Some Third Order Rotatable Designs

Prepared Under Contract No. DA-36-034-ORD-1517 (RD)

(Experimental Designs for Industrial Research)

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Mimeo Series No. 149
April, 1956

Chapter 1

INTRODUCTION

This dissertation considers a problem arising in the design of experiments for empirically investigating the relationship between a dependent and several independent variables, all variables being continuous. It is assumed that the form of the functional relationship is unknown but that within the range of interest the function could be represented by a Taylor Series expansion of moderately low order. For example, in two independent variables and to terms of third order the series has the form

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \beta_{111} x_1^3 + \beta_{222} x_2^3 + \beta_{112} x_1^2 x_2 + \beta_{122} x_1 x_2^2,$$

where η is the expected value of the dependent variable, x_1 and x_2 are the independent variables and where the β's are unknown coefficients in the series.

Specifically, the problem considered herein is that of the choice of the combinations of the independent variables so as to achieve certain desirable properties in the final estimates. The set of such combinations will be called the experimental design. Box and Hunter (1954a) have derived a group of designs for fitting second order Taylor Series. These designs have the desirable property that the variance of estimates of the response made from the least squares estimate of the Taylor Series depends only on the distance from the origin of the independent variables; that is, the reliability of these estimates is constant on circles (or spheres or hyperspheres in three or more independent variables). Such designs have been called rotatable. In this thesis the derivation of rotatable designs for fitting third order Taylor Series is considered.

It will be convenient to think of a specific combination of levels of k independent variables as a point in k-dimensional factor space. Thus, a design, or a set of such combinations of levels, may be viewed as a geometrical configuration of points (in that space), whose coordinates represent the levels of the k independent variables. The designs to be presented were developed by combining geometrical figures in such a way that the coordinates of the composite figure satisfied the criterion of rotatability.

With $k = 2$ only regular figures, that is, points equally spaced on circles were considered. Third order rotatable designs were found which consist of points on two such circles. The experiments required in these designs can be run in two stages in such a way that after completion of the first stage a second order series may be fitted and a decision made as to whether or not to complete the design for third order terms. The designs may also be arranged in blocks so as to balance out certain components of extraneous variation (i.e., batch effects). To achieve both of these purposes it is necessary to choose the ratio of the radii of the two circles in the proper way.

In three dimensions, third order rotatable designs were built up from both regular and semi-regular figures. Regular figures are solids all of whose faces are of the same form and size. Semi-regular figures are those figures whose vertices are symmetrically placed about the origin but whose faces are not all of the same form. Some of these designs were developed so that the experiment could be performed in two stages also.

As the number of factors increased, the number of designs discovered became smaller since the number of regular figures and number of useable semi-regular figures decreases. Also, the number of experimental points necessary to achieve a third order rotatable design increases alarmingly with each increase in the number of dimensions, so that the third order rotatable designs found in the higher dimensions become only of academic interest.

Chapter II

REVIEW OF LITERATURE

Excellent reviews of the literature on the subjects of locating optima and exploring response surfaces are given by Anderson (1953) and Hunter (1954b). Much of the writings cited here are reviewed in those articles.

One of the first papers dealing with the location of an optimum response was written by Hotelling (1941). In this, Hotelling proposed for a one dimensional experiment in which an interval containing the optimum had been determined, a method of selecting experimental points for fitting a quadratic equation. The points were selected in such a way that the coefficients in a quadratic model would be unbiased by cubic effects and so that the bias from quartic effects would be a minimum. For the two-dimensional case and a quadratic model Hotelling set forth conditions on the locations of the experimental points to assure the vanishing of cubic bias.

Friedman and Savage (1947) discussed a sequential scheme for locating an optimum in a multi-factor situation. The method is that in which each factor is varied separately while each of the remaining factors is maintained at the prevailing best estimate of its optimum level.

In contrast with this, Box and Wilson (1951) suggested a method of exploring a response surface in which several factors might be varied simultaneously. Given an experimentally obtained polynomial regression equation, they propose proceeding by further experimentation toward the optimum or stationary point along the "path of steepest ascent". The coordinates of this path are proportional to the first order derivatives of the fitted regression equation. When increases in response are no longer achieved, another experiment, perhaps of the factorial type, is performed in the region of the largest response and a new direction of steepest ascent determined. Box and Wilson give a composite design developed to fit a full quadratic model when a near-stationary region has been reached. The composite design consists of the 2^k vertices of a k-dimensional cube and the 2k vertices of the k-dimensional octahedron. Variations of this composite design form rotatable designs for second order response surfaces (Box and Hunter, 1954a) and will be recognized as integral parts of some third order rotatable designs developed in this thesis.

Box (1952) discussed the problem of optimum designs for multi-factor experiments when the response surface may be approximated by a plane. He showed that the best design, using the minimum number of points, is k + 1 points arranged in a k-dimensional simplex. That is, for k = 2, three points would be arranged in an equilateral triangle, for k = 3, four points would be arranged in a tetrahedron, and so on. In a subsequent paper, Box (1954) discussed the philosophy of the surface fitting problem and reviewed much of the work done up to that time.

Two papers which did much to stir up interest in the general problem of surface fitting were those by Box and Hunter (1954a) and Hunter (1954b). It was in these papers that the criterion of rotatability for multifactor experimental designs was advanced. The authors showed that rotatable designs could be formed from geometrical configurations whose point coordinates had moments identical with those of the spherical distribution up to order 2d, where d is the order of the equation to be fitted. For quadratic response surfaces (d = 2), a class of designs was developed called second order rotatable designs. These designs appear to have met with considerable success in the physical sciences.

In another paper, Hunter (1954a) described the application of a third order composite (but not rotatable) design to a study of the flooding capacity of a pulse column. The study involved three independent variables whose levels were located at the vertices of a cube, an octahedron and a cuboctahedron.

The problem of establishing confidence regions about an experimentally estimated stationary point was considered by Box and Hunter (1954b). Dealing first with the general problem of obtaining confidence regions for the solution of a set of simultaneous equations, they gave an example of a confidence region for the estimated stationary point of a quadratic response surface investigated using a 3^2 factorial design.

Much of the work done on the fitting of response surfaces concerns itself with the fitting of a Taylor Series expansion including terms up to and including order d, say, under the assumption that terms of order higher than d are negligible. A paper by Box, Hunter and Hader (1954) discusses the consequences of fitting a d-th order equation when, unknown to the experimenter, this assumption is not justified. By the use of a device called the alias matrix the nature of the biases so introduced is demonstrated.

De la Garza (1954), for the single factor case, showed that the precision matrix for a polynomial regression equation of order d, based on more than d + 1 distinct points, can be duplicated by placing the levels of the factors at exactly d + 1 judiciously selected locations. An extension of this work to the multi-factor case warrants some attention.

Chapter III

RESPONSE SURFACES, TAYLOR SERIES EXPANSIONS AND LEAST SQUARES

Response Surfaces

Suppose that an experimenter wishes to explore a functional relationship between a response, η, and several quantitative factors, $x_1, x_2, \ldots x_k$. The relationship could be expressed generally as

$$\eta = \phi(x_1, x_2, \ldots x_k). \tag{1}$$

If it were possible to depict graphically this unknown relationship, one might plot η in the k + 1-th dimension over the k-dimensional factor space and the resulting plot would describe a response surface of some form or other. Several excellent diagrams of response surfaces are given by Box (1954) for k = 2 and k = 3. The experimenter's interest in the surface might lie in locating an optimum point on this surface at which the yield is a maximum or at which the cost is a minimum. He might be interested in several responses, $\eta_1, \eta_2, \ldots \eta_m$, over the same factor space. For example, he may wish to find the combinations of factors for which η_1 is a maximum and η_2 is equal to some fixed constant, c. Many examples might be cited but the important thing is that a knowledge of the mathematical form, or an approximation to it, is of paramount concern.

Taylor Series Expansions

If it is assumed that the functional relationship is unknown, one must be satisfied, during the initial stages of experimentation at least, with an attempt to find an approximation to the true form. One such approximation may be obtained from the Taylor Series expansion of equation (1).

Expanding equation (1) in a Taylor Series gives an infinite series which might be expressed as

$$\eta = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i \le j=1}^{k} \beta_{ij} x_i x_j + \sum_{i \le j \le \ell=1}^{k} \beta_{ij\ell} x_i x_j x_\ell + \cdots \qquad (2)$$

where the x_i are measured from an origin in the center of the region of interest. Equation (2) is equivalent to equation (1) and an approximation to either is obtained by disregarding all terms of (2) of a certain order and higher. A second order approximation is obtained by disregarding all terms beyond the second summation sign; a third order approximation results from dropping all terms beyond the third summation sign. In most experimental situations a second order approximation would be all that is required but experience has shown that sometimes second order approximations are not adequate. A logical next step in such cases would be to try a third order approximation.

The experimenter is confronted with the problem of deciding upon the order of approximation he feels is adequate and attempting to obtain estimates, experimentally, of the coefficients, β_0, β_i, β_{ij}, ... The estimates of the coefficients having been obtained, the experimenter then has an estimate of the response surface of his phenomenon which, if adequate, will allow him to explore for maxima or minima or other optimum points. Of equal or greater importance to the experimenter who has found an adequate approximation is the interpretation of the fitted surface in terms of the theory of the scientific field in which the technique has been applied.

Least Squares

To fit the response surface, a model such as the third order model

$$y = \beta_0 x_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i \leq j=1}^{k} \beta_{ij} x_i x_j + \sum_{i \leq j \leq \ell=1}^{k} \beta_{ij\ell} x_i x_j x_\ell + \varepsilon \qquad (3)$$

is postulated. Here y is a measured response, x_0 is a dummy variable always equal to one, the β_i and x_i are defined as before and ε is a random error, independent of the x's and with mean zero and variance σ^2. The x's are considered fixed and measured without error. An experimental design is chosen with which to fit the response surface and which has as its points combinations of levels of the factors, x_i. Following the notation of Box and Hunter, let the u-th experimental point be denoted by the (1 x k) row vector

$$\underline{x}_u' = (x_{1u}, x_{2u}, \ldots x_{ku}). \qquad (4)$$

N such experimental points constitute a design and if the N vectors, $\underline{x}_u'$, are arranged in a column, the design matrix, D, is formed, i.e.,

$$\underline{D} = \begin{bmatrix} \underline{x}_1' \\ \underline{x}_2' \\ \cdot \\ \cdot \\ \cdot \\ \underline{x}_N' \end{bmatrix} \qquad (5)$$

$\underline{D}$ is an (N x k) matrix where N must be greater than or equal to L, the number of coefficients in the series to be fitted, i.e., $N \geqslant \binom{k+d}{d}$, k being the number of factors and d the order of the series. By augmenting $\underline{D}$ with a column of one's on the left and by affixing on the right, columns formed by the appropriate multiples of columns of $\underline{D}$ according to the form of (3), the matrix $\underline{X}$ is formed. Then the model may be written

$$\underline{Y} = \underline{X}\,\underline{\beta} + \underline{\varepsilon} \tag{6}$$

in which $\underline{Y}$ is an (N x 1) column vector of observations, or the response variable, y, $\underline{X}$ is an (N x L) matrix formed by augmenting $\underline{D}$, $\underline{\beta}$ is an (L x 1) vector of coefficients and $\underline{\varepsilon}$ is an (N x 1) vector of errors. Denoting by $\underline{B}$, the (L x 1) vector of the minimum variance unbiased estimates of the coefficients, it can be shown that

$$\underline{B} = (\underline{X}'\underline{X})^{-1}\,\underline{X}'\underline{Y}, \tag{7}$$

provided that $\underline{X}$ is of rank L. The elements of $\underline{B}$ are the least squares estimates of the β's. The matrix, $\sigma^2(\underline{X}'\underline{X})^{-1}$, is the variance-covariance matrix of the estimates, and an unbiased estimate of σ^2 is given by s^2, where

$$(N - L)s^2 = \underline{Y}'(\underline{Y} - \underline{XB}). \tag{8}$$

Chapter IV

CRITERION OF ROTATABILITY

For planar response surfaces, it has been shown by Box (1952), that there is a unique class of designs which will minimize the variances of the estimates of the β's. These are the orthogonal designs and there is a sub-class of these, namely, the designs based upon the simplex, which use the minimum number of experimental points. The criterion of orthogonality, however, does not lead to a unique class of designs for response surfaces of order higher than one and, as was shown by Box and Hunter (1954a), the variances of the coefficients in orthogonal designs, as well as in some other designs, are dependent upon the orientation of the response surface over the region studied. This can be examined by applying an orthogonal transformation to the design matrix, $\underline{D}$, and comparing the variance-covariance matrix after transformation to the variance-covariance matrix before transformation. For most designs these variance-covariance matrices would be different, showing that the variances of coefficients, and consequently of the predictions and estimates made from them, are dependent upon the orientation of the design.

It seemed logical to require that designs used for exploring response surfaces be independent of rotation, that is, to require that the variances of estimated responses be constant on spheres or hyper-spheres with centers at the origin of the design. This is the criterion of rotatability and designs which meet the criterion are termed rotatable designs. Box and Hunter proved that a necessary and sufficient condition for rotatability is that the moments of the independent variables be the same as those of a spherical probability distribution up to order 2d. Thus, the moment matrix, $N^{-1}(\underline{X}'\underline{X})$, of a rotatable design of order 3 in two factors can be written

$$
N^{-1}(\underline{X}'\underline{X}) =
\begin{array}{cccccccccc|c}
x_0 & x_1^2 & x_2^2 & x_1x_2 & x_1 & x_1^3 & x_1x_2^2 & x_2 & x_2^3 & x_1^2x_2 & \\
\hline
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x_0 \\
 & 3\lambda_1 & \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x_1^2 \\
 & & 3\lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x_2^2 \\
 & & & \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & x_1x_2 \\
 & & & & 1 & 3\lambda_1 & \lambda_1 & 0 & 0 & 0 & x_1 \\
 & & & & & 15\lambda_2 & 3\lambda_2 & 0 & 0 & 0 & x_1^3 \\
 & & & & & & 3\lambda_2 & 0 & 0 & 0 & x_1x_2^2 \\
 & & & & & & & 1 & 3\lambda_1 & \lambda_1 & x_2 \\
 & & \text{(symmetric)} & & & & & & 15\lambda_2 & 3\lambda_2 & x_2^3 \\
 & & & & & & & & & 3\lambda_2 & x_1^2x_2
\end{array}
\qquad (9)
$$

in which λ_1 and λ_2 are constants. (λ_1 corresponds to Box and Hunter's λ_4 which they shortened to λ, and λ_2 corresponds to their λ_6.) The independent variables x_1 and x_2 have been coded so that

$$\sum_{u=1}^{N} x_1^2 = \sum_{u=1}^{N} x_2^2 = N$$

to standardize the moment matrix for ease in further investigation. Each term in (9) is a moment of the independent variables. For example, the term in the column headed by x_2^2 and the row labeled x_2^2 is the fourth moment of x_2, i.e.,

$$\frac{1}{N}\sum_{u=1}^{N} x_{2u}^4 = 3\lambda_1 .$$

The term in the column headed by $x_1 x_2^2$ and the row, x_1^3, is a sixth order mixed moment of both x_1 and x_2, i.e.,

$$\frac{1}{N} \sum_{u=1}^{N} x_{1u}^4 \, x_{2u}^2 = 3\lambda_2 .$$

Equation (9) may be generalized to k dimensions by writing

$$N^{-1}(\underline{X}'\underline{X}) = \begin{bmatrix} \underline{G} & 0 & 0 & 0 & \cdots & 0 & 0 \\ & \lambda_1 I & 0 & 0 & \cdots & 0 & 0 \\ & & K & 0 & \cdots & 0 & 0 \\ & & & & \ddots & \vdots & \vdots \\ & & & & & K & 0 \\ & & & & & & \lambda_2 I \end{bmatrix} \tag{10}$$

in which the submatrices are defined as follows:

$$\underline{G} = \begin{array}{c} \begin{array}{ccccc} \underline{x_0} & \underline{x_1^2} & \underline{x_2^2} & \cdots & \underline{x_k^2} \end{array} \\ \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ & 3\lambda_1 & \lambda_1 & \cdots & \lambda_1 \\ & & 3\lambda_1 & \cdots & \lambda_1 \\ & & & \ddots & \vdots \\ & & & & 3\lambda_1 \end{bmatrix} \end{array} , \tag{11}$$

$$\underline{K} = \begin{array}{cccccc} \underline{x_i} & \underline{x_i^3} & \underline{x_i x_1^2} & \underline{x_i x_2^2} & \cdots & \underline{x_i x_k^2} \\ \end{array}$$
$$\left[\begin{array}{cccccc} 1 & 3\lambda_1 & \lambda_1 & \lambda_1 & \cdots & \lambda_1 \\ & 15\lambda_2 & 3\lambda_2 & 3\lambda_2 & \cdots & 3\lambda_2 \\ & & 3\lambda_2 & \lambda_2 & \cdots & \lambda_2 \\ & & & 3\lambda_2 & \cdots & \lambda_2 \\ & & & & \ddots & \vdots \\ & & & & & 3\lambda_2 \end{array}\right], \qquad (12)$$

$$\lambda_1 I = \begin{array}{c} \begin{array}{cccc} \underline{x_1 x_2} & \underline{x_1 x_3} & \cdots & \underline{x_{k-1} x_k} \end{array} \\ \left[\begin{array}{cccc} \lambda_1 & 0 & \cdots & 0 \\ & \lambda_1 & \cdots & 0 \\ & & \ddots & \vdots \\ & & & \lambda_1 \end{array}\right] \end{array}, \qquad (13)$$

$$\lambda_2 I = \begin{array}{c} \begin{array}{cccc} \underline{x_1 x_2 x_3} & \underline{x_1 x_2 x_4} & \cdots & \underline{x_{k-2} x_{k-1} x_k} \end{array} \\ \left[\begin{array}{cccc} \lambda_2 & 0 & \cdots & 0 \\ & \lambda_2 & \cdots & 0 \\ & & \ddots & \vdots \\ & & & \lambda_2 \end{array}\right] \end{array}. \qquad (14)$$

In equation (10), 0 denotes a null matrix of appropriate size and in equation (12) the column corresponding to x_i^3 appears only once and always in the second position.

Equations (9) and (10) will be sufficient for a useable rotatable design provided that

$$\lambda_1 > \frac{k}{k+2} \tag{15}$$

and

$$\lambda_2 > \frac{k+2}{k+4}\lambda_1^2 . \tag{16}$$

If (15) and (16) are not satisfied, (9) and (10) are singular or do not exist.

The moment matrix has been written in this form rather than with the order of the columns corresponding to the order of the coefficients in the model to point out the amount of orthogonality present and to facilitate the calculation of the inverse.

The criterion of rotatability is characterized mathematically by equation (10) with its attendant restrictions, equations (15) and (16). To find a third order rotatable design in k factors, one must discover a set of combinations of factor levels whose moments are those of equation (10).

The inverses of the submatrices of (10) are

$$G^{-1} = A\begin{bmatrix} 2\lambda_1^2(k+2) & -2\lambda_1 & -2\lambda_1 & \cdots & -2\lambda_1 \\ & (k+1)\lambda_1-k+1 & 1-\lambda_1 & \cdots & 1-\lambda_1 \\ & & (k+1)\lambda_1-k+1 & \cdots & 1-\lambda_1 \\ & & & \ddots & \vdots \\ & & & & (k+1)\lambda_1-k+1 \end{bmatrix} \tag{17}$$

$$\underline{K}^{-1} = B \begin{bmatrix} 6(k+4)\lambda_2 & -6\lambda_1 & -6\lambda_1 & -6\lambda_1 & \cdots & -6\lambda_1 \\ & k+1-(k-1)\lambda_1^2\lambda_2^{-1} & 3(\lambda_1^2\lambda_2^{-1}-1) & 3(\lambda_1^2\lambda_2^{-1}-1) & \cdots & 3(\lambda_1^2\lambda_2^{-1}-1) \\ & & 3[k+3-(k+1)\lambda_1^2\lambda_2^{-1}] & 3(\lambda_1^2\lambda_2^{-1}-1) & \cdots & 3(\lambda_1^2\lambda_2^{-1}-1) \\ & & & 3[k+3-(k+1)\lambda_1^2\lambda_2^{-1}] & \cdots & 3(\lambda_1^2\lambda_2^{-1}-1) \\ & & & & \ddots & \vdots \\ & & & & & 3[k+3-(k+1)\lambda_1^2\lambda_2^{-1}] \end{bmatrix} \tag{18}$$

$$(\lambda_1 I)^{-1} = \begin{bmatrix} 1/\lambda_1 & 0 & \cdots & 0 \\ & 1/\lambda_1 & \cdots & 0 \\ & & \ddots & \vdots \\ & & & 1/\lambda_1 \end{bmatrix} \tag{19}$$

$$(\lambda_2 I)^{-1} = \begin{bmatrix} 1/\lambda_2 & 0 & \cdots & 0 \\ & 1/\lambda_2 & \cdots & 0 \\ & & \ddots & \vdots \\ & & & 1/\lambda_2 \end{bmatrix} \tag{20}$$

where the constants, A and B, are given by

$$A^{-1} = 2\lambda_1 [(k + 2)\lambda_1 - k] \tag{21}$$

$$B^{-1} = 6[(k + 4)\lambda_2 - (k + 2)\lambda_1^2]. \tag{22}$$

Chapter V

ROTATABLE DESIGNS FOR SECOND ORDER SURFACES

In this chapter will be reviewed the second order rotatable designs as discovered by Box and Hunter (1954a). Also some second order rotatable arrangements discovered subsequent to that writing will be presented. By rotatable arrangement is meant a configuration of points, the moments of whose coordinates are invariant under rotation, but which does not necessarily constitute a design. For example, a configuration of points may satisfy equation (9) of the previous chapter but may not satisfy either equation (15) or equation (16). It has been shown (Box and Hunter, 1954a) that for a configuration of points equidistant from the origin, even though the moments are those of a spherical distribution,

$$\lambda_1 = \frac{k}{k + 2},$$

which violates equation (15). Thus, such points equidistant from the origin constitute a rotatable arrangement but do not, in themselves, provide a rotatable design. Some rotatable designs are termed _uniform information rotatable designs_. These are designs for which the variance of a predicted response, $V(\dot{y})$ is the same at the center of the design as at a unit distance from the center of the design. Between these two points the variance curve, in general, will be reasonably flat.

Second Order Designs in Two Dimensions

There are an infinite number of rotatable arrangements in two dimensions for any order surface. In two factors a regular figure, that is, points equally spaced on a circle, gives a rotatable second order arrangement provided that the number of points on the circle is greater than four. By adding an observation or observations at the center of the circle a rotatable design is obtained. Each point added at the center increases the value of λ_1. By increasing λ_1 to 0.7844, a uniform information second order rotatable design in two dimensions is obtained.

With $n_2 > 4$ points on the circle and n_1 points at the center, Hunter (1954b) gives the design matrix for a second order rotatable design in two factors as

$$\underline{D} = \begin{array}{c} \begin{array}{cc} \underline{x_1} & \underline{x_2} \end{array} \\ \begin{bmatrix} a \cos \theta & a \sin \theta \\ a \cos 2\theta & a \sin 2\theta \\ a \cos 3\theta & a \sin 3\theta \\ \vdots & \vdots \\ a \cos n_2\theta & a \sin n_2\theta \\ 0 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix} \end{array}$$

where $\theta = \frac{2\pi}{n_2}$ and a is chosen so that $\sum x_i^2 = n_1 + n_2 = N$.

<u>Second Order Designs in Three Dimensions</u>

By concentrating attention on the regular figures in three dimensions, Box and Hunter (1954a) developed three basic rotatable designs for second order equations. One is based on the icosahedron, a 12 pointed, 20 sided regular figure, with additional points at the center of the figure. Its design matrix is

$$
\underline{D} = \begin{array}{c}
\begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\
\begin{bmatrix}
0 & 1.902a & 1.176a \\
0 & 1.902a & -1.176a \\
0 & -1.902a & 1.176a \\
0 & -1.902a & -1.176a \\
1.176a & 0 & 1.902a \\
1.176a & 0 & -1.902a \\
-1.176a & 0 & 1.902a \\
-1.176a & 0 & -1.902a \\
1.902a & 1.176a & 0 \\
1.902a & -1.176a & 0 \\
-1.902a & 1.176a & 0 \\
-1.902a & -1.176a & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0
\end{bmatrix}
\end{array}
$$

with a chosen so that $\sum x_i^2 = N$.

A second design is based on the dodecahedron, which has 20 points and 12 faces. With points added at the center of the arrangement, the design matrix is

$$\underline{D} = \begin{array}{c} \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\ \begin{bmatrix} a & -a & -a \\ -a & a & -a \\ -a & -a & a \\ a & a & a \\ & & \\ a & a & -a \\ 0 & 0.618a & 1.618a \\ -1.618a & 0 & -0.618a \\ 0.618a & -1.618a & 0 \\ & & \\ -a & -a & -a \\ 0 & -0.618a & 1.618a \\ 1.618a & 0 & -0.618a \\ -0.618a & 1.618a & 0 \\ & & \\ a & -a & a \\ 0 & -0.618a & -1.618a \\ -1.618a & 0 & 0.618a \\ 0.618a & 1.618a & 0 \\ & & \\ -a & a & a \\ 0 & 0.618a & -1.618a \\ 1.618a & 0 & 0.618a \\ -0.618a & -1.618a & 0 \\ & & \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 0 & 0 & 0 \end{bmatrix} \end{array}$$

again taking a so that $\sum x_i^2 = N$.

The third second order rotatable design in three dimensions has as its points the vertices of a cube and of an octahedron concentrically placed. This composite configuration needs no points at the center to satisfy equation (10), but a better conditioned moment matrix results if central points are used. (Box and Wilson call this the central composite design.) However, to meet equation (9), the ratio of the radii of the cube to the octahedron must be $\frac{3^{1/2}}{2^{3/4}}$. The design matrix for the cube-plus-octahedron design is

$$
\begin{array}{ccc}
 & \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} & \\
\underline{D} = & \left[\begin{array}{ccc}
-a & -a & -a \\
a & -a & -a \\
-a & a & -a \\
a & a & -a \\
-a & -a & a \\
a & -a & a \\
-a & a & a \\
a & a & a \\
-1.682a & 0 & 0 \\
1.682a & 0 & 0 \\
0 & -1.682a & 0 \\
0 & 1.682a & 0 \\
0 & 0 & -1.682a \\
0 & 0 & 1.682a \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
0 & 0 & 0
\end{array}\right] &
\begin{array}{l}
 \\ \\ \\ \text{------- Cube} \\ \\ \\ \\ \\ \\ \\ \text{------- Octahedron} \\ \\ \\ \\ \\ \\ \text{------- Center} \\ \\ \\ \\
\end{array}
\end{array}
$$

While investigating the geometrical configurations to discover which might be used to make third order rotatable designs, several new second order designs were discovered. All but one of these were based on three-dimensional semi-regular figures. Consider, for example, the truncated cube, which is a 24 point semi-regular figure and which can be visualized by imagining a cube each of whose corners has been cut off in the same amount and at the same angle. Each of the eight points of the cube generates three points of a truncated cube. Together with some center points, the truncated cube affords a second order rotatable design whose matrix is

$$\underline{D} = \begin{array}{c} \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\ \begin{bmatrix} c & b & b \\ b & c & b \\ b & -c & b \\ c & -b & b \\ -c & -b & b \\ -b & -c & b \\ -b & c & b \\ -c & b & b \\ & & \\ c & b & -b \\ b & c & -b \\ b & -c & -b \\ c & -b & -b \\ -c & -b & -b \\ -b & -c & -b \\ -b & c & -b \\ -c & b & -b \\ & & \\ b & b & c \\ b & b & -c \\ b & -b & c \\ b & -b & -c \\ -b & b & c \\ -b & b & -c \\ -b & -b & c \\ -b & -b & -c \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 0 & 0 & 0 \end{bmatrix} \end{array} \tag{23}$$

in which

$$c^2 = \frac{5 + 2\sqrt{10}}{15} \cdot \frac{N}{8}$$

$$b^2 = \frac{N - 8c^2}{16} .$$

If a cube is truncated to the extreme, that is, so that the two points on each edge merge into one, a 12 pointed figure, known as the cuboctahedron, is formed. The same figure results from truncating to the extreme the six vertices of the octahedron. The cuboctahedron, in conjunction with an octahedron, also forms a second order rotatable design. The design matrix for this configuration is

$$
\begin{array}{cc}
 & \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\
\underline{D} = & \begin{bmatrix}
a & 0 & a \\
0 & -a & a \\
-a & 0 & a \\
0 & a & a \\
a & 0 & -a \\
0 & -a & -a \\
-a & 0 & -a \\
0 & a & -a \\
a & a & 0 \\
a & -a & 0 \\
-a & a & 0 \\
-a & -a & 0 \\
 & & \\
ba & 0 & 0 \\
-ba & 0 & 0 \\
0 & ba & 0 \\
0 & -ba & 0 \\
0 & 0 & ba \\
0 & 0 & -ba \\
 & & \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
0 & 0 & 0
\end{bmatrix} .
\end{array}
\tag{24}
$$

Here, a is the scaling factor selected so that $\sum x_i^2 = N$, and

$$b = \left(\frac{1}{2}\right)^{1/4} = 0.8409.$$

A second order rotatable design in three dimensions may also be formed by adding center points to a truncated octahedron. Its design matrix is

$$
\underline{D} = \begin{array}{c} \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\ \left[\begin{array}{ccc}
b & c & 0 \\
b & -c & 0 \\
b & 0 & c \\
b & 0 & -c \\
-b & c & 0 \\
-b & -c & 0 \\
-b & 0 & c \\
-b & 0 & -c \\
c & b & 0 \\
-c & b & 0 \\
0 & b & c \\
0 & b & -c \\
c & -b & 0 \\
-c & -b & 0 \\
0 & -b & c \\
0 & -b & -c \\
c & 0 & b \\
-c & 0 & b \\
0 & c & b \\
0 & -c & b \\
c & 0 & -b \\
-c & 0 & -b \\
0 & c & -b \\
0 & -c & -b \\
 & & \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
0 & 0 & 0
\end{array}\right] \end{array} . \qquad (25)
$$

For equation (25)

$$b^2 = \frac{3 + \sqrt{5}}{2} c^2$$

$$c^2 = \frac{5 - \sqrt{5}}{80} N.$$

Still another configuration, which defies description in terms of the regular or semi-regular figures, may be used to construct a second order rotatable design. Basically, it is a version of the snub-cube. Consider a square parallel to the (x_1, x_2) plane at a distance b from the origin and another square rotated 45^o from the first square and at a distance -b from the origin. In like manner, consider pairs of squares parallel to the (x_1, x_3) plane and (x_2, x_3) plane in similar positions and distances from the origin. With points added at the center, the design matrix is

$$\underline{D} = \begin{array}{c} \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\ \begin{bmatrix} c & c & b \\ c & -c & b \\ -c & c & b \\ -c & -c & b \\ c\sqrt{2} & 0 & -b \\ 0 & c\sqrt{2} & -b \\ -c\sqrt{2} & 0 & -b \\ 0 & -c\sqrt{2} & -b \\ b & c & c \\ b & c & -c \\ b & -c & c \\ b & -c & -c \\ -b & c\sqrt{2} & 0 \\ -b & 0 & c\sqrt{2} \\ -b & -c\sqrt{2} & 0 \\ -b & 0 & -c\sqrt{2} \\ c & b & c \\ -c & b & c \\ c & b & -c \\ -c & b & -c \\ 0 & -b & c\sqrt{2} \\ c\sqrt{2} & -b & 0 \\ 0 & -b & -c\sqrt{2} \\ -c\sqrt{2} & -b & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \end{bmatrix} \end{array} . \qquad (26)$$

In this design

$$b^2 = \frac{6 \pm \sqrt{30}}{2} c^2$$

and

$$c^2 = \frac{N}{40 \pm 4\sqrt{30}} ,$$

where it is understood that the sign used is either plus for both equations or minus for both equations.

Finally, a new design based on two regular figures was discovered. This is a simple offshoot of the cube-plus-octahedron design and consists of a cube plus a doubled octahedron. The doubled octahedron is simply an octahedron with each point repeated. This configuration has an advantage in that it reduces the radius of the octahedron needed to afford rotatability. Its design matrix is as follows:

$$\begin{array}{c} \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\ \underline{D} = \begin{bmatrix} a & a & a \\ a & a & -a \\ a & -a & a \\ a & -a & -a \\ -a & a & a \\ -a & a & -a \\ -a & -a & a \\ -a & -a & -a \\ a\sqrt{2} & 0 & 0 \\ a\sqrt{2} & 0 & 0 \\ -a\sqrt{2} & 0 & 0 \\ -a\sqrt{2} & 0 & 0 \\ 0 & a\sqrt{2} & 0 \\ 0 & a\sqrt{2} & 0 \\ 0 & -a\sqrt{2} & 0 \\ 0 & -a\sqrt{2} & 0 \\ 0 & 0 & a\sqrt{2} \\ 0 & 0 & a\sqrt{2} \\ 0 & 0 & -a\sqrt{2} \\ 0 & 0 & -a\sqrt{2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 0 & 0 & 0 \end{bmatrix} . \end{array} \qquad (27)$$

Again a is the coding factor which guarantees that the sum of squares equals N.

Second Order Designs in More than Three Dimensions

There are few regular figures in four dimensions which may be practically utilized in the formation of rotatable designs. They are the measure polytope of 16 points (the analogue of the cube), the cross polytope of 8 points (the analogue of the octahedron) and a 24 pointed figure which is a combination of the two. The other figures have either too many points to be practically useful or, as in the case of the simplex, too few to estimate all the coefficients. In five dimensions or more only the simplex, measure polytope and cross polytope exist as regular figures. Box and Hunter (1954a) used a combination of the measure polytope and cross polytope as the basis of all their designs in more than three dimensions. In general the design matrix for the design in k dimensions is

$$\underline{D} = \begin{array}{c} \begin{array}{cccc} \underline{x_1} & \underline{x_2} & \cdots & \underline{x_k} \end{array} \\ \left[\begin{array}{cccc} a & a & \cdots & a \\ a & a & \cdots & -a \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ -a & -a & \cdots & -a \\ 2^{k/4}a & 0 & \cdots & 0 \\ -2^{k/4}a & 0 & \cdots & 0 \\ 0 & 2^{k/4}a & \cdots & 0 \\ 0 & -2^{k/4}a & \cdots & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & \cdots & 2^{k/4}a \\ 0 & 0 & \cdots & -2^{k/4}a \\ 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & \cdots & 0 \end{array} \right] \end{array} .$$

To reduce the number of experiments necessary to complete a second order design, fractional replicates of the measure polytope may be used for k greater than or equal to five. The radius of the cross polytope is changed to $a2^{\frac{k-1}{4}}$ if a half replicate is used and to $a2^{\frac{k-2}{4}}$ if a quarter replicate is used. A quarter replicate may be used only when k is greater than seven if the second order effects are to be unconfounded with first or other remaining second order effects.

Some of the second order rotatable designs discovered subsequent to Box and Hunter's paper, in particular the designs of equations (23), (24), (25) and (27), may also be extended to more than three dimensions. The design of equation (26) does not lend itself to extension to 4 or more dimensions. Consider first the design based on the extension to k dimensions of the truncated cube. The coordinates of this design may be written as all possible permutations of the elements of the vector

$$(\pm c, \pm b, \pm b, \ldots, \pm b)$$

together with a number of center points. (See, for example, equation (23) for three variables.) The elements c and b are given by

$$c^2 = (3 + \sqrt{2k + 4})\, b^2$$

$$b^2 = \frac{N}{2^k} \frac{1}{2 + k + \sqrt{2k + 4}} .$$

N in this case is $k2^k$ plus the number of points at the center.

Equation (24), when extended to k dimensions, has as its coordinates the permutations of

$$(0, \pm a, \pm a, \ldots, \pm a)$$

for the k-dimensional cuboctahedron portion, and for the cross polytope portion the permutations of

$$(\pm ba, 0, 0, \ldots, 0),$$

where

$$b = \left[\frac{2k - 5}{(k - 1)^2}\, 2^{k-2} \right]^{1/4} .$$

The number of points in this design is $k(2^{k-1} + 2)$ plus the number of central points.

Equation (25) may be extended only to k = 4 to obtain a second order rotatable design as may be seen by the defining relationship

$$b^2 = \frac{3 + \sqrt{9 - (k - 1)^2}}{k - 1} c^2.$$

When $k = 4$, $b = c = a$, and a 24 point figure results whose coordinates are the permutations of

$$(\pm a, \pm a, 0, 0)$$

where again a is the coding factor, and again points are added at the center to satisfy equation (16).

The design of equation (27) extends to more than three dimensions with the use of the k-dimensional measure polytope, whose coordinates are all possible permutations of

$$(\pm a, \pm a, \ldots, \pm a),$$

and with two cross polytopes with coordinates the permutations of

$$(\pm ba, 0, \ldots, 0).$$

The factor, b, is given by

$$b = 2^{(k-1)/4}.$$

The total number of points is $2^k + 4k$ plus the number of points added at the center.

The new designs presented here, that is, the designs of equations (23), (24), (25), (26) and (27) and their extensions, all require more points than do the designs of Box and Hunter. This disadvantage is partially offset, however, by the fact that the factor space is more fully covered in the region of interest (with (23), (24), (25) and (26)) and in that respect, the design is probably less sensitive to bias from higher order terms. The design of equation (27) can be looked at as a Box-Hunter design, slightly replicated. It has the advantage that it gives a check on whether the experimental error can be regarded as constant in the factor space without repeating the entire experiment. The new designs are of greater interest, however, from the point of view that they may be utilized in the formation of designs for the exploration of third order response surfaces.

Chapter VI

THIRD ORDER ROTATABLE DESIGNS IN TWO DIMENSIONS

In this section only arrangements consisting of points equally spaced on circles will be considered. The conditions necessary for the moments of the coordinates of the points to be invariant under rotation will be set forth. n points on a circle of radius ρ could have as coordinates the following

$$\begin{array}{ll}
\underline{x_1} & \underline{x_2} \\
\rho\cos 0 = \rho & \rho\sin 0 = 0 \\
\rho\cos\theta & \rho\sin\theta \\
\rho\cos 2\theta & \rho\sin 2\theta \\
\vdots & \vdots \\
\rho\cos(n-1)\theta & \rho\sin(n-1)\theta\ ,
\end{array}$$

where $\theta = \frac{2\pi}{n}$.

By varying q, in steps of one, from 0 to p, any p^{th} order moment may be expressed as

$$M = \frac{\rho^p}{n} \sum_{u=0}^{n-1} (\cos u\theta)^{p-q} (\sin u\theta)^q. \tag{28}$$

If the design is rotated through an angle α, the p^{th} order moment becomes

$$M_\alpha = \frac{\rho^p}{n} \sum_{u=0}^{n-1} [\cos(u\theta + \alpha)]^{p-q} [\sin(u\theta + \alpha)]^q . \tag{29}$$

If the p^{th} order moment is to be invariant under rotation the difference between (28) and (29) must be zero.

We may write

$$(\cos u\theta)^{p-q} = \left(\frac{e^{iu\theta} + e^{-iu\theta}}{2}\right)^{p-q} = 2^{-(p-q)} \sum_{t=0}^{p-q} \binom{p-q}{t} e^{iu\theta(p-q-2t)} \tag{30}$$

$$(\sin u\theta)^{q} = \left(\frac{e^{iu\theta} - e^{-iu\theta}}{2i}\right)^{q} = (2i)^{-q} \sum_{r=0}^{q} \binom{q}{r} e^{iu\theta(q-2r)} (-1)^{r} \tag{31}$$

and similarly for $[\cos(u\theta + \alpha)]^{p-q}$ and $[\sin(u\theta + \alpha)]^{q}$. With the above substitutions, the difference between (28) and (29) may be expressed as

$$M_{\alpha} - M = \frac{\rho^{p}}{n} 2^{-p} i^{-q} \sum_{u=0}^{n-1} \sum_{t} \sum_{r} (-1)^{r} \binom{p-q}{t} \binom{q}{r} e^{iu\theta(p-2t-2r)} [e^{i\alpha(p-2t-2r)} - 1]. \tag{32}$$

If the terms of $\sum_{t}\sum_{r} (-1)^{r} \binom{p-q}{t} \binom{q}{r} e^{iu\theta(p-2t-2r)} [e^{i\alpha(p-2t-2r)} - 1]$ were written out in a rectangular array with, for example, the terms in r running laterally and the terms in t vertically, the summation could be performed diagonally and the result expressed as

$$\sum_{m=0}^{p} A_m e^{iu(p-2m)} [e^{i\alpha(p-2m)} - 1],$$

where

$$m = t + r$$

and

$$A_m = \sum_{j=0}^{m} (-1)^{m-j} \binom{p-q}{j} \binom{q}{m-j} \tag{33}$$

with the understanding that

$$\binom{a}{b} = 0 \text{ for } a < b.$$

Then (32) may be written as

$$M_\alpha - M = K \sum_{u=0}^{n-1} \sum_{m=0}^{p} A_m e^{iu\theta(p-2m)} [e^{i\alpha(p-2m)} - 1]. \tag{34}$$

Examining the separate terms in (34), it is seen that (34) vanishes for $p - 2m = 0$, since then

$$e^{i\alpha(p-2m)} - 1 = 0,$$

and (34) vanishes also for $p - 2m \neq In$, I an integer, since then

$$\sum_{u=0}^{n-1} e^{iu\theta(p-2m)} = 0$$

by the property of the summation of roots of unity.

Since m may take the values 0, 1, 2, ..., p,

$$-p \leq p - 2m \leq p,$$

so that for $p < n$, $p - 2m \neq In$ and (34) vanishes. But if $p \geq n$, there is at least one value of $p - 2m = In$ so that

$$\sum_{u=0}^{n-1} e^{iu\theta(p-2m)} = n$$

and for this value of m, say m_0, (34) becomes

$$M_\alpha - M = KnA_{m_0} [e^{i\alpha(p-2m_0)} - 1]. \tag{35}$$

Examination of (33) shows that there is a $q < p$ for which $A_{m_0} \neq 0$, and therefore (35) does not vanish for all q and all α. For example, if $p = 4$, $n = 2$ and $m_0 = 1$, A_1 equals $4 - 2q$ which vanishes only for $q = 2$. Similarly, with $p \geq n$, and more than one value of m for which $p - 2m$ is a multiple of n, it can be shown that there is a q and an α for which (34) is not zero.

It has been shown then that a necessary and sufficient condition for all moments of order p of n points equally spaced on a circle to be invariant under any rotation, α, is that n be greater than p. Therefore, to achieve invariance under rotation, the number of points equally spaced on a circle must be greater than 2d if the equation to be estimated is of degree d.

If the moments of a set of points are invariant under rotation the moments must be those of a spherical distribution and therefore equation (10) is satisfied. But for n = 2d + 1 or more points equally spaced on a circle, it may be verified that

$$\lambda_1 = \frac{n \sum_u x_{1u}^2 x_{2u}^2}{\left[\sum_u x_{iu}^2\right]^2} = \frac{n\rho^4 n/8}{(\rho^2 n/2)^2} = \frac{1}{2}$$

which does not satisfy equation (15). Therefore, these points constitute a rotatable arrangement but not a rotatable design. If n_1 is the number of points on the circle and n_2 points are added at the center, λ_1 becomes

$$\lambda_1 = \frac{(n_1 + n_2)\rho^4 n_1/8}{(\rho^2 n_1/2)^2} = \frac{1}{2}\left(1 + \frac{n_2}{n_1}\right) > \frac{1}{2}$$

which satisfies (15), but then

$$\lambda_2 = \frac{(n_1 + n_2)^2 \rho^6 n_1/16}{3(\rho^2 n_1/2)^3} = \frac{1}{6}\left(1 + \frac{n_2}{n_1}\right)^2 = \frac{2}{3}\lambda_1^2,$$

and equation (16) is not satisfied. Equally spaced points on a circle with additional points at the center, then, do not constitute a third order rotatable design.

Now consider an arrangement of N points on two circles with

n_1 points equally spaced on a circle of radius ρ_1

and n_2 points equally spaced on a circle of radius ρ_2,

where n_1 and $n_2 = N$, $\rho_1 \neq \rho_2$, $\rho_1 > 0$, $\rho_2 > 0$.

Let the u^{th} point on the first circle have coordinates

$$x_{11u} = \rho_1 \cos \frac{2\pi u}{n_1} = \rho_1 \cos u\theta$$

$$x_{21u} = \rho_1 \sin \frac{2\pi u}{n_1} = \rho_1 \sin u\theta$$

and the v^{th} point on the second circle have coordinates

$$x_{12v} = \rho_2 \cos\left(\frac{2\pi v}{n_2} + \beta\right) = \rho_2 \cos(v\phi + \beta)$$

$$x_{22v} = \rho_2 \sin\left(\frac{2\pi v}{n_2} + \beta\right) = \rho_2 \sin(v\phi + \beta)$$

where

$$u = 0, 1, 2, \ldots, n_1 - 1$$

$$v = 0, 1, 2, \ldots, n_2 - 1$$

$$0 \leq \beta \leq 2\pi.$$

By allowing β to be arbitrary it is not required that a point on the first circle and a point on the second circle be on the same vector through the origin.

Any p^{th} order moment may be given by

$$NM = \rho_1^p \sum_{u=0}^{n_1-1} (\cos u\theta)^{p-q}(\sin u\theta)^q + \rho_2^p \sum_{v=0}^{n_2-1} [\cos(v\phi+\beta)]^{p-q}[\sin(v\phi+\beta)]^q \quad (36)$$

and the moment after rotation through an angle, α, by

$$NM_\alpha = \rho_1^p \sum_u [\cos(u\theta+\alpha)]^{p-q}[\sin(u\theta+\alpha)]^q$$

$$+ \rho_2^p \sum_v [\cos(v\phi+\beta+\alpha)]^{p-q}[\sin(v\phi+\beta+\alpha)]^q \quad (37)$$

If the arrangement of points is to be invariant under rotation, the difference between (36) and (37) must be zero. By using substitutions similar to (30), (31) and (33), this difference may be written

$$N(M_\alpha - M) = K\sum_{m=0}^{p} A_m[e^{i\alpha(p-2m)}-1][\rho_1^p \sum_u e^{iu\theta(p-2m)} + \rho_2^p e^{i\beta(p-2m)} \sum_v e^{iv\phi(p-2m)}]. \quad (38)$$

By the same arguments as before (38) will vanish if either

$$p - 2m = 0$$

or $\quad p - 2m \neq In_1$ and In_2

and a sufficient condition for the vanishing of (38) is $p < n_1$ and $p < n_2$.

However, if

$$n_1 > p \geq n_2,$$

then

$$\sum_u e^{iu\theta(p-2m)} = 0$$

but

$$\sum_v e^{iv\phi(p-2m)} = n_2 \text{ for some } p_0 \leq p \text{ and for}$$

$$m = 0,\ p_0/2,\ p_0$$

in which case (38) becomes, apart from the constant,

$$A_0(e^{i\alpha p_0} - 1)e^{i\beta p_0} + A_{p_0}(e^{-i\alpha p_0} - 1)e^{i\beta p_0}. \tag{39}$$

There are a $p_0 > 0$, and a q such that (39) is a non-zero quantity except for certain α. A similar result obtains for

$$n_2 > p \geqslant n_1$$

and it remains therefore to investigate the case in which

$$n_1 = n_2 \leqslant p.$$

Let $$n_1 = n_2 = p_0 \leqslant p.$$

Then all terms in (38) will vanish except those terms for which $m = 0$ and $m = p_0$. (38) then becomes, apart from a constant factor,

$$A_0(e^{i\alpha p_0} - 1)(\rho_1^{p_0} + \rho_2^{p_0}\, e^{i\beta p_0}) + A_{p_0}(e^{-i\alpha p_0} - 1)(\rho_1^{p_0} + \rho_2^{p_0}\, e^{-i\beta p_0}). \tag{40}$$

There exists a q such that $A_0 = A_{p_0}$, and if (40) is to vanish in this case, independent of α,

$$\pm 1 = -\left(\frac{\rho_1}{\rho_2}\right)^{p_0},$$

which is not allowed. The case in which n_1 and n_2 are both less than or equal to p gives the same results as (39), for then there is a p_1, say, less than p for which

$$n_1 > p_1 \geqslant n_2$$

or $$n_2 > p_1 \geqslant n_1.$$

We may find a p_0, such that

$$0 < p_0 \leqslant p_1,$$

and a q for which (39) does not vanish except for certain α. Therefore all moments up to order p are not invariant to rotation.

The conclusion is, then, if points equally spaced on two circles of unequal radii are to have all moments to order p invariant under rotation, that the number of points on each, that is, both n_1 and n_2, must be greater than p. From this it may be concluded that a rotatable arrangement of order d is provided by points equally spaced on two circles if and only if the number of points on each circle is greater than 2d.

It is easily shown that this type of arrangement, in actuality, provides a third order rotatable design if n_1, $n_2 > 6$. For then

$$\lambda_1 = \frac{N(n_1\rho_1^4 + n_2\rho_2^4)/8}{[n_1\rho_1^2 + n_2\rho_2^2]^2/4} = \frac{1}{2}\,\frac{n_1^2\rho_1^4 + n_2^2\rho_2^4 + n_1n_2(\rho_1^4 + \rho_2^4)}{n_1^2\rho_1^4 + n_2^2\rho_2^4 + 2n_1n_2\rho_1^2\rho_2^2},$$

and since $\rho_1^4 + \rho_2^4 > 2\rho_1^2\rho_2^2$, for $\rho_1 \neq \rho_2$,

$$\lambda_1 > \frac{1}{2}.$$

Therefore, equation (15) is satisfied. Similarly

$$\lambda_2 = \frac{N^2}{3}\,\frac{(n_1\rho_1^6 + n_2\rho_2^6)/16}{[n_1\rho_1^2 + n_2\rho_2^2]^3/8} > \frac{2}{3}\lambda_1^2$$

since
$$\frac{\lambda_2}{\lambda_1^2} = \frac{2}{3}\,\frac{n_1^2\rho_1^8 + n_2^2\rho_2^8 + n_1n_2\rho_1^2\rho_2^2(\rho_1^4 + \rho_2^4)}{n_1^2\rho_1^8 + n_2^2\rho_2^8 + n_1n_2\rho_1^2\rho_2^2(2\rho_1^2\rho_2^2)}$$

which is greater than $\frac{2}{3}$ for $\rho_1 \neq \rho_2$ and so equation (16) is satisfied, also.

Thus, it has been shown that a simple class of third order rotatable designs in two factors exists. This class consists of designs which have seven or more points equally spaced on each of two concentric circles. Each of the circles may be rotated independently of the other and therefore there are an infinite number of configurations possible for designs with a given n_1 and n_2. Since points located at the center of the circles do not disturb the moment properties of the configuration, these may be added at will to achieve variations in the parameters λ_1 and λ_2.

The variance profiles of these designs are interesting to note. Consider first, the variance of a response predicted from a third order rotatable design in k factors. Define $\underline{x}'$ as the vector

$$\underline{x}' = (1, x_1^2, \ldots, x_k^2, x_1x_2, \ldots, x_{k-1}\, x_k, x_1, x_1^3, x_1x_2^2, \ldots x_1x_k^2, \\ \ldots x_k, x_k^3, x_kx_1^2, \ldots, x_kx_{k-1}^2, x_1x_2x_3, \ldots, x_{k-2}\, x_{k-1}\, x_k). \tag{41}$$

By least squares theory

$$V(\mathring{y}) = \underline{x}' \left[\underline{X}'\underline{X} \right]^{-1} \underline{x}\, \sigma^2 \tag{42}$$

where $\mathring{y}$, and $\left[\underline{X}'\underline{X} \right]^{-1}$ are defined as in Chapter III. If the $\left[\underline{X}'\underline{X} \right]^{-1}$ matrix of a third order rotatable design is substituted in (42), and the variables expressed in terms of their distance, ρ, from the center, there results

$$\frac{N}{\sigma^2} V(\dot{y}) = 2\lambda_1^2(k+2)A + \rho^2 \left[6(k+4)\lambda_2 B - 4\lambda_1 A \right]$$

$$+ \rho^4 \left\{ \left[(k+1)\lambda_1 - (k-1) \right] A - 12\lambda_1 B \right\} + \rho^6 \left[(k+1) - (k-1)\lambda_1^2\lambda_2^{-1} \right] B, \tag{43}$$

where A and B are as defined in Chapter IV. After substituting for k, A and B, the variance equation for this type of design in two dimensions is

$$\frac{N}{\sigma^2} V(\dot{y}) = \frac{2\lambda_1}{2\lambda_1 - 1} + \rho^2 \left[\frac{3\lambda_2}{3\lambda_2 - 2\lambda_1^2} - \frac{1}{2\lambda_1 - 1} \right]$$

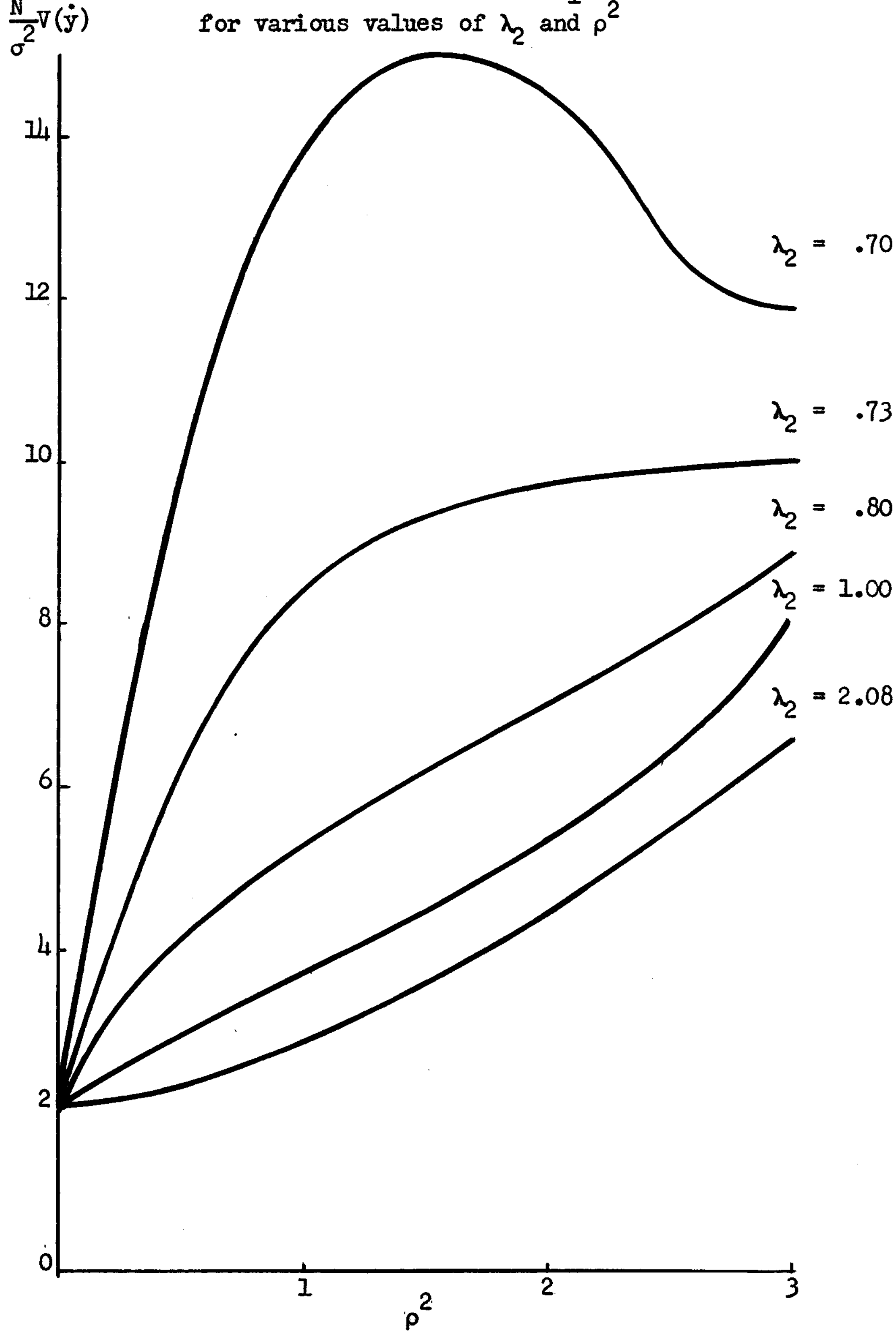
$$+ \rho^4 \left[\frac{3\lambda_1 - 1}{4\lambda_1(2\lambda_1 - 1)} - \frac{\lambda_1}{3\lambda_2 - 2\lambda_1^2} \right] + \rho^6 \left[\frac{3 - \lambda_1^2\lambda_2^{-1}}{12(3\lambda_2 - 2\lambda_1^2)} \right]. \tag{44}$$

Equation (44) was used to plot $\frac{N}{\sigma^2} V(\dot{y})$ against ρ^2 for $\lambda_1 = 1$ and several values of λ_2 in Figure 1. This figure shows quite clearly the effect on the variance profile of increasing λ_2. The same effect would be noticed on a graph in which λ_1 was increased for a constant λ_2.

For the two dimensional third order rotatable design in which $n_1 = n_2$, variance profiles were drawn and are shown in Figure 2. In this figure the horizontal scale is the squared ratio of the distance of a point from the center of the design to the radius of the outer circle. Each curve in Figure 2 represents the variance profile of a design with a specific ratio of radii of the two circles. If $\rho_1 > \rho_2$ and $\theta^2 = \frac{\rho_1^2}{\rho_2^2}$, it is seen that as θ^2 increases from $\frac{3}{2}$ to about 3 the

FIGURE 1

Variance Profiles, $k = 2$, $\lambda_1 = 1$ for various values of λ_2 and ρ^2



variance profile tends to be lower and flatter. However, as θ^2 increases beyond 3, the center of the profile rises. Although Figure 2 represents only those two dimensional designs in which the number of points on each circle is the same, and which contain no central points, it is apparent that every profile will drop at its extreme left if points are added at the center. For then $\rho = 0$ and (44) will decrease since each point added to the center increases λ_1. Adding points on the outer circle so that $n_2 < n_1$ will cause a drop in the profiles at the extreme right (where $\rho = 1$) since λ_1 will increase faster than λ_2, causing (44) to be smaller. Similarly, it may be shown that the central portion of the profiles will decrease if $n_1 < n_2$. The criterion of uniform information advanced by Box and Hunter (1954a) does not appear to be useful for third order designs because an excessive number of points would be required to achieve this property.

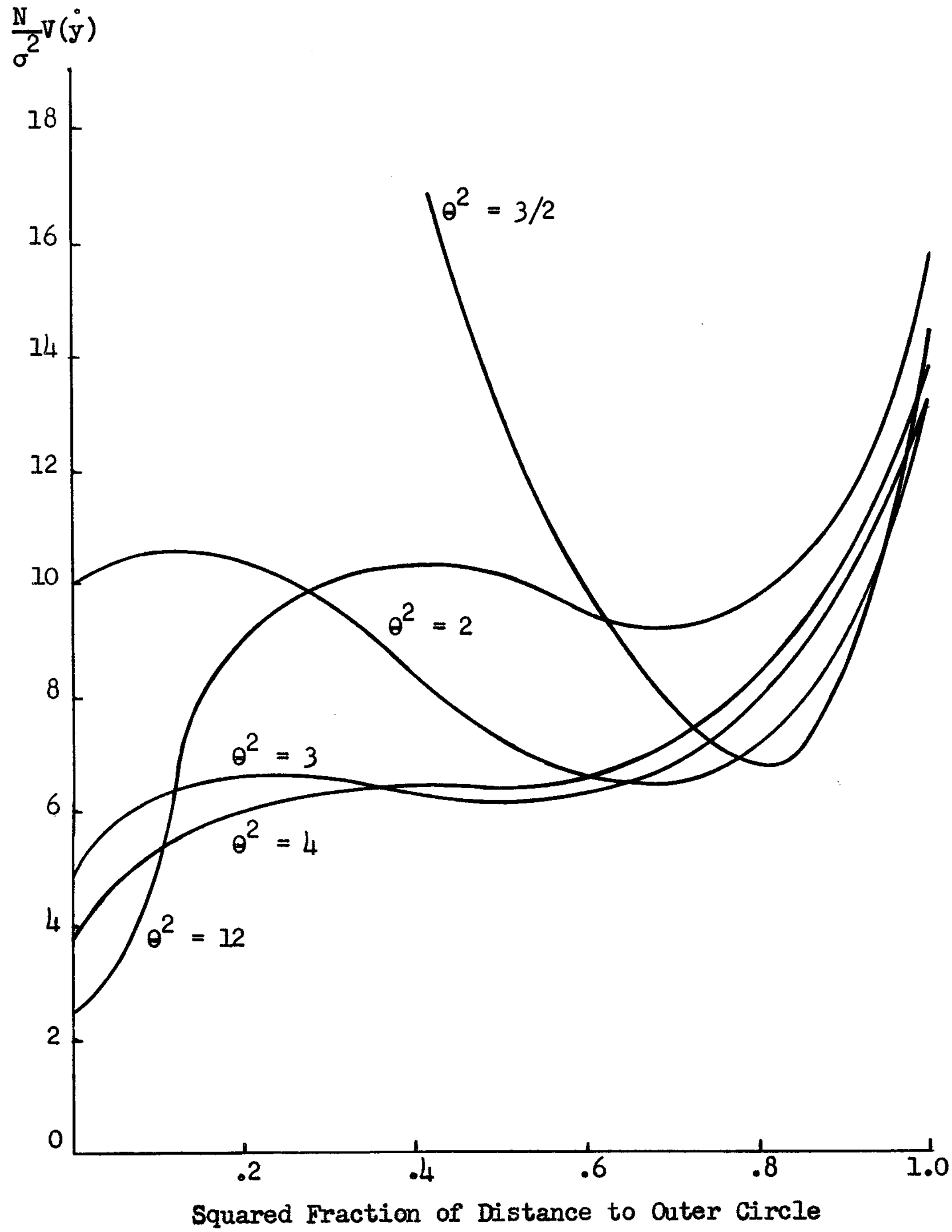
Since there are ten coefficients to estimate in a third order expansion in two factors and since the third order rotatable design with the minimum number of points requires 14 experiments without any replication, it would not seem warranted to suggest the addition of points to the center of the design or to either of the two circles in order to achieve a particular variance curve. Rather, it would appear reasonable to adjust the radii of the two circles in order to obtain a relatively low variance profile and one which was relatively flat in the interior of the region studied, in the absence of any additional information concerning the response surface explored. This would suggest that the ratio of the radii of the circles be given approximately by

FIGURE 2

Variance Profiles

$k = 2,\ n_1 = n_2$

for various values of θ^2



$$\frac{\rho_1^2}{\rho_2^2} = 3$$

But this is arbitrary and there is another line of thought which suggests a more useful method of deciding upon a particular design. This method is discussed in the following section.

Sequential Third Order Rotatable Designs in Two Factors

It can be assumed that an experimenter interested in exploring a response surface would prefer the simplest solution to his problem. That is, if a planar approximation would suffice, he would prefer a first order approximation to a second order approximation; if the planar equation is not satisfactory, he would prefer a second order approximation, if adequate, to a third order equation. It is possible for an experimenter to proceed in an investigation in such a manner that he may stop experimenting when he feels that his latest approximation is sufficient for his purposes. This type of experimentation could be called sequential experimentation and designs which accommodate this approach may be called sequential designs.

For example, an experimenter could apply a first order 2-dimensional rotatable design consisting of 3 points on an equilateral triangle with a point or points at the center to his problem. If he found that the planar fit were inadequate he could superpose a second equilateral triangle with central points on the first (so that the six points of the triangles described a hexagon) and add further points at the center. The combined configurations would constitute a second order rotatable design and a quadratic equation could be fit. It is not possible, however, to extend this example to a third order approximation without duplicating the arrangement (which would require too many points), since six points on a circle do not afford a third order rotatable arrangement.

If the experimenter had begun with 4 points on a square for his planar fit, superposed another square rotated 45° from the first and added points at the center to achieve a second order rotatable design, it would be possible then, at a later date, to augment this configuration with a circle of seven or more points to obtain a third order rotatable design.

Assume, now, that a second order rotatable design in two factors, is to be augmented by another set of points to obtain a third order rotatable design in two factors. The second order design can be considered as one "block" of points and the added points a second "block" of points. It is desirable to estimate block coefficients and to arrange the points so that estimates of the coefficients in the Taylor Series expansion are unconfounded with block effects.

Suppose the first block consists of seven or more points equally spaced on a circle with some points at the center. This allows the estimation of polynomial coefficients up to and including the second order. Now add a second block consisting of seven or more points equally spaced on a circle of different radius from the first. Let n_1 be the number of points in the first block and n_2 the number of points in the second block. Let δ_1 be the effect of the first block, δ_2 the effect of the second block, and let $Z_{wu} = 1$ if the u^{th} observation occurs in the w^{th} block, $w = 1, 2$, and $Z_{wu} = 0$ otherwise. Then, the expectation of the u^{th} observation can be written

$$\eta_u = \beta_0 + \sum_i \beta_i x_{iu} + \sum_i \sum_j \beta_{ij} x_{iu} x_{ju} + \sum_i \sum_j \sum_\ell \beta_{ij\ell} x_{iu} x_{ju} x_{\ell u}$$

$$+ \sum_w \delta_w (Z_{wu} - \bar{Z}_{wu}) \tag{45}$$

in which

$$\bar{Z}_w = \sum_u Z_{wu}/N$$

$$N = n_1 + n_2.$$

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

$$\sum_u (Z_{wu} - \bar{Z}_w) = 0 \tag{46}$$

$$\sum_u (Z_{wu} - \bar{Z}_w) x_{iu} = 0 \tag{47}$$

$$\sum_u (Z_{wu} - \bar{Z}_w) x_{iu} x_{ju} = 0 \tag{48}$$

$$\sum_u (Z_{wu} - \bar{Z}_w) x_{iu} x_{ju} x_{\ell u} = 0 \tag{49}$$

for $w = 1, 2$ and $i, j, \ell = 1, 2$. (46) is satisfied by the definition of $\bar{Z}_w$, while (47), (48) and (49) are satisfied with one exception, by the fact that $Z_{wu} - \bar{Z}_w$ is constant within blocks and each block contains a rotatable arrangement of points. The exception is in (48) when $i = j$. For this case, if n_{01} = the number of points at the center in the first block, (48) becomes

$$(1 - \frac{n_1}{N})(n_1 - n_{01}) \frac{\rho_1^2}{2} + (\frac{-n_1}{N}) n_2 \frac{\rho_2^2}{2} = 0$$

or

$$\frac{\rho_2^2}{\rho_1^2} = \frac{n_1 - n_{01}}{n_1} \; . \tag{50}$$

Therefore, by selecting ρ_2, the radius of the circle in the second block, in accordance with (50) the experiment may be performed sequentially and estimates of polynomial coefficients will be free of block effects. It is interesting to note that (50) is independent of the number of points in the second block, it being required only that $n_2 > 6$.

The design parameters for designs constructed in this manner are

$$\lambda_1 = \frac{1}{2} \frac{\frac{n_1^2}{n_1 - n_{01}} + n_2}{n_1 + n_2}$$

$$\lambda_2 = \frac{1}{6} \frac{\frac{n_1^3}{(n_1 - n_{01})^2} + n_2}{n_1 + n_2} \; . \tag{51}$$

Similarly, it is possible to construct a sequential third order rotatable design in four blocks, the first two of which constitute a complete second order rotatable design and the last two of which constitute the additional points necessary to convert the whole into a third order design. The first two blocks, or the second order portion, would contain an even number of points (greater than 6) on a circle of radius ρ_1 with an even number of points at the center. Each of the blocks would comprise a regular figure of half the number of points on the circle and half the number of central points.

The second two blocks must also contain an even number of points (greater than 6) equally spaced on a circle whose radius is determined by (50). Half of these points constituting a regular figure would make up the third block and the remaining points the fourth.

Again, let n_1 be the number of points in the second order portion of the design, n_{01} of which are at the center and n_2 the number of points on the added circle. The four blocks would contain points as follows:

Block	Total Points	Number of Points on Circle	Number of Central Points
I	$\frac{n_1}{2}$	$\frac{n_1 - n_{01}}{2}$	$\frac{n_{01}}{2}$
II	$\frac{n_1}{2}$	$\frac{n_1 - n_{01}}{2}$	$\frac{n_{01}}{2}$
III	$\frac{n_2}{2}$	$\frac{n_2}{2}$	0
IV	$\frac{n_2}{2}$	$\frac{n_2}{2}$	0

The relationship between the radii of the two circles is again given by (50) and the parameters by (51).

Since Block I is a complete first order rotatable design an experiment using this design could be performed sequentially in three stages. That is, an experimenter could apply Block I and analyze the results; if he felt that a planar equation was not sufficient he could then perform Block II and fit a second order equation; if this fit were inadequate he could then perform Blocks III and IV. In all stages the estimates of polynomial coefficients would be unconfounded with block effects.

As an example of a three stage sequential design consider the following 20 point design:

Block I - 4 points on a square of radius 1 with 2 points in the center

Block II - 4 points on a square of radius 1, rotated 45° from the square in Block I, with 2 points in the center

Block III - 4 points on a square of radius $\sqrt{2/3}$

Block IV - 4 points on a square of radius $\sqrt{2/3}$ rotated 45° from the square in Block III.

The parameters are $\lambda_1 = \frac{13}{20}$, and $\lambda_2 = \frac{7}{24}$. Block I is a complete first order rotatable design, Blocks I and II are a complete second order rotatable design and Blocks I, II, III, and IV constitute a third order rotatable design.

Sequential third order rotatable designs may also be constructed by an additional circle of $n_2 - n_{02} > 6$ points with n_{02} points at the center. Consider the second order rotatable design as one block and the n_2 additional points as a second block. Then, to avoid confounding polynomial coefficients with block coefficients the relationship between the radii of the circles must be

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

A third order rotatable design with these blocking properties is not possible, however, if $n_2 n_{01} = n_1 n_{02}$; that is, if the ratio of the total number of points in the first block to the total number of points in the second block is the same as the ratio of the number of center points in the first block to the number of center points in the second block.

Three sequential third order rotatable designs in which

$$\frac{\rho_2^2}{\rho_1^2} = \frac{2}{3}$$

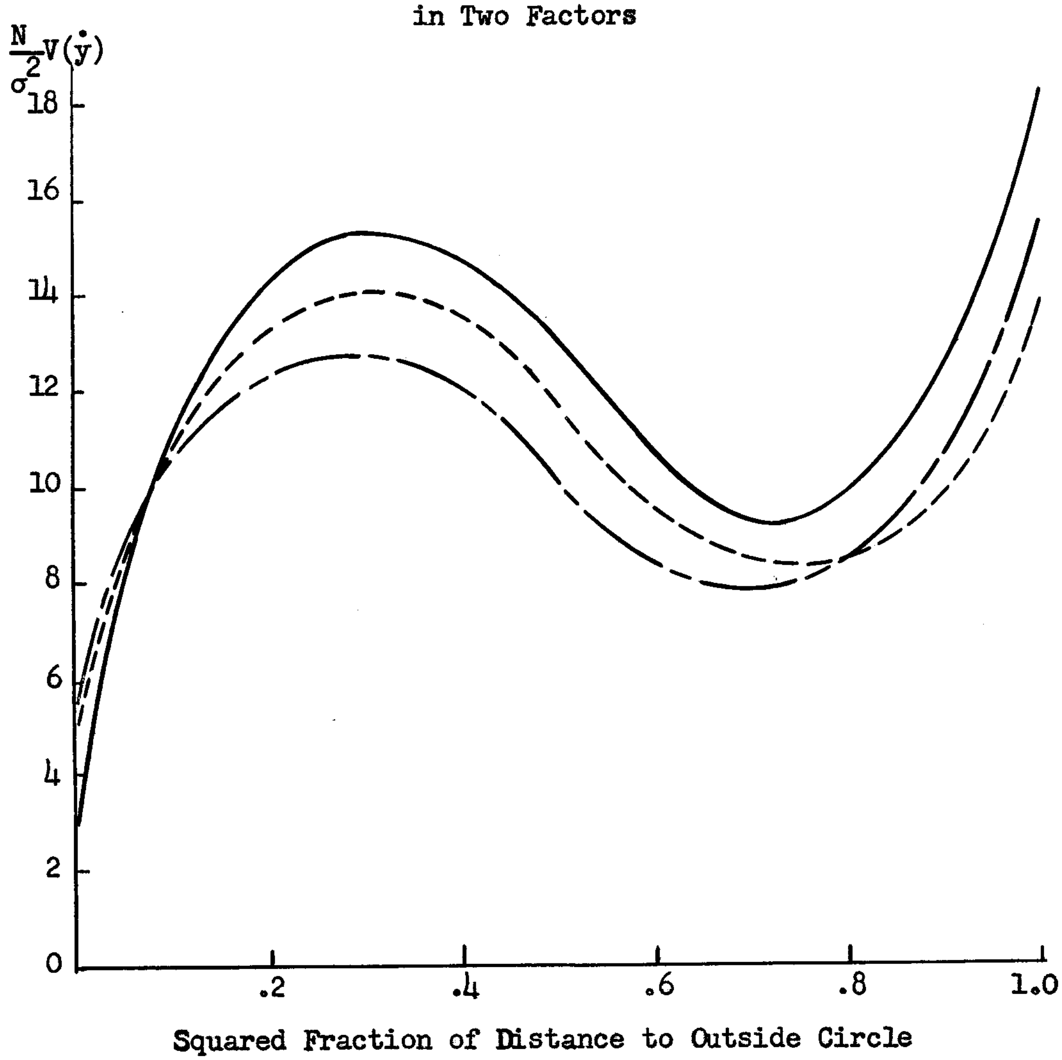
are compared by their variance profiles in Figure 3. As would be expected, the designs with 8 points on the outside circle have lower variance at the periphery of the design than does the design with only 7 points on the outer circle. Also, the design with the most central points has the lowest variance at the center of the design. Similarly the design with 12 points on the inside circle has lower variance in the intermediate area than do the designs with 8 and 7 points on the inner circle.

FIGURE 3

Variance Profiles for Three

Sequential Third Order Rotatable Designs

in Two Factors



First Stage	Second Stage
7 points on inner circle 1 central point	7 points on outer circle 5 central points
8 points on outer circle 4 central points	8 points on inner circle no central points*
8 points on outer circle 4 central points	12 points on inner circle no central points*

*May be run in four blocks

Chapter VII

THIRD ORDER ROTATABLE DESIGNS IN THREE FACTORS

Proceeding in the same manner as with the 2 dimensional designs, that is, by examining the regular figures, it is soon apparent that of the five regular figures in three dimensions, i.e., the

a) tetrahedron
b) octahedron
c) cube
d) dodecahedron
e) icosahedron,

none will by itself constitute a third order rotatable design. In fact only one composite design is possible and that is the design composed of a dodecahedron and an icosahedron.

Let ρ_1 be the radius of the icosahedron and ρ_2 the radius of the dodecahedron. Then a third order rotatable design of 32 points is possible if

$$\frac{\rho_2^6}{\rho_1^6} = \frac{2\tau + 1}{2\tau - 1} = \frac{\tau^3}{\sqrt{5}}$$

where τ is the parameter of the "Golden Section" and is given by

$$\tau = \frac{\sqrt{5} + 1}{2} = 1.61803399.$$

Thus if $\rho_1 = 1$, then $\rho_2 = 1.012910$. But, this design has $\lambda_1 = .60009$, which is almost pathological, hence points should be added at the center. If 8 points are so added the resulting 40 point design has

$$\lambda_1 = .7501$$

$$\lambda_2 = .4020.$$

The design matrix for this type of third order rotatable design is

$$
D = \begin{array}{c}
\begin{matrix} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{matrix} \\
\begin{bmatrix}
ca & da & 0 \\
ca & -da & 0 \\
-ca & da & 0 \\
-ca & -da & 0 \\
da & 0 & ca \\
da & 0 & -ca \\
-da & 0 & ca \\
-da & 0 & -ca \\
0 & ca & da \\
0 & ca & -da \\
0 & -ca & da \\
0 & -ca & -da \\
fa & -fa & -fa \\
-fa & fa & -fa \\
-fa & -fa & fa \\
fa & fa & fa \\
fa & fa & -fa \\
0 & ga & ha \\
-ha & 0 & -ga \\
ga & -ha & 0 \\
-fa & -fa & -fa \\
0 & -ga & ha \\
ha & 0 & -ga \\
-ga & ha & 0 \\
fa & -fa & fa \\
0 & -ga & -ha \\
-ha & 0 & ga \\
ga & ha & 0 \\
-fa & fa & fa \\
0 & ga & -ha \\
ha & 0 & ga \\
-ga & -ha & 0 \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0
\end{bmatrix}
\end{array}
$$

where $c = .850651$, $d = .525731$, $f = .584810$, $g = .361432$, $h = .946242$, and a is selected so that $\sum x_i^2 = N$.

Another 32 point design can be constructed by resorting to the use of a semi-regular figure. This is a composite design consisting of the points of a cube, two octahedra and a cuboctohedron as defined in Chapter V. Let the cube have radius $\rho_1 = \sqrt{3}$, one octahedron a radius $\rho_2 = 1.82969$, the cuboctahedron have radius $\rho_3 = 2^{1/3}$, and the other octahedron radius $\rho_4 = 1.16343$. Without central points the design has parameters

$$\lambda_1 = .638$$

$$\lambda_2 = .300.$$

The design matrix with center points is

$$\underline{D} = \begin{array}{c} \begin{array}{ccc} \underline{x_1} & \underline{x_2} & \underline{x_3} \end{array} \\ \left[\begin{array}{ccc}
a & a & a \\
a & a & -a \\
a & -a & a \\
a & -a & -a \\
-a & a & a \\
-a & a & -a \\
-a & -a & a \\
-a & -a & -a \\
1.82969a & 0 & 0 \\
-1.82969a & 0 & 0 \\
0 & 1.82969a & 0 \\
0 & -1.82969a & 0 \\
0 & 0 & 1.82969a \\
0 & 0 & -1.82969a \\
2^{1/3}a & 0 & 2^{1/3}a \\
0 & -2^{1/3}a & 2^{1/3}a \\
-2^{1/3}a & 0 & 2^{1/3}a \\
0 & 2^{1/3}a & 2^{1/3}a \\
2^{1/3}a & 0 & -2^{1/3}a \\
0 & -2^{1/3}a & -2^{1/3}a \\
-2^{1/3}a & 0 & -2^{1/3}a \\
0 & 2^{1/3}a & -2^{1/3}a \\
2^{1/3}a & 2^{1/3}a & 0 \\
2^{1/3}a & -2^{1/3}a & 0 \\
-2^{1/3}a & -2^{1/3}a & 0 \\
-2^{1/3}a & 2^{1/3}a & 0 \\
1.16343a & 0 & 0 \\
-1.16343a & 0 & 0 \\
0 & 1.16343a & 0 \\
0 & -1.16343a & 0 \\
0 & 0 & 1.16343a \\
0 & 0 & -1.16343a \\
0 & 0 & 0 \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
0 & 0 & 0
\end{array}\right] \end{array}$$

in which a is chosen so that $\sum x_i^2 = N$.

The addition of center points increases the parameters as follows:

No. of Center Points	λ_1	λ_2	$5\lambda_1^2/7$
1	.658	.319	.309
2	.678	.339	.328
3	.698	.359	.348
4	.718	.380	.368
5	.738	.402	.389
6	.758	.423	.410
7	.778	.446	.432
8	.798	.469	.455

This design has an advantage over the icosahedron-dodecahedron design in that it requires fewer central points to achieve a certain λ_1 and λ_2.

Neither of the 3rd order rotatable designs in three factors presented thus far have analogues in higher dimensions. There are no 4 dimensional analogues of the icosahedron or dodecahedron. The k-dimensional cuboctahedron does not have the proper moment properties for $k > 3$.

Of greater interest than a third order rotatable design *per se* is the third order rotatable design which can be performed sequentially, and particularly those sequential designs in three factors which may be extended to higher dimensions.

Consider the sequential design as being performed in two parts: the first part to be a second order rotatable design and the second part a set of points which, when added to the first part, makes a third order design. If the second order moment properties are to be preserved after the addition of the second set of points, it is obvious that both parts of the design must be complete second order designs in themselves.

For the first of these 3 dimensional sequential designs consider the design whose initial portion is the cube + octahedron configuration with points at the center. By adding to this, the points of a truncated cube and of another octahedron, a third order rotatable design results. This design would not be recommended in practice because the resultant matrix of normal equations is poorly conditioned. That is, although the inequalities (15) and (16) of Chapter IV are satisfied, (16) is very close to an equality. Consequently, the linear and cubic coefficients are very poorly estimated. The design is presented here for academic interest only.

The coordinates of a truncated cube in 3 dimensions can be written as all 24 permutations of the elements of the vector,

$$(\pm c,\ \pm d,\ \pm d)$$

where the radius of the figure is given by

$$\rho^2 = c^2 + 2d^2$$

and where c is a measure of the amount of truncation. For example, if $c = d$ the figure is not truncated at all and the 24 points make up a triply replicated cube. If $c = 0$, the truncation is extreme and the figure becomes a doubly replicated cuboctahedron. It can be shown that if

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

the 24 points constitute a second order rotatable design. Unfortunately, this value of c will not help to make a third order rotatable design.

For the first portion of the sequential design let the cube have radius ρ_1 and an octahedron have radius

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

Box and Hunter (1954a) show that this arrangement of 14 points comprises a second order rotatable design. To this add a truncated cube of radius ρ_3 and coordinates

$$(\pm c, \pm d, \pm d)$$

and another octahedron with coordinates $(\pm\rho_4, 0, 0)$. All moments having one or more odd exponents are then zero. The other fourth order moments must be in the relation

$$\frac{1}{N}\sum x_i^4 = \frac{3}{N}\sum x_i^2 x_j^2$$

or

$$\frac{24}{9}\rho_1^4 + 12c^4 - 8c^2\rho_3^2 + 4\rho_3^4 + 2\rho_4^4 = 3\left[\frac{8}{9}\rho_1^4 + 2(\rho_3^2 - c^2)(3c^2 + \rho_3^2)\right]$$

which establishes the condition

$$\rho_4^4 = \rho_3^4 + 10c^2\rho_3^2 - 15c^4. \tag{52}$$

Also, there must hold

$$\sum x_i^6 = 5\sum x_i^4 x_j^2, \quad i \neq j$$

$$\text{or } \frac{8 + 32\sqrt{2}}{27}\rho_1^6 + 6c^6 + 6c^4\rho_3^2 - 6c^2\rho_3^4 + 2\rho_3^6 + 2\rho_4^6 =$$

$$5\left[\frac{8}{27}\rho_1^6 + \rho_3^6 - c^2\rho_3^4 + 3c^4\rho_3^2 - 3c^6\right]$$

from which results

$$\frac{32(1-\sqrt{2})}{27}\rho_1^6 = 2\rho_4^6 + 21c^6 - 9c^4\rho_3^2 - c^2\rho_3^4 - 3\rho_3^6. \tag{53}$$

A third condition is that

$$\sum x_i^4 x_j^2 = 3\sum x_1^2 x_2^2 x_3^2$$

or

$$\frac{8}{27}\rho_1^6 + \rho_3^6 - c^2\rho_3^4 + 3c^4\rho_3^2 - 3c^6 = 3\left[\frac{8}{27}\rho_1^6 + 6c^6 - 12c^4\rho_3^2 + 6c^2\rho_3^4\right]$$

which gives

$$\frac{16}{27}\rho_1^6 = \rho_3^6 - 19c^2\rho_3^4 + 39c^4\rho_3^2 - 21c^6. \tag{54}$$

Equations (52), (53) and (54) may be solved jointly if either ρ_1, ρ_3 or ρ_4 is specified. For convenience let $\rho_1 = \sqrt{3}$. Then an admissible solution of the three equations is

$$\begin{aligned} \rho_3 &= 1.657765 \\ \rho_4 &= 1.705945 \\ c &= 0.184388 \\ d &= 1.164944. \end{aligned} \tag{55}$$

The design parameters are given below for various numbers of points added at the center

No. of Central Points	λ_1	λ_2	$5\lambda_1^2/7$
0	.6007	.2581	.2577
1	.6144	.2700	.2696
2	.6280	.2821	.2817
3	.6417	.2945	.2941
4	.6553	.3071	.3067
5	.6690	.3201	.3197
6	.6826	.3333	.3328
7	.6963	.3467	.3463
8	.7099	.3605	.3600
9	.7236	.3745	.3740
10	.7372	.3887	.3882

The relationship between λ_1 and λ_2 for each number of central points above is almost pathological.

However, the difficulty of the ill-conditioned matrix may be avoided by modifying the design slightly. This is accomplished by using a cube and doubled octahedron, as in (27), instead of a cube and octahedron in the first stage. Let ρ_1, ρ_2, ρ_3 and ρ_4 designate the radii of a cube, doubled octahedron, truncated cube and octahedron respectively. If the first portion, consisting of the cube and doubled octahedron is to be second order rotatable, then

$$\rho_2 = \rho_1 \sqrt{2/3} \ . \tag{56}$$

Keeping in mind that the doubled octahedron has 12 points, equations (52), (53) and (54) become

$$\rho_4^4 = \rho_3^4 + 10c^2\rho_3^2 - 15c^4 \tag{57}$$

$$2\rho_4^6 = -21c^6 + 9c^4\rho_3^2 + c^2\rho_3^4 + 3\rho_3^6 \tag{58}$$

$$\frac{16}{27}\rho_1^6 = \rho_3^6 - 19c^2\rho_3^4 + 39c^4\rho_3^2 - 21c^6 \tag{59}$$

If ρ_1 again equals $\sqrt{3}$, and hence $\rho_2 = \sqrt{2}$, then a solution of (57), (58) and (59) is

$$\rho_3 = 1.851208$$

$$\rho_4 = 1.985406$$

$$c = 0.341564$$

The coordinates of the resultant design are

$$\underline{D} = \begin{bmatrix}
a & a & a \\
a & a & -a \\
a & -a & a \\
a & -a & -a \\
-a & a & a \\
-a & a & -a \\
-a & -a & a \\
-a & -a & -a \\
\sqrt{2}a & 0 & 0 \\
\sqrt{2}a & 0 & 0 \\
-\sqrt{2}a & 0 & 0 \\
-\sqrt{2}a & 0 & 0 \\
0 & \sqrt{2}a & 0 \\
0 & \sqrt{2}a & 0 \\
0 & -\sqrt{2}a & 0 \\
0 & -\sqrt{2}a & 0 \\
0 & 0 & \sqrt{2}a \\
0 & 0 & \sqrt{2}a \\
0 & 0 & -\sqrt{2}a \\
0 & 0 & -\sqrt{2}a \\
ca & da & da \\
ca & da & -da \\
ca & -da & da \\
ca & -da & -da \\
-ca & da & da \\
-ca & da & -da \\
-ca & -da & da \\
-ca & -da & -da \\
da & ca & da \\
da & ca & -da \\
-da & ca & da \\
-da & ca & -da \\
da & -ca & da \\
da & -ca & -da \\
-da & -ca & da \\
-da & -ca & -da \\
da & da & ca \\
-da & da & ca \\
da & -da & ca \\
-da & -da & ca \\
da & da & -ca \\
-da & da & -ca \\
da & -da & -ca \\
-da & -da & -ca \\
fa & 0 & 0 \\
-fa & 0 & 0 \\
0 & fa & 0 \\
0 & -fa & 0 \\
0 & 0 & fa \\
0 & 0 & -fa \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0
\end{bmatrix} \tag{60}$$

in which c = .341564, d = 1.286527, f = ρ_4 = 1.985406 and again a is the factor guaranteeing that $\sum x_i^2 = N$. The values of the parameters for number of central points to 10 are:

Number of Central Points	λ_1	λ_2	$5\lambda_1^2/7$
0	.6271	.2902	.2809
1	.6396	.3019	.2922
2	.6522	.3139	.3038
3	.6647	.3261	.3156
4	.6773	.3385	.3277
5	.6898	.3511	.3399
6	.7023	.3640	.3523
7	.7149	.3771	.3651
8	.7274	.3905	.3779
9	.7400	.4041	.3911
10	.7525	.4179	.4045

The distribution of the points in any two of the dimensions of the factor space is shown in Figure 4. The points are dispersed quite well and there should be little difficulty in differentiating between points.

Block coefficients may be introduced into the model with this design also. Now $n_1 = 20$ and $n_2 = 30$ and so the equation which expresses the condition for orthogonal blocking is

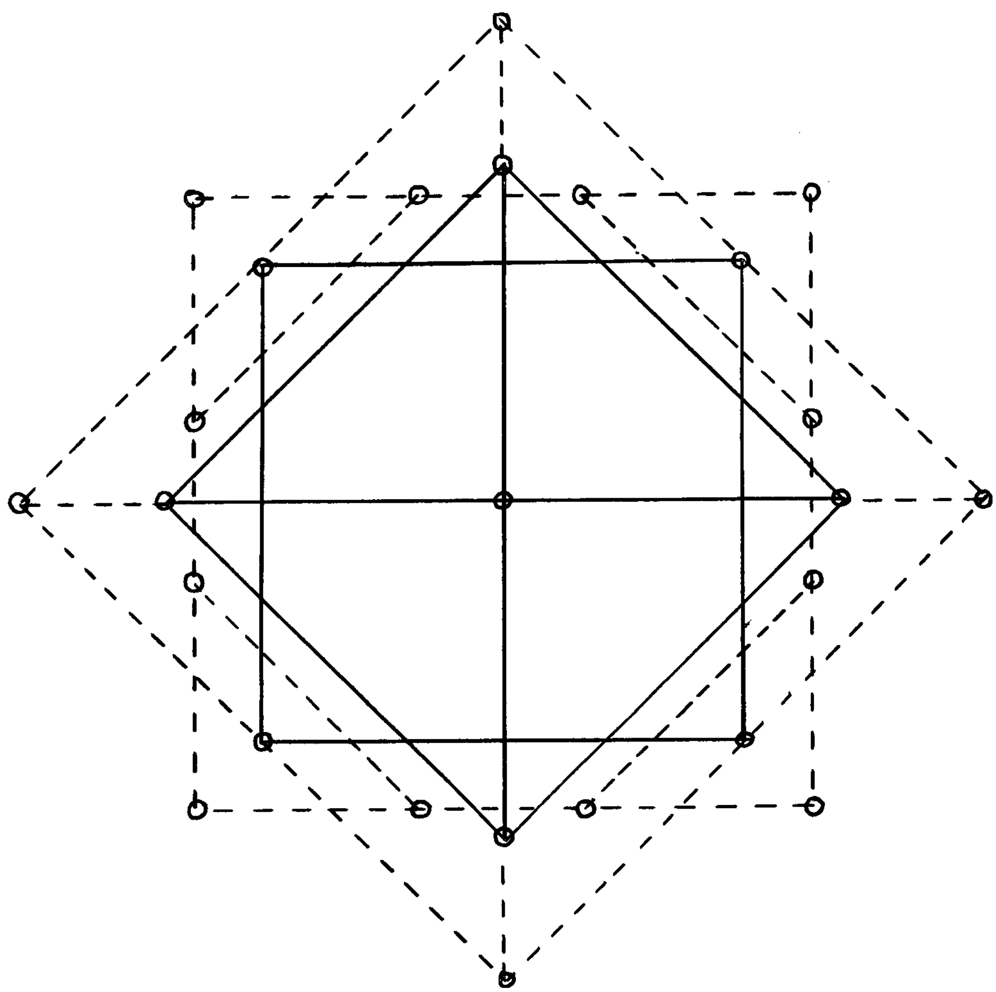
$(30 + n_{02})$(Sum of squares for first stage) = $(20 + n_{01})$(Sum of squares for second stage)

or
$$n_{02} = 2.206 n_{01} + 14.124 \tag{61}$$

Applying equation (61), the following table of design numbers for approximately orthogonal blocking results.

FIGURE 4

Three Dimensional Sequential
Third Order Rotatable Design
in 50 points
(plan view)



Solid lines denote figures of the first stage of the design, consisting of

1 cube
1 doubled octahedron

Broken lines denote figures of the second stage of the design, consisting of

1 truncated cube
1 octahedron

(Experimental points are denoted by circles)

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

Chapter VIII

THIRD ORDER ROTATABLE DESIGNS IN MORE THAN THREE FACTORS

Geometrical Figures in Higher Dimensions

As was pointed out in Chapter V, only the analogues of the tetrahedron, the octahedron and the cube exist, as regular figures in more than four dimensions. The latter two were used successfully by Box and Hunter (1954a) in their development of second order rotatable designs in the higher dimensional factor spaces. In Chapter V some semi-regular figures were described which provided second order rotatable designs for three dimensions. Of these semi-regular figures, the truncated cube was of particular interest in that it provided a basis for the construction of three dimensional sequential third order rotatable designs.

The higher dimensional analogue of the truncated cube is not easy to identify. The obvious extension from three dimensions to k dimensions would be the figure whose coordinates are the permutations of the elements of

$$(\pm c, \pm d, \pm d, \ldots, \pm d),$$

there being $k - 1$ elements $\pm d$. Call this "truncated cube (1)". A less obvious, but nevertheless reasonable extension to k dimensions is the figure whose coordinates are the permutations of

$$(\pm c, \pm c, \ldots, \pm c, \pm d, \pm d, \ldots, \pm d)$$

with, say, r elements $\pm c$ and $k - r$ elements $\pm d$, and with $1 < r < \frac{k+1}{2}$. Let this figure be called "truncated cube (r)".

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

Consider the configuration made up of the k-dimensional "truncated cube (1)" and a k-dimensional octahedron of radius ρ. For a sequential design of the type described in Chapter VII, this composite configuration would comprise the second stage of experimentation and therefore the coordinates must satisfy the requirement (among others)

$$\sum x_i^4 = 3 \sum x_i^2 x_j^2, \qquad i, j = 1, 2, \ldots, k. \tag{62}$$

For this configuration

$$\sum x_i^4 = 2^k [c^4 + (k-1)\, d^4] + 2\rho^4$$

$$\sum x_i^2 x_j^2 = 2^k d^2 [2c^2 + (k-2)\, d^2].$$

Substitution of the above into (62), requires

$$c^2 = 3d^2 \pm [(4 + 2k)\, d^4 - 2\rho^4]^{1/2}. \tag{63}$$

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

$$\sum x_i^4 x_j^2 = 3 \sum x_i^2 x_j^2 x_\ell^2, \; i, j, \ell = 1, 2, \ldots, k. \tag{64}$$

For the combined configurations (64) requires

$$c^2 = \frac{4d^4 \pm [(9 + 2k)d^8 + 2d^2]^{1/2}}{d^2}. \tag{65}$$

The minus sign in (65) will give a negative c^2 (with $k > 3$) and therefore must be disregarded. Equating (63) to (65) (with the plus sign) and simplifying gives

$$3d^6 + d^2 \left[\rho^4 + \sqrt{(9 + 2k)d^8 + 2d^2}\right] + 2 = 0, \qquad (66)$$

which is impossible since each term on the left of (66) must be a positive quantity. Therefore, "truncated cube (1)" cannot be used in a third order rotatable design of this form if k is greater than 3.

A Sequential Third Order Rotatable Design in Four Factors

With $k = 4$ a sequential third order rotatable design was discovered. The first stage of the design consists of a four dimensional cube of radius 2 and a 4-dimensional octahedron, also of radius 2. (Actually, this is a 4-dimensional regular figure of 24 points.) The second stage is comprised of a 4-dimensional "truncated cube (2)", with coordinates

$$(\pm c, \pm c, \pm d, \pm d)$$

and another 4-dimensional octahedron of radius ρ. To satisfy equation (10) of Chapter III, we must have

$$c = 1.200919$$

$$d = .256303$$

$$\rho = 1.736604.$$

This design contains 16 points on the cube, 8 points on the first octahedron, 96 points on the truncated cube and 8 points on the second octahedron for a total of 128 points without center points. The design parameters are

$$\lambda_1 = .676$$

$$\lambda_2 = .349.$$

The design matrix for the design with center points is

$$\underline{D} = \begin{array}{c} \begin{array}{cccc} \underline{x_1} & \underline{x_2} & \underline{x_3} & \underline{x_4} \end{array} \\ \begin{bmatrix} a & a & a & a \\ a & a & a & -a \\ \vdots & \vdots & \vdots & \vdots \\ -a & -a & -a & -a \\ 2a & 0 & 0 & 0 \\ -2a & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & -2a \\ 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 \\ & & & \\ ca & ca & da & da \\ ca & ca & da & -da \\ \vdots & \vdots & \vdots & \vdots \\ -ca & -ca & -da & -da \\ \rho a & 0 & 0 & 0 \\ -\rho a & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & -\rho a \\ 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{l} \text{(first stage)} \\ \\ \\ \\ \text{(second stage)} \end{array}$$

where a, again is the constant assuring that $\sum x_i^2 = N$.

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

n_{01}	n_{02}	n_1	n_2	N	λ_1	λ_2
8	0	32	104	136	.719	.394
9	4	33	108	141	.745	.423
10	7	34	111	145	.766	.447
11	10	35	114	149	.787	.472

The radii of the two octahedra are sufficiently different so that investigation of the design with a doubled octahedron (and 8 additional points) appears unwarranted.

Designs in More than Four Dimensions

No attempt has been made to extend the concept of third order rotatable designs to more than four dimensions, chiefly because the approach pursued in this thesis required the use of an excessive number of experimental points. Investigations were made, following this approach, only of the sequential type of rotatable design because this is the type which seems likely to be most useful to an experimenter. But even in the non-sequential type of experiment the indications are that third order rotatable designs in the higher dimensions require too many points.

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

If a full replicate, 5-dimensional design of this type were possible, 372 points would be required. The same design in six factors would require 1,048. For practical reasons the criterion of rotatability for the investigation of third order response surfaces in more than four dimensions will apparently have to be sacrificed.

Chapter IX

SUMMARY

This work has concerned itself with extending the criterion of rotatability, as advanced by Box and Hunter (1954a), to experimental designs for estimating response surfaces by third order polynomial equations. The method of attack has been to examine combinations of regular and semi-regular geometrical figures and find those combinations whose coordinate points satisfy the moment properties, to order six, of spherical distributions. Designs with these properties and the attendant restrictions were shown by Box and Hunter to have spherical variance contours when the polynomial coefficients were estimated by the method of least squares.

It was found that third order rotatable designs in two factors could be attained by locating seven or more experimental points equally spaced on each of two concentric circles of different non-zero radii. Also it was shown that certain rotatable designs in two factors can be performed in two stages, the first of which will enable the experimenter to fit a second order polynomial equation and the second of which will enable him to estimate a third order polynomial equation if this is necessary. By choosing the radii of the two circles in the proper ratio it is possible to obtain estimates of the polynomial coefficients which are independent of "block" effects due to running the experiments in two stages. Such designs were termed sequential third order rotatable designs.

In three factors, third order rotatable designs were presented which consisted of composites of cubes, truncated cubes, octahedra, cuboctahedra, icosahedra and dodecahedra. Three of these designs in three factors were constructed so that they might be performed sequentially. The design matrix of each was presented in a standard form.

One sequential third order rotatable design in four factors was also presented. This design has as its experimental points the vertices of the 4-dimensional analogues of a cube, a truncated cube and two octahedra of specific dimensions.

It was discovered that the approach used in this thesis for constructing rotatable designs for estimating third order coefficients resulted in the requirement of an excessive number of experimental points in four or more factors. Indeed it is realized that even in the lower dimensions designs with fewer points are desirable. Consequently, further research directed toward minimizing the number of experimental points in rotatable designs is suggested. In this regard, the extension of the work of De la Garza (1954) to two and more dimensions would seem to warrant some attention. Also, research on the problem of augmenting a second order rotatable design to explore more thoroughly a specific area of the factor space can be recommended. Once an experimenter has applied a second or third order rotatable design to a problem, the criterion of rotatability is of lesser importance. For then the general orientation of the response surface will presumably be determined and the experimenter will wish to concentrate further attention in a particular direction. Non-central composite designs have been proposed for this purpose, but a more thorough examination, especially of sequential designs with orthogonal blocking properties, is in order.

Because of the increased complexity of the polynomial equation future research on fourth order rotatable designs is not recommended, even should a method requiring a minimum number of points be discovered. The experimenter is looking for a simple approximation to the phenomenon he studies and rarely would he be willing to use a polynomial of the fourth order for this purpose. Fourth order rotatable designs would appear to be of limited practical value.

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APPENDIX

EXAMPLE OF SEQUENTIAL THIRD ORDER ROTATABLE DESIGN APPLIED TO A HYPOTHETICAL EXPERIMENT

Suppose an experimenter is desirous of exploring the response surface of a chemical reaction with a view toward locating an economical point of operation at which a given viscosity of liquid can be attained. That is, the experimenter is manufacturing a liquid; he wants the liquid to have a specific viscosity and he wishes to know what combinations of the levels of his variables will produce a liquid of this viscosity so that he might choose the optimum point of operation from those combinations. Suppose further that there are three variables of interest

Variable	Range of Variable	Symbol
Temperature of Reaction	70 - 95°C	z_1
Monomer Concentration	40 - 70%	z_2
Time of Reaction	15 - 240 minutes	z_3

which can be varied throughout the ranges noted and there is reason to believe that the relationship between viscosity and these variables is not linear.

The statistician can reason that the experimenter is looking for a contour of constant viscosity, say y_0, which is a non-linear function of the variables, z_1, z_2 and z_3. This function, in the absence of information to the contrary, may be approximated by a Taylor Series expansion to terms of the second or perhaps the third order. With little or nothing known about the orientation of the response surface a rotatable design can be recommended since the variance of predicted viscosities will be independent of the orientation if the predictions are determined from a rotatable design. In particular a sequential third order rotatable design will have merit in that it will allow the experimenter to discontinue experimenting if a second order approximation proves adequate or allow him to use a complete third order design if a second order approximation is not sufficient.

Let us suppose that the experimenter has no limitations on the number of experimental points he may run. Also let us suppose that he desires to mix a batch of his raw materials exclusive of the monomer and for each experimental point add an amount of monomer to a portion of this batch to achieve a specific monomer concentration. Suppose that there will be no difference in the monomer used over time, but that each batch of the other materials can be expected to vary. If the experiment is to be carried out in two stages, the experimenter would like to prepare a batch of the basic materials for each stage. Under these conditions the design of equation (60), Chapter VII, can be recommended using 14 central points in the second stage, as per equation (61), to achieve approximately orthogonal blocking.

For convenience in theoretical study the independent variables x_i are always measured from the origin of the design and are further coded so that $\sum' x_i^2 = N$. Thus the relation between the actual operating variables z_i and the "design" variables, x_i, is of the form

$$x_i = \frac{z_i - z_{i0}}{k},$$

where z_{i0} is the middle of the range of z_i to be included in the experiment and k is a constant which can easily be found by substituting the extreme value of z_i and the corresponding extreme value of x_i from the design matrix. Thus, for example, if the range of z_1 is to be from 70° to 95° C, and we use the design of equation (60) the relation is

$$x_1 = \frac{z_1 - 82.5}{k}$$

where k is found from

$$1.98554a = \frac{95 - 82.5}{k},$$

whence

$$k = \frac{12.5}{1.98554a}$$

and

$$x_1 = \left(\frac{1.98554a}{12.5}\right)(z_1 - 82.5).$$

A table showing the complete relation between the design variables, x_i, and the experimental variables, z_i, for the design of equation (60) is given below:

x_1, x_2, x_3	$z_1(^\circ$ C)	z_2(%)	z_3(min.)
-1.98554a	70.0	40.0	15.0
-1.8512a	70.845	41.014	22.604
- 2a	73.596	44.316	47.366
-1.2865a	74.400	45.280	54.602
- a	76.204	47.355	70.836
- .34156a	80.350	52.419	108.146
0	82.5	55.0	127.5
.34156a	84.650	57.581	146.854
a	88.796	62.555	184.164
1.2865a	90.600	64.720	200.398
2a	91.404	65.684	207.634
1.8512a	94.155	68.986	232.396
1.98554a	95.0	70.0	240.0

First Stage

The first stage of the experiment will consist of those runs which will enable the experimenter to estimate all the coefficients in a Taylor Series expansion to the second order. The experimental points will have as combinations of levels of the three variables the first 20 lines of equation (60) with the levels of z substituted for x. For example, line 3 would read

$$88.8^{\circ} \qquad 47.4\% \qquad 184.2 \text{ minutes},$$

lines 9 and 10 would read

$$91.4^{\circ} \qquad 55.0\% \qquad 127.5 \text{ minutes},$$

and lines 19 and 20

$$82.5^{\circ} \qquad 55.0\% \qquad 47.4 \text{ minutes}.$$

The experimenter may now perform these 20 runs in a random order and record the viscosity of the liquid, y, measured after each run.

After identifying the line in equation (60) with the appropriate run of the experiment, the following quantities may be calculated

$$\begin{array}{ll} \sum y & \sum x_2^2 y \\ \sum x_1 y & \sum x_3^2 y \\ \sum x_2 y & \sum x_1 x_2 y \\ \sum x_3 y & \sum x_1 x_3 y \\ \sum x_1^2 y & \sum x_2 x_3 y \end{array}$$

using for "a" the value

$$a = (20/16)^{1/2} = 1.118034$$

in which 20 is the number of runs and 16 the sum of squares of x_i if a were equal to 1. Then the values λ_1 and A may be calculated as follows:

$$\lambda_1 = \frac{\sum x_i^4}{(20)(3)} = .6250$$

$$A = [2\lambda_1(5\lambda_1 - 3)]^{-1} = 6.4000.$$

Referring to equations (17) and (19) of Chapter IV, the estimates of the coefficients of the second order expansion may be computed.

$$\begin{bmatrix} b_0 \\ b_{11} \\ b_{22} \\ b_{33} \end{bmatrix} = \frac{1}{20} \begin{bmatrix} 25.0 & -8 & -8 & -8 \\ & 3.2 & 2.4 & 2.4 \\ & & 3.2 & 2.4 \\ & & & 3.2 \end{bmatrix} \begin{bmatrix} \sum y \\ \sum x_1^2 y \\ \sum x_2^2 y \\ \sum x_3^2 y \end{bmatrix}$$

(from equation 17)

$$\begin{bmatrix} b_{12} \\ b_{13} \\ b_{23} \end{bmatrix} = \frac{1}{20} \begin{bmatrix} 1.6 & 0 & 0 \\ & 1.6 & 0 \\ & & 1.6 \end{bmatrix} \begin{bmatrix} \sum x_1 x_2 y \\ \sum x_1 x_3 y \\ \sum x_2 x_3 y \end{bmatrix}$$

(from equation 19)

The linear coefficients are not given _per se_ by any equations in Chapter IV since the matrices in Chapter IV were prepared for a third order model in which linear and third order coefficients are dependent. However, they are simply calculated as

$$b_1 = \sum x_1 y/20$$
$$b_2 = \sum x_2 y/20$$
$$b_3 = \sum x_3 y/20.$$

An analysis of variance may now be performed and the fit of the second order equation tested in the standard manner. Let us assume that the fit is not adequate and proceed to augment the experiment by additional runs in order to fit a third order equation.

Second Stage

In the second stage of the experiment 44 additional runs will be made. The combinations of the levels of the z_i may be obtained by transforming lines 21 through 50 of equation (60) according to the table of transformation given earlier and adding 14 runs with levels $z_1 = 82.5^\circ$ C, $z_2 = 55.0\%$ and $z_3 = 127.5$ minutes.

These 44 runs may now be performed in a random order and at their completion the following calculations made:

$$\begin{array}{llll}
\sum y & \sum x_2^2 y & \sum x_1^3 y & \sum x_1 x_2^2 y \\
\sum x_1 y & \sum x_3^2 y & \sum x_2^3 y & \sum x_2^2 x_3 y \\
\sum x_2 y & \sum x_1 x_2 y & \sum x_3^3 y & \sum x_1 x_3^2 y \\
\sum x_3 y & \sum x_2 x_3 y & \sum x_1^2 x_2 y & \sum x_2 x_3^2 y \\
\sum x_1^2 y & \sum x_1 x_3 y & \sum x_1^2 x_3 y & \sum x_1 x_2 x_3 y
\end{array}$$

where the summations extend over all 64 runs and where a new "a" is used;

$$a = (64/51.299452)^{1/2} = 1.116950.$$

64 is the total number of runs made and 51.299452 is the sum of squares of the 64 x's if a were equal to 1. The parameters for this design with 14 central points are

$$\lambda_1 = .80269$$

$$\lambda_2 = .47545.$$

The constants A and B are calculated as

$$A = [2\lambda_1(5\lambda_1 - 3)]^{-1} = .61465$$

$$B = [6(7\lambda_2 - 5\lambda_1^2)]^{-1} = 1.56270.$$

These constants may then be substituted into equations (17), (18), (19) and (20) and the coefficients of the third order equation obtained as follows:

$$\begin{bmatrix} b_0 \\ b_{11} \\ b_{22} \\ b_{33} \end{bmatrix} = \frac{1}{64} \begin{bmatrix} 3.960 & -.9867 & -.9867 & -.9867 \\ & .7442 & .1213 & .1213 \\ & & .7442 & .1213 \\ & & & .7442 \end{bmatrix} \begin{bmatrix} \sum y \\ \sum x_1^2 y \\ \sum x_2^2 y \\ \sum x_3^2 y \end{bmatrix}$$

$$\begin{bmatrix} b_1, & b_2, & b_3 \\ b_{111}, & b_{222}, & b_{333} \\ b_{122}, & b_{112}, & b_{113} \\ b_{133}, & b_{233}, & b_{223} \end{bmatrix} = \frac{1}{64} \begin{bmatrix} 31.205 & -7.526 & -7.526 & -7.526 \\ & 2.015 & 1.665 & 1.665 \\ & & 2.716 & 1.665 \\ & & & 2.716 \end{bmatrix}$$

$$\times \begin{bmatrix} \sum x_1 y, & \sum x_2 y, & \sum x_3 y \\ \sum x_1^3 y, & \sum x_2^3 y, & \sum x_3^3 y \\ \sum x_1 x_2^2 y, & \sum x_1^2 x_2 y, & \sum x_1^2 x_3 y \\ \sum x_1 x_3^2 y, & \sum x_2 x_3^2 y, & \sum x_2^2 x_3 y \end{bmatrix}$$

$$\begin{bmatrix} b_{12} \\ b_{13} \\ b_{23} \end{bmatrix} = \frac{1}{64} \begin{bmatrix} 1.246 & 0 & 0 \\ & 1.246 & 0 \\ & & 1.246 \end{bmatrix} \begin{bmatrix} \sum x_1 x_2 y \\ \sum x_1 x_3 y \\ \sum x_2 x_3 y \end{bmatrix}$$

$$b_{123} = \sum x_1 x_2 x_3 y/(64)(.47545).$$

With the estimates of the coefficients of the third order model now determined the experimenter may use the equation

$$y_0 = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_{11}x_1^2 + b_{22}x_2^2 + b_{33}x_3^2 + b_{12}x_1x_2$$
$$+ b_{13}x_1x_3 + b_{23}x_2x_3 + b_{111}x_1^3 + b_{222}x_2^3 + b_{333}x_3^3 + b_{122}x_1x_2^2$$
$$+ b_{133}x_1x_3^2 + b_{112}x_1^2x_2 + b_{233}x_2x_3^2 + b_{113}x_1^2x_3 + b_{223}x_2^2x_3$$
$$+ b_{123}x_1x_2x_3$$

together with whatever restrictions he may have on his operating variables to select optimum values of x_1, x_2, and x_3 for his purposes. Then after transforming the x_i to z_i a solution to his problem will have been obtained.