions again corresponding to the semicolons, and since $(1/2)(k+1)(k+2)$ is the number of elements in $\underline{x}_1$, $p = (1/2)(k+1)(k+2) - (2k-1) = (1/2)(k+1)k$. Similarly

$$\Omega\int_R \underline{x}_2\underline{x}_1' \, dx = v \left(\begin{array}{c|cccc|c} & \begin{matrix}3\\1\\1\\ \vdots\\1\end{matrix} & & & & \\ 0 & & \begin{matrix}3\\1\\1\\ \vdots\\1\end{matrix} & & & 0 \\ & & & \ddots & & \\ & & & & \begin{matrix}3\\1\\1\\ \vdots\\1\end{matrix} & \\ \hline 0 & & & 0 & & 0 \end{array}\right)$$

where $v(k+2)(k+4) = 1$. This matrix has the same dimensions and is similiar element-wise to the transpose A' of A. Again similarly

$$\Omega\int_R \underline{x}_2\underline{x}_2' \, dx = w \left(\begin{array}{c|c|c|c|c} \underline{G}_1 & & & & \\ \hline & \underline{G}_2 & & & \\ \hline & & \ddots & & \\ \hline & & & \underline{G}_k & \\ \hline & & & & \underline{I}_q \end{array}\right)$$

where

$$\underline{G}_i = \begin{pmatrix} 15 & 3 & 3 & \cdots & 3 \\ 3 & 3 & 3 & \cdots & 1 \\ 3 & 1 & 3 & & 1 \\ \cdot & & & \cdot & \cdot \\ \cdot & & & \cdot & \cdot \\ \cdot & & & \cdot & \cdot \\ 3 & 1 & 1 & \cdots & 3 \end{pmatrix} \text{, all } i,$$

and $w(k+2)(k+4)(k+6) = 1$.

The matrix divisions correspond to the semicolons in the vector $\underline{x}_2$ (16). Hence, since each $\underline{G}_i$ is a k by k matric,
$q = [k(k+1)(k+2)/6] - k^2 = k(k-1)(k-2)/6$.

Substituting in equation (23), one finds that the bias contribution B is given by $B = \alpha_2 \, \underline{Q} \, \alpha_2$, where

$$\underline{Q} = \left(\begin{array}{c|c|c|c|c} \underline{Q}_1 & & & & \\ \hline & \underline{Q}_1 & & & \\ \hline & & \ddots & & \\ \hline & & & \underline{Q}_1 & \\ \hline & & & & \underline{Q}_2 \end{array}\right)$$

$$\underline{Q}_1 = \begin{array}{cc} \begin{array}{ccccc} \alpha_{i11} & \alpha_{i22} & \alpha_{i33} & \cdots & \alpha_{ikk} \end{array} & \\ \begin{bmatrix} A & E & E & \cdots & E \\ E & C & D & \cdots & D \\ E & D & C & \cdots & \vdots \\ \vdots & \vdots & \vdots & C & D \\ E & D & \cdots & D & C \end{bmatrix} & \begin{array}{c} \alpha_{i11} \\ \alpha_{i22} \\ \alpha_{i33} \\ \vdots \\ \alpha_{ikk} \end{array} \end{array}$$

and

$$\underline{Q}_2 = \underline{I}_q/(k+2)(k+4)(k+6) = w\,\underline{I}_q \; .$$

The α_{ijj} indicate the positions of the elements of $\underline{Q}_1$ and show how the quadratic form will arise. The elements of $\underline{Q}_2$ will be multiplied by terms like α_{ijl} where i, j and l are different.

If one defines

$$\theta = 3\,\lambda_4/\lambda_2, \qquad U = [\theta-3/(k+4)]^2/9(k+2), \qquad W = 1/(k+2)(k+4)^2(k+6);$$

then $\quad A = 9U+6(k+1)W, \quad E = 3U-6W, \quad C = U+2(k+3)W, \quad D = U-2W$.

Evaluation of the quadratic form now gives $B = PU + [(k+4)Q-2P]W$.
Where U and W are as defined above and where

$$\sigma^2\,P/N = (3\beta_{111} + \beta_{122} + \ldots + \beta_{1kk})^2 + \ldots + (3\beta_{kkk} + \beta_{k11} + \beta_{k22} + \ldots + \beta_{k,k-1,k-1})^2$$

$$\sigma^2\,Q/N = 2(3\beta_{111}^2 + \beta_{122}^2 + \ldots + \beta_{1kk}^2) + \ldots + 2(3\beta_{kkk}^2 + \beta_{k11}^2 + \ldots + \beta_{k,k-1,k-1}^2) + (\beta_{123}^2 + \ldots + \beta_{k-2,k-1,k}^2).$$

It was shown in [3] Appendix 2 that P and Q are both invariant under rotation.

The matrix $(\underline{X}_1' \, \underline{X}_1)^{-1}$ is found from the formulae given in Box and Hunter [4] for the inverse of certain matrices which frequently arise in response surface work, where the matrix $\underline{X}_1' \, \underline{X}_1$ contains the sums of squares and products of the independent variables. Notice that $N^{-1} \, \underline{X}_1' \, \underline{X}_1$ may be viewed as a matrix of moments of the design. From [4] the odd moments of a second-order rotatable design of k-variables are zero, and the remaining moments are shown as equation (24). Thus for a second-order rotatable design the moment matrix is of the form

$$
N^{-1}\underline{X}_1\underline{X}_1 =
\begin{array}{c|c|c|c|c}
 & 0 & 1 \; 2 \cdots k & 11 \;\; 22 \cdots kk & 12 \;\; 13 \cdots k-1,k \\
\hline
0 & 1 & 0 & 1 \;\; 1 \cdots 1 & 0 \\
\hline
\begin{matrix} 1 \\ 2 \\ \vdots \\ k \end{matrix} & 0 & \begin{matrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{matrix} & 0 & 0 \\
\hline
\begin{matrix} 11 \\ 22 \\ \vdots \\ kk \end{matrix} & \begin{matrix} 1 \\ 1 \\ \vdots \\ 1 \end{matrix} & 0 & \begin{matrix} 3\lambda_4 & \lambda_4 & \cdots & \lambda_4 \\ \lambda_4 & 3\lambda_4 & \lambda_4 \cdots & \lambda_4 \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_4 & \lambda_4 & \cdots & 3\lambda_4 \end{matrix} & 0 \\
\hline
\begin{matrix} 12 \\ 13 \\ \vdots \\ k-1,k \end{matrix} & 0 & 0 & 0 & \begin{matrix} \lambda_4 & & & \\ & \lambda_4 & & \\ & & \ddots & \\ & & & \lambda_4 \end{matrix}
\end{array}
$$

where $\lambda_2 = 1$.

The inverse matrix is obtained by inversion of the partitioned matrix [7].

$N(\underline{X}_1\underline{X}_1)^{-1}$ is equal to

$$
\begin{array}{cc}
 & \begin{array}{ccccccc} 0 & 12\cdots k & 11 & 22 & \cdots & kk & 12\cdots k-1,k \end{array} \\
\begin{array}{c} 0 \\ 1,2,\ldots,k \\ 11 \\ 22 \\ \vdots \\ kk \\ 12,\ldots,k-1,k \end{array} &
\left(\begin{array}{c|c|cccc|c}
2\lambda_4^2(k+2)a & 0 & -2\lambda_4 a & -2\lambda_4 a & \cdots & -2\lambda_4 a & 0 \\
\hline
0 & \begin{matrix} 1 & & \\ & \ddots & \\ & & 1 \end{matrix} & & 0 & & & 0 \\
\hline
-2\lambda_4 a & & [(k+1)\lambda_4-(k-1)]a & (1-\lambda_4)a & \cdots & (1-\lambda_4)a & \\
-2\lambda_4 a & & (1-\lambda_4)a & [(k+1)\lambda_4-(k-1)]a & \cdots & (1-\lambda_4)a & \\
\vdots & 0 & \vdots & \vdots & & \vdots & 0 \\
-2\lambda_4 a & & (1-\lambda_4)a & (1-\lambda_4)a & & [(k+1)\lambda_4-(k-1)]a & \\
\hline
0 & 0 & & 0 & & & \begin{matrix} \lambda_4^{-1} & & \\ & \ddots & \\ & & \lambda_4^{-1} \end{matrix}
\end{array}\right)
\end{array}
$$

where $a = [2\lambda_4\big((k+2)\lambda_4-k\big)]^{-1}$.

Then from equation (17) one can find that

$$V = \frac{1}{2} + \frac{3(k+1)}{2(k+4)\theta\lambda_2} + \frac{(k+2)(k+4)\theta\lambda_2 + 3 - 2(k+4)\theta}{(k+4)\lambda_2\ [(k+2)\theta - 3\lambda_2]} \ .$$

If θ is fixed, and P, Q, which are functions of the β_{ijk}, are constants, then, it is possible to choose λ_2 as a function of θ. So one has

$$J = V(\lambda_2, \theta) + B(\theta,\ P,\ Q)\ . \tag{26}$$

Since θ is fixed and P and Q are constants, then B is fixed. As indicated in section 2 one must choose $\lambda_2 = \lambda_2(\theta)$ so that V (and hence J) is minimized for this θ. Thus set

$$\frac{\partial V}{\partial \lambda_2}(\lambda_2, \theta) = 0 ,$$

which leads to

$\lambda_2(\theta) =$

$$\theta\left\{\frac{\{6[2(k+4)\theta+3(k+1)][(k+2)^2(k+4)\theta^2-6k(k+4)\theta+9k]\}^{\frac{1}{2}}-3k[2(k+4)\theta+3(k+1)]}{3[2\theta^2(k+2)(k+4)-6k(k+4)\theta-9k(k-1)]}\right\} . \quad (27)$$

Now differentiate J with respect to θ, and obtain

$$\frac{\partial V}{\partial \lambda_2}\frac{d\lambda_2}{d\theta} + \frac{\partial V}{\partial \theta} + \frac{dB}{d\theta} = 0, \quad \text{or} \quad \frac{\partial V}{\partial \theta} + \frac{dB}{d\theta} = 0, \quad \text{and since} \quad \frac{\partial V}{\partial \lambda_2} \equiv 0 ,$$

$$\frac{\partial V}{\partial \theta} = -\frac{3}{(k+4)\lambda_2}\left\{\frac{k-1}{2\theta^2} + \frac{k(k-2)(k+4)\lambda_2^2 - 2k(k+4)\lambda_2 + (k+2)}{[(k+2)\theta - 3k\lambda_2]^2}\right\}$$

and $\dfrac{dB}{d\theta} = \dfrac{2}{9(k+2)}\left(\theta - \dfrac{3}{k+4}\right)P$.

Thus $\dfrac{\partial V}{\partial \theta} + \dfrac{dB}{d\theta} = 0$ implies that

$$P = \frac{27(k+2)}{2\lambda_2[(k+4)\theta - 3]}\left\{\frac{k-1}{2\theta^2} + \frac{k(k+2)(k+4)\lambda_2^2 - 2k(k+4)\lambda_2 + (k+2)}{[(k+2)\theta - 3k\lambda_2]^2}\right\} , \quad (28)$$

where $\lambda_2 = \lambda_2(\theta)$ as in equation (27).

If a value for k is selected, then a value for θ, equations (27) and (28) can be used to tabulate sets of values of (θ, λ_2, P). On the other hand, for a given P, one can find the appropriate value for θ from equation (28) and the appropriate design is chosen so that it has moments related by the equation $\lambda_2 = \lambda_2(\theta)$. Therefore, for a given P one can find the moment values $\lambda^{1/2}$, $\lambda = 3\lambda_4/\lambda_2^2$ and V/B, when there is a contribution from V.

In most situations the appropriate experimental designs to use to minimize J have moments slightly larger than the moments of the appropriate all-bias design where $P = \infty$. As a pratical matter in situations where no information about the possible size of P exists, about 10% greater is suggested as a rough rule.

3.2 Designs Obtained From Consideration of Detection of the Inadequacy of Model

If one uses this criterion to select a design, a design is chosen such that the quantity

$$\sum_{u=1}^{N} [E(\hat{y}_u) - \psi_u]^2 = E(S_R) - \omega\,\sigma^2 = NF, \text{ say,}$$

is large. As explained in Box and Draper (1959) [3], this quantity can be written

$$NF = -\underline{\beta}_2'\underline{X}_2'\underline{X}_1 A\underline{\beta}_2 + \underline{\beta}_2'\underline{X}_2'\underline{X}_2\underline{\beta}_2 \; .$$

The matrix $N^{-1}(\underline{X}_2'\underline{X}_1 A)$ is square and of dimension $k(k-1)(k-2)/6$. It consists of a number of submatrices down the main diagonal. The first k of these are of dimension k by k and have the form

$$\frac{\lambda_4^2}{\lambda_2} \begin{bmatrix} 9 & 3 & \cdots & 3 \\ 3 & 1 & \cdots & 1 \\ 3 & 1 & \cdots & 1 \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & & \cdot \\ 3 & 1 & & 1 \end{bmatrix} .$$

All other elements are zero. Thus

$$N^{-1}\underline{\beta}_2'\underline{X}_2'\underline{X}_1 A\underline{\beta}_2 = \lambda_4^2\, \lambda_2^{-1}\, [9(\beta_{111}^2 + \ldots) + 6(\beta_{111}\, \beta_{122} + \ldots) + \\ + (\beta_{122}^2 + \ldots) + 2(\beta_{122}\, \beta_{133} + \ldots)]$$

$$= \lambda_4^2\, \lambda_2^{-1}\, [(3\beta_{111} + \beta_{122} + \ldots + \beta_{1kk})^2 + \ldots + \\ (3\beta_{kkk} + \beta_{k11} + \ldots + \beta_{k,\ k-1,\ k-1})^2]$$

$$= \lambda_4^2\, \lambda_2^{-1}\, P\, \sigma^2/N .$$

The matrix $N^{-1}(\underline{X}_2'\underline{X}_2)$ is also square of dimension $k(k-1)(k-2)/6$. It consists of $(k+1)$ submatrices down the main diagonal. The first of these is of the form

$$N^{-1} \begin{bmatrix} \sum x_{1u}^6 & \sum x_{1u}^4 x_{2u}^2 & \cdots & \sum x_{1u}^4 x_{ku}^2 \\ \sum x_{1u}^4 x_{2u}^2 & \sum x_{1u}^2 x_{2u}^4 & \cdots & \sum x_{1u}^2 x_{2u}^2 x_{ku}^2 \\ \vdots & & & \\ \sum x_{1u}^2 x_{ku}^2 & \sum x_{1u}^2 x_{2u}^2 x_{ku}^2 & \cdots & \sum x_{1u}^2 x_{ku}^4 \end{bmatrix}$$

and the second, third $\cdots$ down to the k^{th} are similar but with the obvious variation in suffixes. The (k+1) the matrix is diagonal with terms such as $N^{-1} \sum x_{1u}^2 x_{2u}^2 x_{3u}^2$. The other elements of $\underline{x}_2'\underline{x}_2$ are zero.

As discussed in [3], one has the average value $\bar{F}$ of F over all orthogonal rotations.

$$N\bar{F}/\sigma^2 = (P + Q) \sum_{u=1}^{N} r_u^6/N(k+2)(k+4)k - \lambda_4^2\lambda_2^{-1} P ,$$

where $r_u^2 = x_{1u}^2 + x_{2u}^2 + \ldots + x_{ku}^2$. Since λ_2 and λ_4 can be obtained from equation (28) and (24) for a given P, it follows that the design should be such that $\bar{F}$ is made large implies that $\sum_{u=1}^{N} r_u^6$ should be large.

4. SECOND-ORDER ROTATABLE DESIGNS IN THREE DIMENSIONS

If there are three factors to be considered in an experimental design, one may use second order rotatable designs in three dimensions.

Assume that the measurements of the factors have been coded and Cartesian axes in three dimensional space are used to describe an experimental design. In [4], Box and Hunter have shown that the necessary and sufficient condition for forming a rotatable design of second order is

$$\lambda_4/\lambda_2^2 > k/(k+2) . \tag{29}$$

This condition may always be satisfied merely by the addition of points at the center of design.

When presenting a rotatable design, it is customary to choose $\lambda_2 = 1$ as the scale of the coded controllable variables. Hence it fixes a particular design and enables better comparison between two designs with different values of λ_4/λ_2^2 .

Let $W(x,y,z) = (y,z,x)$, $W^2(x,y,z) = (z,x,y)$, $W^3(x,y,z) = (x,y,z)$. Thus W, W^2 and $W^3 = I$ form a cyclincal 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 W, R_1, R_2 and R_3 generate a group G of transformations of order 24 with elements

$$W^j,\ W^jR_1,\ W^jR_2,\ W^jR_3,\ W^jR_2R_3,$$

$$W^jR_1R_3,\ W^jR_1R_2,\ W^jR_1R_2R_3\ . \qquad (j = 1,\ 2,\ 3)$$

While R_1, R_2, and R_3 commute, W^j and R_i do not. $(j = 1, 2;\ i = 1, 2, 3)$.

Given a general point (x,y,z) in three dimensions, one may apply to it all the transformation of the group G. In this way one obtains

$$(\pm x,\ \pm y,\ \pm z),\ (\pm y,\ \pm z,\ \pm x),\ (\pm z,\ \pm x,\ \pm y)\ . \tag{30}$$

Denote it by $G(x,y,z)$ and it satisfies all the moment conditions (24), except

$$\sum_{u=1}^{N} x_{iu}^4 = 3 \sum_{\substack{u=1 \\ i\neq j}}^{N} x_{iu}^2\, x_{ju}^2 \qquad (i,j = 1,\ 2,\ 3)\ . \tag{31}$$

Now define a function K of the point (x, y, z) as

$$K(x,y,z) = \frac{1}{3}\,(x^4 + y^4 + z^4 - 3y^2z^2 - 3z^2x^2 - 3x^2y^2)\ . \tag{32}$$

This function is constant for all of the 24 points of $G(x,y,z)$. Furthermore, if it is zero then $G(x,y,z)$ is a rotatable design, because the condition (31) becomes satisfied.

Let

$$x^2 = sz^2,\ y^2 = tz^2,\ z \neq 0\ . \tag{33}$$

If $K(x,y,z) = 0$, then

$$t^2 - 3t(s+1) + (s^2-3s+1) = 0\ .$$

Solving for t in terms of s, one obtains

$$t = (1/2)[3(x+1) \pm \sqrt{5(s^2+6s+1)}\ . \tag{34}$$

If $s^2 - 3s+1 > 0$, then

$$s \geq (3 + \sqrt{5}\ )/2 \quad \text{or} \quad 0 \leq s \leq (3 - \sqrt{5}\ )/2\ .$$

Otherwise there is only one positive solution for each value of $s = 0$.

If N_0 center points are added at the center to form the design, then $N = 24 + N_0$ and $\lambda_2 N = 8(x^2 + y^2 + z^2) = 8(s + t + 1)z^2$. Then if one applies the scaling condition $\lambda_2 = 1$,

$$z^2 = N/8(s + t + 1),\quad z = [N/8(s + t + 1)]^{1/2}\ . \tag{35}$$

Thus there is an infinite class of second order designs which depends on the parameters. For if $s \geq 0$ is specified, one can have all design points fixed from equation (33), (34) and (35).

Suppose $K(x, y, z) \neq 0$ for the points of the set $G(x, y, z)$. Define $\sum K(x, y, z)$ over a point set S to be the excess of the set and write it $Ex(S)$. Thus

$$Ex[G(x,y,z)] = 8(x^4 + y^4 + z^4 - 3y^2z^2 - 3z^2x^2 - 3x^2y^2)\ . \tag{36}$$

This can take both positive and negative values according to the choice of x, y and z. If a number of sets $S_1, S_2, \ldots, S_m$ satisfy, either separate or together, the moment conditions (24) except the condition (31), then

$$Ex(S_1 + S_2 + \ldots + S_m) = Ex(S_1) + Ex(S_2) + \ldots + Ex(S_m) = 0 \tag{37}$$

is a necessary and sufficient condition for the points of the whole set $S_1 + S_2 + \ldots + S_m$ to form a rotatable arrangement of second order.

5. SECOND ORDER ROTATABLE DESIGNS IN FOUR OR MORE DIMENSIONS

In the previous section the method for obtaining infinite classes of second order rotatable designs in three dimensions has been shown. Now one may use the method previously employed to obtain infinite classes of second order rotatable designs in dimensions higher than three by a suitable generation and combination of basic sets.

Let $(x_1, x_2, x_3, \ldots, x_k)$ be a point in k dimensions and let P_k be the symmetric group of order k; that is, the group of all permutations of k elements. Thus one can obtain k points by operating upon $(x_1, x_2, \ldots, x_k)$ with the elements of P_k. Let R_{ik} be the transformation on k-space which takes the point $(x_1, x_2, \ldots, x_i, \ldots, x_k)$ into the point $(x_1, x_2, \ldots, -x_i, \ldots, x_k)$.

From a single point $(x_1, x_2, \ldots, x_k)$, by an application of the k elements of P_k and/or the k transformations $R_{ik}(i = 1, 2, \ldots k)$, one can obatin a set $H(x_1, x_2, \ldots, x_k)$ of $2^k\, k!$ distinct points. It consists of the points

$$(\pm x_{i_1}, \pm x_{i_2}, \ldots, \pm x_{i_k}), \tag{38}$$

where $i_1, i_2, \ldots, i_k$ run through every possible permutation of $1, 2, \ldots, k$. It satisfies the following conditions

$$\sum_{u=1}^{N} x_{iu}^2 = (k-1)!\ 2^k\ (x_1^2 + x_2^2 + \ldots + x_k^2)\ ,$$

$$\sum_{u=1}^{N} x_{iu}^4 = (k-1)!\ 2^k\ (x_1^4 + x_2^4 + \ldots + x_k^4)\ , \tag{39}$$

$$\sum_{\substack{u=1 \\ i\neq j}}^{N} x_{iu}^2\, x_{ju}^2 = (k-2)!\ 2^k \sum_{i\neq j}^{k} x_i^2\, x_j^2\ ,$$

$$(i,\ j = 1,\ 2,\ \ldots,\ k)$$

and all odd sums of squares and products up to and including order four are zero. Therefore,

$$Ex[H(x_1,\ x_2,\ \ldots,\ x_k)] = (k-2)!\ 2^k[(k-1)\sum_{i=1}^{k} x_i^4 - 3\sum_{i\neq j}^{k} x_i^2\, x_j^2] \tag{40}$$

where $Ex[H(x_1, x_2, \ldots, x_k)]$ is the excess of the point set H and was defined in section 4. However, the number of points in this set is too large for use in a design and it will be necessary to reduce the size of the set by making several of the x_i equal to one another and/or putting some of the x_i equal to zero.

If one wishes to use half of the set of $2^{k-1}\ k!$ points; that is, the group of all the even permutations, one can achieve the reduction only under the circumstance such that its moments are symmetrical in the way one desired. However, when $k > 3$, a cyclic permutation of coordinates does not achieve symmetry.

When there are k factors, the number of constants to be estimated for a second order model is $1 + k + k + \left(k(k-1)/2\right)$ or $(k^2 + 3k + 2)/2$. For $4 \leq k \leq 7$, one has the table

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

To obtain a design, consisting of a number of points equal to twice the number of constants to be estimated, will be regarded here as a desirable achievement. Unfortunately, because of the large number of moments to be balanced when selecting design points, such an achievement is rarely possible with the method of this section. Thus, some of the designs to be presented are useful only when a fairly large number of design points is allowable.

In order to restrict the number of points in a generated set, one considers only cases where no more than three of $x_1, x_2, \ldots, x_k$ are distinct. Consider the fraction of $H(p, p, \ldots, p; q, q, \ldots, q; r, r, \ldots, r)$ which contains all possible points once and once only.

Let p occur t times, q occur m times and r occur n times, so that $t + m + n = k$. Let v be the number of zeros if any of p, q and r are zero. For example if $p \neq 0$, $q \neq 0$, $r = 0$, then $v = n$. Hence the desire fraction $H(p^t, q^m, r^n)$ or the whole set contains

$$\frac{k!}{t!\, m!\, n!}\, 2^{k-v} \tag{41}$$

points. This set has sums of powers and products as follows:

$$\begin{aligned}
\sum_u x_{iu}^2 &= \frac{(k-1)!}{t!\, m!\, n!}\, 2^{k-v}\, [tp^2 + mq^2 + nr^2]\,, \\
\sum_u x_{iu}^4 &= \frac{(k-1)!}{t!\, m!\, n!}\, 2^{k-v}\, [tp^4 + mq^4 + nr^4]\,, \\
\sum_u x_{iu}^2 x_{ju}^2 &= \frac{(k-2)!}{t!\, m!\, n!}\, 2^{k-v}\, [t(t-1)p^4 + m(m-1)\, q^4 + n(n-1)\, r^4 \\
&\qquad + 2\, tmp^2q^2 + 2\, mnq^2r^2 + 2\, ntr^2p^2]\,,
\end{aligned} \tag{42}$$

and all other sums of powers and products up to and including order four are zero. Hence by equations (39) and (40), the excess of this generated set of $\frac{k!}{t!m!n!} 2^{k-v}$ points is obtained as

$$\mathrm{Ex}[(t!m!n!2^v)^{-1} H(p^t, q^m, r^n)]$$
$$= \frac{(k-2)!}{t!m!n!} 2^{k-v} [t(k-3t+2)p^4 + m(k-3m+2)q^4 + n(k-3n+2)r^4$$
$$- 6\, tmp^2q^2 - 6\, mnq^2r^2 - 6\, ntr^2p^2] \;. \tag{43}$$

By giving specific values to p, q, r, t, m, and n the more useful sets of this type will be achieved. In particular, any set that contains more than 48 in four dimensions will be rejected. Thus if there are three distinct values for p, q, r, one must put $r = 0$ and allow p and q to occur once only in order to maintain a reasonable number of points. This leads to consider the generated set $S(p, q, 0^{k-2}) = [4(k-2)!]^{-1} H(p, q, 0, 0, \ldots, 0)$ obtained by setting $r = 0$, $t = m = 1$. Then the set has

$$\frac{k!}{t!m!n!} 2^{k-v} = 4\, k(k-1)$$

points and its excess is

$$\mathrm{Ex}[(k-2)!\; 2^v]^{-1} H(p, q, 0^{k-2}) = 4(k-1)(p^4+q^4) - 24\, p^2q^2 \;.$$

A short table of the number of points in this set follows:

k	4	5	6	7
4k(k-1)	48	80	120	168

If $4(k-1)(p^4 + q^4) - 24\, p^2q^2 = 0$, then

$$(p^2/q^2)^2 - (6/(k-1))(p^2/q^2) + 1 = 0 \;,$$

$$p^2/q^2 = [3 \pm 9 - (k-2)^2]/(k-1) \;.$$

Since $k = 4$, $p^2/q^2 = 1$, is possible only when $k=4$. But if $p^2/q^2 = 1$ the set can be reduced by half so that $S(p, q, 0^{k-2}) = [8(k-2)!]^{-1} H(p,p,0, \ldots ,0)$ consisting of

$$\frac{k!}{2!\ (k-2)!\ 0!}\ 2^{k-(k-2)} = 2k(k-1)$$

points, form a rotatable arrangement. It becomes clear that the only point sets which are a fraction of $H(p^t, q^m, r^n)$ and which obey all the required moment conditions, except that their excess is not zero and which, in addition, contain a reasonable number of points are obtained by setting $n = 0$, $q = 0$ (i.e.; letting the coordinate take two distinct values, one of which is zero) or setting $n = m = 0$ (i.e., allowing only one possible value for the coordinate). The generated sets may be combined in the same way as was done previously in the three dimensional case.

6. CONCLUSION

The second-order rotatable design is a design based on the closeness of fitting a response surface by a polynomial and on the high power of the test for goodness of fit. One can choose N points by minimizing the difference between the true response surface and the polynomial used to fit it, or by maximizing the power of the test for the goodness of fit.

Sometimes one may obtain a fairly large number of points, therefore making it impossible to perform the design. This usually happens when there are more than three factors to be considered. In this case the k factors must be reduced into three, or less, distinct factors so that a reasonable number of points can be obtained.

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SECOND - ORDER ROTATABLE DESIGNS

by

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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 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; that is, an experimental design must be selected prior to experimentation. G. E. P. Box and J. S. Hunter suggested designs of rotatability as being suitable for such experimentation.

For a second-order design with two factors one can obtain N points for a particular group of experiments in which he is interested by the following method:

(i) minimizing the difference between the true response surface and the polynomial used to fit it, or

(ii) maximizing the power of the test for the goodness of fit.

From the designs used for two factors, one can obtain the designs for three or more factors. Sometimes a fairly large number of points may be obtained, hence making it impossible to perform the design. Usually this happens when there are more than three factors to be considered. If a large number of points are obtained, the k factors must be reduced into three or less than three distinct factors so that a reasonable number of points can be obtained.