V 95

ON INVESTIGATION OF RESPONSE SURFACES

By

P.J. THAKER.

Dissertation submitted in partial fulfilment of the requirements for the award of Diploma in Agricultural and Animal Husbandry Statistics of the Institute of Agricultural Research Statistics (I.C.A.R.), New Delhi.

- 1960 -

...

ACKNOWLEDGEMENT

I have great pleasure in expressing my deep sense of gratitude to Shri M.N. Das, Professor of Statistics, Institute of Agricultural Research Statistics, for his valuable guidance, keen interest and valuable criticisms throughout the course of the investigation and writing this thesis.

(P.J. THAKER)

INTRODUCTION

During the last three decades, the statistical theory of designs and analysis of experiments has developed with remarkable rapidity, largely due to close cooperation between theoreticians on the one hand and the experimenters on the other. In recent years numerous important and comprehensive works on agricultural and industrial experiments have appeared, explaining the basic principles of the theory and discussing the available statistical techniques. The practical applications of the theory in engineering and other physical sciences have also become increasingly popular.

In statistical design of experiments in the fields of agriculture and industry, numerous problems have involved exploration of functional relationship. In last decade, a fundamentally new approach to the problems for exploration of functional relationship was initiated by Box (1951, 1952, 1954, 1955, & 1957). He and his coworkers studied the relationship such as exists between a quantitative response such as yield of product, cost or purity on one hand and sets of controlled variables such as temperature, pressure, amount of nitrogen, acidity, etc. on the other. Suppose we have k quantitative factors or variables $x_1, x_2, \ldots, x_k$ on which depend some response η in accordance with the unknown relationship,

$$\eta = \phi(x_1, x_2, \ldots, x_k) \quad \ldots\ldots\ldots \quad (1)$$

In order to explore this relationship, let N experiments be performed. The uth of these experiments consists in adjusting the factor levels to a certain set of predetermined values $x_{1u}, x_{2u}, \ldots, x_{ku}$ and of observing the corresponding response, y_u. The observed response y_u, varies about a mean of η_u, with a common variance of σ^2 for all values of u, these errors being uncorrelated. The problem of experimental design discussed is that of choosing the N sets of levels at which observations are to be made. It is often convenient to view the problem geometrically and to regard equation (1) as defining a surface referred to as the "response surface". The N sets of factor levels at each of which response is observed will then correspond to N points in the space of variables called experimental points.

When the mathematical form of ϕ is not known, this function can be approximated by a polynomial of degree d, within the experimental region so that the true response at the uth point is

$$\eta_u = \beta_0 + \beta_1 x_{1u} + \cdots + \beta_k x_{ku} + \beta_{11} x_{1u}^2 + \cdots + \beta_{kk} x_{ku}^2 + \beta_{12} x_{1u} x_{2u} + \cdots + \beta_{k-1,k} x_{k-1,u} x_{ku} + \beta_{111} x_{1u}^3 + \cdots + \text{etc.} \quad \ldots\ldots (2)$$

The independent variables when d = 1 (i.e. first order model) are functionally independent, while the independent variables for $d \geq 2$, include terms like $x_i^2, x_i x_j$, etc. which are obviously not functionally independent of $x_1, x_2, \ldots, x_k$ but they are still referred to as "independent" variables to contrast them with the dependent variable (or in our terminology the "response").

A design which includes k variables and allows all constants involved in a polynomial of order d to be determined will be called a k-dimensional experimental design of order d. In a approximated polynomial of order d there are $\binom{k+d}{d}$ terms, so that for a k-dimensional design of order d, the number of experimental points must be atleast $\binom{k+d}{d}$.

The factorial experiments are extensively used for agricultural experimentation. Naturally, one very useful method of analysis of results of factorial experiments, when quantitative factors are studied, is to explore the pattern of functional relationship (1). An attempt has been made in this thesis to evolve systematic and simplified method for exploring response surfaces with the help of the data collected from the usual 3^k factorial experiments.

From the results of any factorial experiment we can obtain "information" at any point of the factor space, information being defined as reciprocal of the variance of the response at that point estimated from the response relation. Box and Hunter (1957) introduced a class of designs called "rotatable" designs in which such information contours are circles, spheres and hyperspheres centred at the point defined by the means of the different levels of the factors introduced in the design. A design is said to be a dth order rotatable design if it permits estimation of all the terms of equation (2) and provides spherical information contours.

This dissertation concerns with the following problems:

(1) to use the data collected from different usual 3^k factorial experiments for fitting the

second degree (i.e. quadratic) response surface by expressing terms involved in second degree surface as functions of the different main effects and two factor interaction components.

(2) construction of a series of second order rotatable designs for four, five, six, seven and other even number of factors.

(3) construction of third order rotatable designs for k = 2, 3, 4, ..., 11 factors, taking into account the requirements of "blocking".

REVIEW OF LITERATURE

Excellent literature is available on response surface techniques. Probably the one man most responsible for promoting the construction of designs useful in fitting response surfaces is G.E.P. Box. His first article with Wilson (1951), threw new light on the nature of the factorial experimentation and constitute a landmark in the history of experimental design. Their problem may be stated briefly as follows: Suppose the true response surface, expressed as function of k controllable variables $x_1, x_2, \ldots\ldots, x_k$ is $\eta = \phi\ (x_1, x_2, \ldots\ldots, x_k)$. It is required to find, with a minimum number of experiments, a maximum or minimum of the response surface (i.e. an optimum operating set of conditions) within the region of interest in the k-dimensional factor space, which is fixed by the experimental conditions.

Box (1952), thereafter, discussed the construction and properties of multifactor first order designs. The method of steepest ascent proposed by Box and Wilson has been developed and expounded by Box and others (1954, 1955). Box and Hunter (1957) introduced the concept of "rotatibility" and derived the necessary and sufficient conditions for a design to be rotatable of order d. They also derived the "blocking" arrangements and constructed many practically useful rotatable designs upto second order.

Uptil now, the construction of rotatable designs mainly rested on the geometrical configurations of regular and semi-regular solid figures. Bose and Draper (1959) and Draper (1960) presented new line of approach for construction of infinite classes of second order rotatable designs. To provide higher order rotatable designs, Gardiner et al (1959) investigated third order rotatable designs upto four factors. More recently Das (1960) has suggested a further method using a modified form of factorial design for the construction of rotatable designs.

In recent years, attention has been focussed on examining the optimality of any specific relationship based on the results of study of any other polynomial relationship of lower order. Dealing with this, Box and Draper (1959) and Folks (1959) developed optimal criteria for judging goodness of a design and investigated optimal designs upto second degree polynomial relationships.

EXPLORATION OF RESPONSE SURFACES WITH THE HELP OF DATA COLLECTED FROM USUAL FACTORIAL EXPERIMENTS

Yates (1937) defines factorial experiments as "experiments which include all combinations of several different treatments or factors". The advantages of a factorial experiment, as compared with a series of separate experiments on separate factors, are economy and the possibility of investigating interactions between the different factors, i.e. of examining the extent to which the effect of one factor is different for different levels of another factor. The usefulness of factorial experiments in agricultural and industrial experiments is well known.

Factors that may arise for consideration can be classified in various ways. First there is a distinction between factors representing treatments applied to the experimental units, and factors which represent simply a classification, outside the experimenter's control, of the experimental units into different types. Secondly there is a distinction between

(a) factors such as volume, temperature, pressure and amount of nitrogen for which different levels correspond to well defined values of a quantitative variable. These factors are called quantitative variables.

(b) factors such as varieties of wheat and different forms of fertilizer for which the different levels represent qualitatively different treatments of intrinsic interest. These factors are called qualitative variables.

The interpretation of the results of factorial experiments raises various problems. When quantitative variables are studied, one very useful method of analysis of the results of a factorial experiment is to explore the pattern of response surface between yield or response and the levels of these quantitative variables.

Let each quantitative variable have three equispaced levels denoted by q_1, q_2 and q_3 such that $q_2 - q_1 = q_3 - q_2 = d'$. For transforming q_i's to s_i's such that $s_1 = 0$, $s_2 = 1$, and $s_3 = 2$, we must have $s_1 = \frac{q_1}{d'} - \frac{q_1}{d'}$, $s_2 = \frac{q_2}{d'} - \frac{q_1}{d'}$, and $s_3 = \frac{q_3}{d'} - \frac{q_1}{d'}$. We shall define for the sake of convenience the response surface in terms of the transformed levels, s_1, s_2 and s_3.

Suppose the true response at the uth experimental point expressed as polynomial of second degree in k quantitative variables with levels 0, 1 and 2 is

$$\eta_u = B_0 x_{0u} + \sum_{i=1}^{k} B_i x_{iu} + \sum_{i \leq j=1}^{k} B_{ij} x_{iu} x_{ju} \quad \ldots\ldots(3)$$

where x_{0u} is the dummy variate conventionally defined as unity. Let N experiments $(u = 1, 2, \ldots N)$ be performed to explore the relationship (3). The observed response y_u, varies about a mean of η_u with a common variance of σ^2 for all values of u, these N errors being uncorrelated.

Our main object, here is to explore the relationship (3) through data obtained from factorial experiments of 3^k series by expressing terms involved in equation (3) as functions of main effects and two factor interaction components of various factors. A direct fit to the surface at (3) is difficult and does not utilise the results of a factorial experiment. As such, an alternative method is sought which expedites the fitting of equation (3) and makes use of the usual results of a factorial experiment.

For alternative method, we redefine the levels 0,1 and 2 of the independent variables in terms of orthogonal polynomials as

$$x'_{iu} = x_{iu} - \bar{x}_i \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

$$x'^2_{iu} = (x_{iu} - \bar{x}_i)^2 - 2/3 \quad \ldots\ldots\ldots\ldots\ldots(5)$$

where x_{iu} denotes the uth level of the ith factor and $\bar{x}_i$ is 1.

Then we shall fit the equation

$$\eta_u = b_0 x'_{0u} + \sum_{i=1}^{k} b_i x'_{iu} + \sum_{i=1}^{k} b_{ii} x'^2_{iu} + \sum_{i<j=1}^{k} b_{ij} x'_{iu} x'_{ju} \ldots(6)$$

by use of the redefined levels (4) and (5). Fitting of this equation (6) is easy and utilizes the results of a factorial experiment as the different coefficients of equation (6) come as simple functions of main effects and two factor interaction components. This method of attack, also, helps in examining the extent to which the terms of equation (6) are affected in case of confounded and fractionally replicated designs. The actual solutions for b_i's are given below for a 3^k unconfounded factorial design:

b_0 = grand mean $= 1/N \sum_{u=1}^{N} y_u$

$b_i = 1/2 \times 3^{k-1}$ (linear effect of the ith factor)

$b_{ii} = 1/6 \times 3^{k-2}$ (quadratic effect of the ith factor)

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

$b_{ij} = 1/4 \times 3^{k-2}$ (linear x linear effect of the two factor interaction i and j)

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

These designs are called "orthogonal" designs, since the moment matrix of the independent variables of (6) is diagonal. Using (4) and (5) in equation (6) and equating the coefficients of $x_1, x_2, \ldots\ldots, x_k, x_1^2, x_2^2 \ldots\ldots x_k^2, x_1 x_2, x_1 x_3, \ldots x_{k-1} x_k$

in (3) and (6), we get the following structural relationship between B_i's and b_i's.

$$B_0 = b_0 - \sum_{i=1}^{k} b_i + 1/3 \sum_{i=1}^{k} b_{ii} + \sum_{i<j=1}^{k} b_{ij}$$

$$B_i = b_i - 2b_{ii} - \sum_{\substack{j \neq i \\ j=1}}^{k} b_{ij} \qquad (i = 1,2,\ldots\ldots k)$$

$$B_{ii} = b_{ii} \qquad (i = 1,2,\ldots\ldots k)$$

$$B_{ij} = b_{ij} \qquad (i \neq j = 1,2,\ldots\ldots k)$$

Once the b_i's are obtained, the B_i's can easily be accomplished through the above structural relationship. There are two reasons for studying problems of fitting equations such as (3):

(i) to find that combination of the variables $x_1, x_2, \ldots, x_k$ which in some sense give the "best" value of η.

(ii) to know the characteristics of the response function in the neighbourhood of the optimum generating conditions.

For practical illustration, a 3^2 factorial design is studied below:

Numerical example for a 3^2 factorial:-

As an illustration of the general approach, a quadratic equation (6) will be fitted to the results of a 3^2 factorial. The data is taken from (Ref. 19) where the effect of application of phosphate, to green manure, combined with different levels of lime is studied. The levels of phosphate (x_1) are $q_1 = 0$, $q_2 = 20$, and $q_3 = 40$ lbs/acre and the levels of lime (x_2) are $q_1 = 0$, $q_2 = 200$, and $q_3 = 400$ lbs/acre. The values of d* for phosphate and lime are 20 and 200 respectively.

Then the quadratic equation (3) in two variables with levels 0, 1, and 2 , is

$$y_u = B_0 x_{0u} + B_1 x_{1u} + B_2 x_{2u} + B_{11} x_{1u}^2 + B_{22} x_{2u}^2 + B_{12} x_{1u} x_{2u} \quad \ldots\ldots\ldots (7)$$

Using the redefined levels (4) and (5), we fit the quadratic equation (6) in two factors,

$$y_u = b_0 x'_{0u} + b_1 x'_{1u} + b_2 x'_{2u} + b_{11} x'^2_{1u} + b_{22} x'^2_{2u} + b_{12} x'_{1u} x'_{2u} \quad \ldots\ldots\ldots (8)$$

and therefore the design points to fit (8) appear in table 1. The response is yield of green manure in lbs/acre averaged over four replications.

<u>TABLE 1</u>: Fitting the quadratic equation (8) to a 3^2 factorial.[@]

Treatment PL	x'_0	x'_1	x'_2	x'^2_1	x'^2_2	$x'_1 x'_2$	yield - y
(00)	1	-1	-1	1/3	1/3	1	3809.25
(11)	1	0	0	-2/3	-2/3	0	8489.91
(22)	1	1	1	1/3	1/3	1	9286.62
(01)	1	-1	0	1/3	-2/3	0	3983.54
(12)	1	0	1	-2/3	1/3	0	7319.25
(20)	1	1	-1	1/3	1/3	-1	8788.68

(02)	1	-1	1	1/3	1/3	-1	6224.28
(10)	1	0	-1	-2/3	1/3	0	7518.92
(21)	1	1	0	1/3	-2/3	0	8913.16

-.-

@ The purpose of separating the treatments with dotted lines will be explained later.

Solutions for b_i's are:

$$b_0 = 1/9 \sum_{u=1}^{9} y_u = 7148.2400$$

$$b_1 = P_1/6 = 12971.37/6 = 2161.8950$$

$$b_2 = L_1/6 = 2713.80/6 = 452.3000$$

$$b_{11} = P_q/6 = -5651.61/6 = -941.9350$$

$$b_{22} = L_q/6 = 174.30/6 = 29.0500$$

$$b_{12} = P_1L_1/4 = -1917.09/4 = -479.2725$$

Thus the fitted relation (8) is

$$y = 7148.240 + 2161.895\, x_1' + 452.300\, x_2' - 941.935\, x_1'^2 + 29.050\, x_2'^2 - 479.272\, x_1'x_2'$$

From the structural relationship, we have

$$B_0 = b_0 - (b_1 + b_2) + 1/3\,(b_{11} + b_{22}) + b_{12} = 3750.477$$

$$B_1 = b_1 - 2b_{11} - b_{12} = 4525.037$$

$$B_2 = b_2 - 2b_{22} - b_{12} = 873.472$$

$$B_{11} = b_{11} = -941.935$$

$B_{22} = b_{22} = 29.050$

$B_{12} = b_{12} = -479.272$

and thus the fitted equation (7) is

$$\hat{y} = 3750.477 + 4525.037\, x_1 + 873.472\, x_2 - 941.935\, x_1^2$$

$$+ 29.050\, x_2^2 - 479.272\, x_1 x_2 \qquad \ldots\ldots \quad (8\,A)$$

The information contained in this quadratic equation is most readily comprehended by rewriting this equation in the canonical form

$$y - Y_s = \overset{\circ}{B}_{11} X_1^2 + \overset{\circ}{B}_{22} X_2^2 \qquad \ldots\ldots\ldots\ldots\ldots\ldots(9)$$

where Y_s is the response predicted at the centre S (stationary point) of the system whose coordinates (X_{1s}, X_{2s}) are the solutions of the equations

$$\left.\begin{array}{l} 4525.037 - 1883.870\, x_1 - 479.272\, x_2 = 0 \\ 873.472 + 58.100\, x_2 - 479.272\, x_1 = 0 \end{array}\right\} \ldots\ldots\ldots(10)$$

obtained by differentiating partially the fitted equation (8 A) with respect to x_1 and x_2 respectively. $\overset{\circ}{B}_{11}$ and $\overset{\circ}{B}_{22}$ are the latent roots of the matrix

$$\begin{Bmatrix} B_{11} & B_{12}/2 \\ B_{12}/2 & B_{22} \end{Bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots(11)$$

where B_{11}, B_{12}, and B_{22} are second order coefficients of the equation (7) and X_1 and X_2 are "canonical" variables of the form

$$X_1 = m_{11}(x_1 - X_{1s}) + m_{12}(x_2 - X_{2s})$$
$$X_2 = m_{21}(x_1 - X_{1s}) + m_{22}(x_2 - X_{2s}) \quad \ldots\ldots\ldots(12)$$

and $\begin{pmatrix} m_{11} \\ m_{12} \end{pmatrix}$, $\begin{pmatrix} m_{21} \\ m_{22} \end{pmatrix}$ are the normalised latent vectors of the matrix (11). From this canonical equation (9), it is frequently possible to secure an understanding of the factor dependencies intrinsic to the system under study. There are basically only two types of surfaces which this second degree equation (8 A) can represent. The contours of these two basic surfaces are given by Box (1954) and Cochran and Cox (1957).

The coordinates (X_{1s}, X_{2s}) of the centre of the canonical system are

$$X_{1s} = 2.009 \qquad X_{2s} = 1.542$$

Substituting these values of X_{1s} and X_{2s} in the fitted equation (8 A) we get the predicted response (Y_s) as 8970.65. This is the maximum of the fitted response surface (8 A).

The latent roots of (11) are obtained by expanding the determinantal equation

$$\begin{vmatrix} -941.935 - B^{\circ} & -239.636 \\ -239.636 & 29.050 - B^{\circ} \end{vmatrix} = 0 \quad \ldots\ldots\ldots (13)$$

i.e. $B^{\circ 2} + 912.885\, B^{\circ} - 84788.624 = 0$

Whence we obtain $B^{\circ}_{11} = 84.97$, $B^{\circ}_{22} = -997.85$

The canonical equation (9) is therefore

$$y - 8970.65 = 84.97\, X_1^2 - 997.85\, X_2^2$$

The contour system is obtained by setting, for example, $y = 5000$ lbs into the above equation and solving for values of X_1 and X_2 that will satisfy the resultant equation, thus generating a contour estimating yield everywhere equal to 5000 lbs. The fitted contour system is given in Fig. 1. Since $\overset{\circ}{B}_{11}$ and $\overset{\circ}{B}_{22}$ are of opposite signs we have a saddle point (i.e. col or minimax) shown in Fig.1. It can easily be seen from Fig.1 that the surface is attenuated along X_1 axis since $\overset{\circ}{B}_{11}$ is smaller than $\overset{\circ}{B}_{22}$ in magnitude. Since contours in Figure 1 are running from the top right to the bottom left, it indicates that the contour systems are associated with postive two factor interaction between phosphate and lime. Again the positive coefficient $\overset{\circ}{B}_{11}$ suggests that the response is expected to increase by trying the factor combinations of phosphate and lime which give higher values of X_1.

To determine the equation of the canonical axes X_1 and X_2 as given by (12), we construct an orthogonal matrix

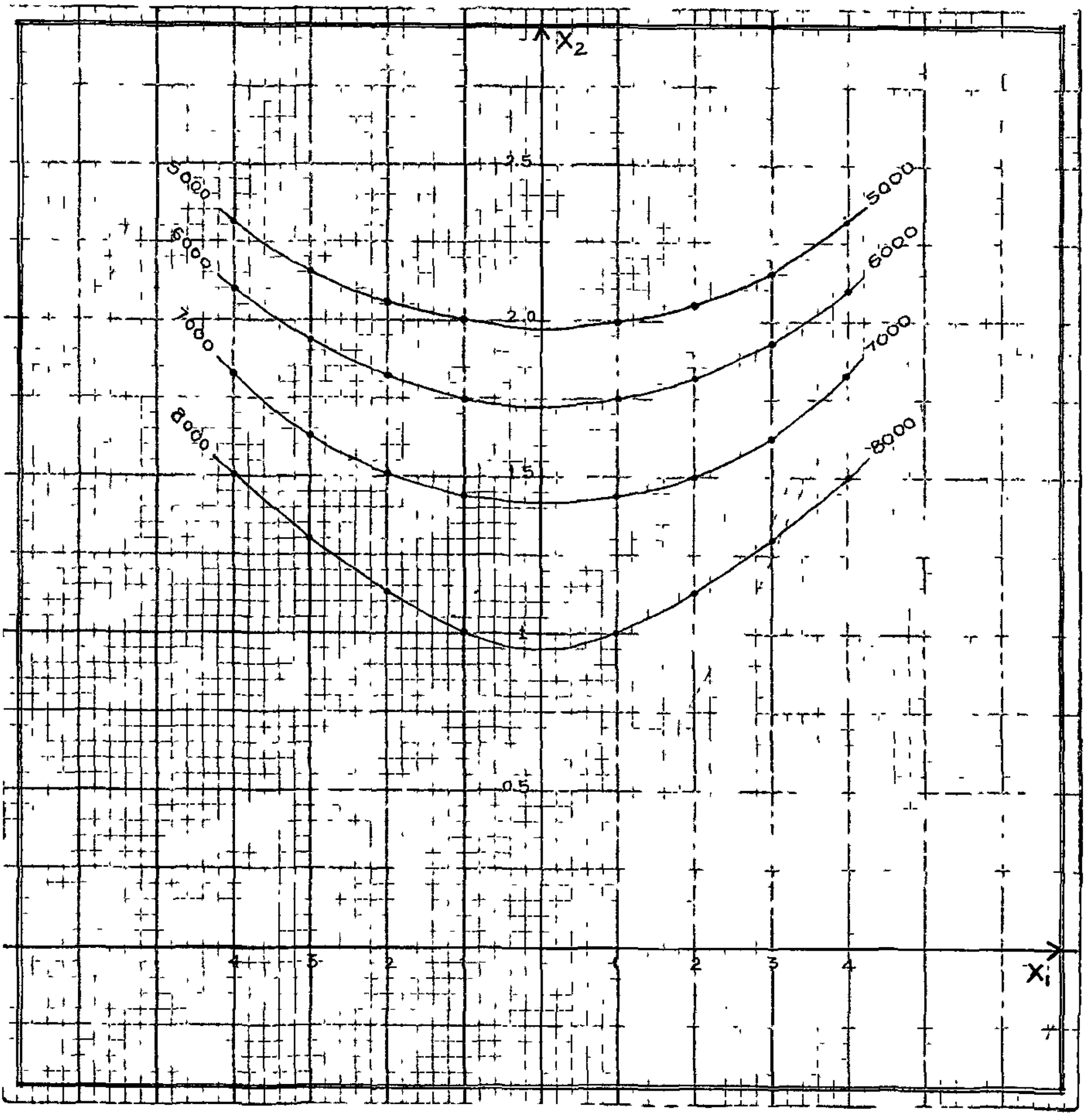
$$\underline{M} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \quad \ldots\ldots\ldots\ldots (14)$$

where $\sum_{t=1}^{2} m_{it}^2 = 1$ and $\sum_{t=1}^{2} m_{1t}\, m_{2t} = 0$

The knowledge of the equations of canonical axes is essential in order to go from coordinates (X_1, X_2) to coordinates (x_1, x_2) or vice versa. The coefficients of x_1 and x_2 of

Fig. 1: The contours of the fitted canonical equation

$$y - 8970.65 = 84.97 X_1^2 - 997.85 X_2^2$$



Scale: .5 inch = 1 unit of X_1

2.0 inches = 1 unit of X_2

canonical equations X_1 and X_2 in (12) are the direction cosines of the canonical axes with respect to design axes. Hence a coefficient near unity would indicate that a canonical axis was nearly parallel to a design axis, and therefore that both axes measured the same quantity. This matrix $\underline{M}$ will rotate our fitted system of axes to the other about the origin (X_{1s}, X_{2s}). To determine the elements of the first row of M in (14), we substitute $\overset{\circ}{B}_{11} = 84.97$ in equation (13) giving the coefficients of a homogeneous set of equations in the m_{ij}'s as follows:

$$\left.\begin{aligned} -1026.900\, m_{11} - 239.636\, m_{12} &= 0 \\ -239.636\, m_{11} - 55.97\, m_{12} &= 0 \end{aligned}\right\} \quad \ldots\ldots\ldots\ldots(15)$$

These equations do not have a unique solution. Setting $m_{11}=1.000$ we obtain $m_{12} = -4.285$. In order that the restraint $\sum_{u=1}^{2} m_{iu}^2 = 1$ be satisfied, these values of m_{ij} are standardized by dividing by $\sqrt{m_{11}^2 + m_{12}^2} = 4.4$, giving finally $m_{11} = 1/4.4 = 0.227$ and $m_{12} = -4.285/4.4 = -0.974$. To determine the elements of the second row of M, the procedure is repeated now using $\overset{\circ}{B}_{22} = -997.85$ which gives $m_{21} = 0.974$ and $m_{22} = 0.227$. We note that

$$\sum_{t=1}^{2} m_{1t}\, m_{2t} = 0$$

Thus the orthogonal matrix of the transformation is

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0.227 & -0.974 \\ 0.974 & 0.227 \end{bmatrix} \begin{bmatrix} x_1 - 2.009 \\ x_2 - 1.542 \end{bmatrix}$$

and we quickly see that the equations of the lines forming the canonical axes X_1 and X_2 are

$$X_1 = 0.227\, x_1 - 0.974\, x_2 + 1.046$$

$$X_2 = 0.227\, x_2 + 0.974\, x_1 - 2.289$$

The coefficients of x_1 and x_2 in both equations are the direction cosines of the canonical axes with respect to the design axes.

A measure of over-all degree of association of y and a set of independent variables x_1, x_2, x_1^2, x_2^2 and $x_1 x_2$ is the multiple correlation coefficient R. It is actually the simple correlation between the observed value y and those predicted by the fitted equation (7). The calculated value of multiple correlation coefficient R is 0.961 and to test significance of R^2, the value of F is 8.00 with 5 and 3 degrees of freedom. It is significant at 5% level of significance and thus the fit is good. The percentage standard error of the maximum response is 0.70 lbs/acre, since the variance of maximum response $V(Y_s)$ is 11.1054 and σ^2 is estimated by 353.31(lbs/acre)^2.

When no two factor interaction or main effect is confounded, the coefficients of equation (6) remain unaffected. But in case of confounded and fractionally replicated designs where the main effect and/or some two factor interactions are lost, the coefficients of equation (6) corresponding to these effects may or may not be estimable. We have examined below the various confounded and fractionally replicated 3^k designs.

CONFOUNDED DESIGNS:

We mentioned that when no main effect or two factor interaction is confounded, the coefficients of equation (6) are fully estimable. When all the four degrees of freedom of any two-factor interaction is confounded, the corresponding "linear x linear" coefficient of that two factor interaction cannot be estimated. But if only two degrees of freedom of a two factor interaction is confounded, the "linear x linear" coefficient of that interaction is estimable though with less precision. Similarly when two degrees of freedom for any main effect is confounded, the coefficients in equation (6) corresponding to "linear" and "quadratic" terms of that factor are not estimable. For instance, let PL^2 be confounded in 3^2 factorial design of the previous example. The three blocks are separated by dotted lines. To fit equation (8), we calculate the moment matrix of the independent variables from within the blocks as given in Table 2.

TABLE: 2 Moment matrix of independent variables for a 3^2 design when PL^2 is confounded.

****

x_0'	x_1'	x_2'	x_1^2	x_2^2	$x_1' x_2'$
9	0	0	0	0	0
	6	0	0	0	0
		6	0	0	0
			2	0	0
				2	0
					2

Due to confounding b_{12}, the term corresponding to two factor interaction PL, is estimated by $\frac{1}{2} P_1 L_1$ instead of $\frac{1}{4} P_1 L_1$.

In general, for a 3^k confounded design, when only two d.f. of any two factor interaction is confounded, say, i and j, the term of equation (6) corresponding to this interaction, namely b_{ij} is estimated by

$$1/2 \times 3^{k-2} \text{ (linear x linear effect of the two factor interaction i and j) } \quad (i \neq j = 1,2,\ldots\ldots,k)$$

FRACTIONALLY REPLICATED DESIGNS:

The importance of fractionally replicated designs in agriculture and industry is well realized. Naturally, the next step is to fit equation (6) and thereby the equation (3) for fractionally replicated designs. Let us take 1/3 replicate of 3^3 design. Let $ABC = I$ be the defining contrast. The alias group is

$$A = BC = AB^2C^2$$
$$B = AC = AB^2C$$
$$C = AB = ABC^2$$
$$AB^2 = AC^2 = BC^2$$

The equation (6) to be fitted in three variables is

$$y_u = b_0 x'_{ou} + b_1 x'_{1u} + b_2 x'_{2u} + b_3 x'_{3u} + b_{11} x'^2_{1u} + b_{22} x'^2_{2u} + b_{33} x'^2_{3u} + b_{12} x'_{1u} x'_{2u} + b_{13} x'_{1u} x'_{3u} + b_{23} x'_{2u} x'_{3u} \quad \ldots\ldots\ldots\ldots (16)$$

The design points and the moment matrix of the independent variables to fit the equation (16) appear in Table 3. Let

x_1, x_2, and x_3 correspond to factors A, B, and C respectively.

<u>TABLE: 3</u> Fitting a quadratic model to $1/3\ (3^3)$ fractional factorial.

Design points:-

Treatment.	x'_0	x'_1	x'_2	x'_3	x_1^2	x_2^2	x_3^2	$x'_1x'_2$	$x'_1x'_3$	$x'_2x'_3$
(000)	1	-1	-1	-1	1/3	1/3	1/3	1	1	1
(012)	1	-1	0	1	1/3	-2/3	1/3	0	-1	0
(021)	1	-1	1	0	1/3	1/3	-2/3	-1	0	0
(111)	1	0	0	0	-2/3	-2/3	-2/3	0	0	0
(120)	1	0	1	-1	-2/3	1/3	1/3	0	0	-1
(210)	1	1	0	-1	1/3	-2/3	1/3	0	-1	0
(222)	1	1	1	1	1/3	1/3	1/3	1	1	1
(201)	1	1	-1	0	1/3	1/3	-2/3	-1	0	0
(102)	1	0	-1	1	-2/3	1/3	1/3	0	0	-1

Moment matrix:-

x'_0	x'_1	x'_2	x'_3	x_1^2	x_2^2	x_3^2	$x'_1x'_2$	$x'_1x'_3$	$x'_2x'_3$
9	0	0	0	0	0	0	0	0	0
	6	0	0	0	0	0	0	0	0
		6	0	0	0	0	0	0	0
			6	0	0	0	0	0	0
				2	0	0	0	0	2
					2	0	0	2	0
						2	2	0	0
							4	2	2
								4	2

Normal Equations:-

$$\sum_{u=1}^{9} y_u = 9\, b_0$$

$$\sum_{u=1}^{9} y\,(x_i') = 6\, b_i \qquad (i = 1,2,3)$$

$$\sum_{u=1}^{9} y\,(x_1'^2) = 2\, b_{11} + 2\, b_{23}$$

$$\sum_{u=1}^{9} y\,(x_2'^2) = 2\, b_{22} + 2\, b_{13}$$

$$\sum_{u=1}^{9} y\,(x_3'^2) = 2\, b_{33} + 2\, b_{12}$$

$$\sum_{u=1}^{9} y\,(x_1' x_2') = 2\, b_{12} + 2\, b_{33} + 2 \sum_{i<j=1}^{3} b_{ij}$$

$$\sum_{u=1}^{9} y\,(x_1' x_3') = 2\, b_{13} + 2\, b_{22} + 2 \sum_{i<j=1}^{3} b_{ij}$$

$$\sum_{u=1}^{9} y\,(x_2' x_3') = 2\, b_{23} + 2\, b_{11} + 2 \sum_{i<j=1}^{3} b_{ij}$$

There are 10 terms in equation (16) and with 9 observations, we can atmost estimate 9 unknown constants. From the normal equations, it becomes evident that

$$\sum y\,(x_1' x_2') - \sum y\,(x_3'^2) = \sum y\,(x_1' x_3') - \sum y(x_2'^2)$$

$$= \sum y(x_2' x_3') - \sum y(x_1'^2) = 2(b_{12} + b_{13} + b_{23})$$

Thus b_{ij}'s ($i \neq j$) are not separately estimable, but the estimation of one is possible when the other two can be assumed zero. The result is quite analogus to fractional replication theory. The solutions for constants of (16) are given below.

$$b_0 = 1/9 \sum_{u=1}^{9} y_u = \text{grand mean}$$

b_i = 1/6 (linear effect of ith factor) i=1,2,3.

When $b_{12} = 0, b_{13} = 0$ then

$b_{22} = 1/6 \ (B_q)$

$b_{33} = 1/6 \ (C_q)$

$b_{11} = 1/3 \ (A_q) - \frac{1}{2} \ (B_1 C_1)$

$b_{23} = \frac{1}{2} \ (B_1 C_1) - 1/6 \ (A_q)$

When $b_{12} = 0, \ b_{23} = 0$ then

$b_{11} = 1/6 \ (A_q)$

$b_{33} = 1/6 \ (C_q)$

$b_{22} = 1/3 \ (B_q) - \frac{1}{2} \ (A_1 C_1)$

$b_{13} = \frac{1}{2} \ (A_1 C_1) - 1/6 \ (B_q)$

Similarly when $b_{13} = 0 \ , \ b_{23} = 0$ then

$b_{11} = 1/6 \ (A_q)$

$b_{22} = 1/6 \ (B_q)$

$b_{33} = 1/3 \ (C_q) - \frac{1}{2} \ (A_1 B_1)$

$b_{12} = \frac{1}{2} \ (A_1 B_1) - 1/6 \ (C_q)$

Once the b_i's are obtained, the B_i's can be accomplished through the structural relationship and thereby we explore the quadratic equation (3).

Let us examine the design $1/3 \ (3^3)$ when defining contrast is AB = I.

The alias group is

$$\begin{array}{lllll} A & = & B & = & AB^2 \\ C & = & ABC & = & ABC^2 \\ AC & = & AB^2C^2 & = & BC^2 \\ BC & = & AB^2C & = & AC^2 \end{array}$$

From the alias group, it is quite evident that b_{12} cannot be estimated as $AB = I$ is the defining contrast and $A = B = AB^2$ Moreover, we can estimate only one of the pairs b_1, b_{11} and b_2, b_{22} since $A = B$. Again, as $AC = BC^2$ and $BC = AC^2$, we see that the terms b_{13} and b_{23} are correlated and estimable with less precision. The solutions for the constants of (16) are given below when $b_{12} = 0$, $b_j = 0$, $b_{jj} = 0$ $(j \neq i = 1,2)$

$b_0 = 1/9 \sum_{u=1}^{9} y_u =$ grand mean

$b_i = 1/6$ (linear of the ith factor) $(i \neq j = 1,2)$

$b_3 = 1/6 \; (C_1)$

$b_{ii} = 1/6$ (quadratic effect of the ith factor) $(i \neq j = 1, 2)$

$b_{33} = 1/6 \; (C_q)$

$b_{13} = 1/3 \; (A_1 C_1) - 1/6 \; (B_1 C_1)$

$b_{23} = 1/3 \; (B_1 C_1) - 1/6 \; (A_1 C_1)$

This study shows that the study of response surface should not be undertaken with the data collected from such designs with $1/3\,(3^3)$. But this has been presented just as an illustration of the method involved.

1/3 replicate of 3^4 design:

The layout of the design is given in plan 6 A .18 of Cochran and Cox (1957). The defining contrast is $A B C^2 D^2 = I$ and the design is arranged in blocks of 9 units confounding $C D^2$. This shows that by confounding the alias group gives

$$
\begin{aligned}
A B &= C D \\
A C^2 &= B D^2 \\
A D^2 &= B C^2
\end{aligned}
$$

From the alias group, it becomes clear that b_{13} and b_{24} are correlated since $A C^2 = B D^2$. Similarly b_{14} and b_{23} are correlated as $A D^2 = B C^2$. The solutions for b_i's are given below:

$$b_o = \text{grand mean} = 1/27 \cdot \sum_{u=1}^{27} y_u$$

$$b_i = \frac{1}{2\left\{\frac{1}{3} \cdot 3^{k-1}\right\}} \text{ (linear effect of ith factor)} \quad (i = 1, 2, 3, 4)$$

$$= 1/2 \times 9 \text{ (linear effect of ith factor)}$$

$$b_{ii} = \frac{1}{6\left\{\frac{1}{3} \, 3^{k-2}\right\}} \text{ (quadratic effect of ith factor)}$$

$$= 1/6 \times 3 \text{ (quadratic effect of ith factor)} \quad (i = 1, 2, 3, 4)$$

$$b_{13} = 1/9\ (A_1 C_1) - 1/18\ (B_1 D_1)$$

$$b_{24} = 1/9\ (B_1 D_1) - 1/18\ (A_1 C_1)$$

$$b_{14} = 1/9\ (A_1 D_1) - 1/18\ (B_1 C_1)$$

$$b_{23} = 1/9\ (B_1 C_1) - 1/18\ (A_1 D_1)$$

As $C D^2$ is lost by confounding and $A B = C D$, we estimate b_{34} with less precision as will be evident below.

$$b_{12} = 1/3 (A_1 B_1) - 1/6 (C_1 D_1)$$

$$b_{34} = 1/6 (C_1 D_1) - 1/6 (A_1 B_1)$$

1/3 replicate of 3^5 design:-

The layout of the design is given in plan 6 A.19 of Cochran and Cox (1957). The two degrees of freedom from A B C D E is being used for defining contrast. The design is arranged in blocks of 9 units. The interaction A E is confounded with blocks. The solutions for terms of equation (6) with five variables are given below:

$$b_o = \text{grand mean} = 1/81 \sum_{u=1}^{81} y_u$$

$$b_i = \frac{1}{2\left\{\frac{1}{3}\, 3^{k-1}\right\}} \text{ (linear effect of ith factor)}$$

$$(i = 1, 2, \ldots\ldots, 5)$$

$$b_{ii} = \frac{1}{6\left\{\frac{1}{3}\, 3^{k-2}\right\}} \text{ (quadratic effect of ith factor)}$$

$$(i = 1, 2, \ldots\ldots 5)$$

$$b_{ij} = \frac{1}{4\left\{\frac{1}{3}\, 3^{k-2}\right\}} \text{ (linear x linear effect of i and j factors) } (i \neq j)$$

(except b_{15})

While due to confoudning

$$b_{15} = \frac{1}{2\left\{\frac{1}{3}\, 3^{k-2}\right\}} (A_1 E_1)$$

Where $k = 5$ and $(i \neq j = 1, 2, \ldots\ldots 5)$.

For clarity and appreciation, we discussed designs of the type 3^k for the exploration of second degree equation (3). The approach adopted is quite general and can easily be extended to s^k factorial designs for the exploration of second degree response surface.

SECOND ORDER ROTATABLE DESIGNS

Plackett (1951) defines experiments with factors as factorial experiments. If we adopt this implied definition then response surface techniques are generalization of factorial designs. Since the total set of treatments in the conventional factorial is the set of all combinations of the factors taken at fixed levels, the sample points form a rectangular lattice in the factor space (whose dimension is the number of factors). The physical law relating the response with the controllable factors may be represented by a k-dimensional surface in the (k+1)-dimensional space defined by the factors and the response, this surface is known as the "response surface". The exploration of this response surface may often be performed more efficiently if the concept of the factorial design is extended to include any configuration of sample points whatever within the factor space.

The designs suitable for fitting response surfaces, first introduced by Box and Wilson (1951), took advantage of the continuity of the levels of the variables and capitalized on the fact that the experiments can be performed sequentially, thereby using information available at any stage for planning further stages of the investigation. In a recent paper, this problem was further investigated by Box and Hunter (1957).

It is assumed that the response surface may be approximated by a polynomial of degree d within the range of interest, that is,

$$\eta = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \dots + \beta_{111} x_1^3 + \beta_{222} x_2^3 + \dots \qquad (17)$$

where in the subscript of β, the number of times each factor number appears is the appropriate power of that factor (and x_0 is conventionally defined as unity). The notations and terminology of Box and Wilson (1951) are used but the values of the x_{iu} are subject to the scaling conventions (Box and Hunter, 1957) $\sum_{u=1}^{N} x_{iu} = 0$, $\sum_{u=1}^{N} x_{iu}^2 = N$ for all i. (i=1,2,..k).

Box and Hunter (1957) obtained a general expression for variance funtion of the estimated response for the design, and considered the advantages of using "rotatable" designs in which the variances of the estimates of the response made from the least squares estimates of the graduating polynomial (17) are constant on circles, spheres and hyperspheres about the centre of the design.

They proved that the necessary and sufficient condition for the design to be rotatable of order d is that the generating function ϕ of the moments upto order 2d, given by

$$Q = N^{-1} \sum_{u=1}^{N} (1+t_1 x_{1u} + t_2 x_{2u} + \ldots\ldots + t_k x_{ku})^{2d}, \quad \ldots\ldots(18)$$

should be of the form

$$Q = \sum_{s=0}^{d} a_{2s} (t_1^2 + t_2^2 + \ldots\ldots\ldots + t_k^2)^s, \quad \ldots\ldots\ldots (19)$$

where a_{2s} are constants independent of $t_1^{\alpha_1}, t_2^{\alpha_2}, \ldots\ldots, t_k^{\alpha_k}$.

Denoting the moments

$$N^{-1} \sum_{u=1}^{N} x_{1u}^{\alpha_1} x_{2u}^{\alpha_2} \ldots\ldots x_{ku}^{\alpha_k} \text{ by } (1^{\alpha_1}, 2^{\alpha_2}, \ldots\ldots, k^{\alpha_k}),$$

they deduced by equating the coefficients of $t_1^{\alpha_1} t_2^{\alpha_2} \ldots . t_k^{\alpha_k}$ in

(18) and (19), that for rotatibility of order d, it is necessary and sufficient that

$$(1^{\alpha_1}, 2^{\alpha_2}, \ldots\ldots, k^{\alpha_k}) = 0 \quad \text{if one or more } \alpha_i \text{ are odd,}$$

$$= \lambda_\alpha \frac{\prod_{i=1}^{k} \alpha_i!}{2^{\alpha/2} \prod_{i=1}^{k} (\frac{1}{2}\alpha_i)} \; ,$$

if all α_i are even,

where $\alpha = \alpha_1 + \alpha_2 + \cdots + \alpha_k \leq 2d$ and λ_α is a constant depending on α, but independent of the way in which α is partitioned into $\alpha_1, \alpha_2, \ldots, \alpha_k$. It may be noted that $\lambda_0 = 1$, since $x_0 = 1$ and $\lambda_2 = 1$ by the scaling convention. A distinction is made between an "arrangement" and a "design" of order d, the former being any configuration of sample points satisfying the necessary moment properties, and the latter being an arrangement which also permits estimation of the constants in the dth order polynomial (17).

Suppose, in the experimental investigation with k factors, N combinations of levels are employed. Thus the group of N experiments which arises can be described by the N points in a k-dimensional space:

$$(x_{1u}, x_{2u}, \ldots\ldots, x_{ku}) \quad \ldots\ldots\ldots\ldots \quad (20)$$

$(u = 1, 2, \ldots\ldots, N)$; where in the uth experiment the factor i is at level x_{iu}. This set of points (20) is said to form a rotatable design of the second order if the following relations hold:

(A) $\sum_{u=1}^{N} x_{1u}^2 = \sum_{u=1}^{N} x_{2u}^2 = \ldots\ldots\ldots = \sum_{u=1}^{N} x_{ku}^2 = \lambda_2 N$

(B) $\sum_{u=1}^{N} x_{1u}^4 = \sum_{u=1}^{N} x_{2u}^4 = \ldots\ldots\ldots = \sum_{u=1}^{N} x_{ku}^4 = 3 \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = 3\lambda_4 N$

$(i \neq j)$

(C) $\lambda_4 / \lambda_2^2 > k/k+2$

and all other sums of powers and products upto and including order four are zero. The relation (C), ensures the estimation of the constants in the second degree polynomial. This condition can always be satisfied merely by adding atleast one point at the centre of the design.

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

Let $(x_1, x_2, \ldots\ldots, x_k)$ be a point set and let C_k be the cyclical group of order k, that is, the group of cyclical permutations of k elements. Thus, we have k point sets, by operating upon $(x_1, x_2, \ldots\ldots, x_k)$, given by

$$(x_1, x_2, \ldots\ldots, x_k),$$
$$(x_2, x_3, \ldots\ldots, x_1),$$
$$\vdots \qquad\qquad \vdots$$
$$(x_k, x_1, \ldots\ldots, x_{k-1}).$$

There will be $k \times 2^k$ total number of points, since each point set will give 2^k permutations of the form $(\pm x_1, \pm x_2, \ldots, \pm x_k)$ if none of the elements is zero. When there are k factors, the number of constants to be estimated for a second order polynomial is $1 + k + k + k(k-1)/2$ or $k^2 + 3k + 2/2$. For $4 \leq k \leq 7$, we have the following table:

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

The desirable property for a practically useful design is that it should not contain excessively large number of experimental points. To obtain a design consisting of a number of points equal to twice the number of constants to be estimated was regarded as a very desirable achievement by Draper (1960). Draper (1960) constructed second order rotatable designs with more than three factors by taking symmetric group of elements of the point set $(x_1, x_2, \ldots, x_k)$. The total number of points in the design with k factors will be $k\ 2^k$. Thus the reduction in total number of points by this method is $(k! - k)2^k$, which is desirably a very good achievement. Of course, the exploration of designs by this method becomes difficult with more than six factors, but we will discuss how the difficulties can be overcome by proper selection of initial point set in case of even number of factors.

Designs with four factors:-

Let (a,b,c,d) be a point set, then the cyclical group C_4 obtained by the cyclical permutations of 4 elements is given by

(a, b, c, d)
(b, c, d, a)
(c, d, a, b)
(d, a, b, c)

The 64 points of the resultant design are:

the 16 points of $(\pm a, \pm b, \pm c, \pm d)$

the 16 points of $(\pm b, \pm c, \pm d, \pm a)$

the 16 points of $(\pm c, \pm d, \pm a, \pm b)$

and the 16 points of $(\pm d, \pm a, \pm b, \pm c)$

As there are two types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ $(i \neq j)$, the relation (B) gives

$$16\,(a^4 + b^4 + c^4 + d^4) = 3\left\{16(a^2 b^2 + b^2c^2 + c^2d^2 + d^2a^2)\right\}$$
$$= 3\left\{16(a^2c^2 + b^2d^2 + c^2a^2 + d^2b^2)\right\} \qquad \text{.......(21)}$$

Let $a^2 = s\,d^2$, $b^2 = t\,d^2$, and $c^2 = u\,d^2$, then (21) gives

$$s^2 + t^2 + u^2 + 1 = 6\,(us + t) \qquad \text{........ (22)}$$

$$s\,t + u\,t + u + s = 2\,(us + t) \qquad \text{........ (23)}$$

These two equations (22) and (23), in three unknown variables u, s and t will furnish infinite positive solutions for (u , s, t). Geometrically this can be viewed as points of intersection, of the surfaces (22) and (23), lying in the first (i.e. positive) quadrant in three dimensions. For instance, the design with 64 non-central points is obtained for the solutions $u = 3 + 2\sqrt{3}$, $s = 1$, and $t = 1$.

When any one of u, s, and t is zero, the resultant design will contain 32 points which is desirably a good achievement. There are only two designs with 32 points and solutions for these designs are:

Design 1:	$u = 0$	Design 2:	$u = 3.13720$
	$s = 1.68125$		$s = 0.59480$
	$t = 5.27452$		$t = 0$

The designs with the solutions $s = 0$, $u = 1.68125$, and $t = 5.27452$ will be regarded as indentical with design 1, since simply by designating x_1 as x_3 and x_3 as x_1 we get the same design matrix. The designs presented in this chapter will give "singular" value of λ_4 (i.e. $\lambda_4/\lambda_2^2 = k/ k+2$), because the design points are equidistant from the centre of the design. To satisfy the relation (C), atleast one point is to be added at the centre of the design.

Designs with five factors:

Let (a , b , c , d , e) be a point set then the cyclical group C_5 is

(a , b , c , d , e) ,
(b , c , d , e , a) ,
(c , d , e , a , b) ,
(d , e , a , b , c) ,
(e , a , b , c , d) .

To reduce the size of the experiment, a suitable fractional replicate can replace the full factorial. Since a second order moment matrix identical with that of the full factorial will be obtained with any fractional replicate of the 2^k design in which no main effects and two factor interactions are confounded. Therefore, select that fractional replicate, for $k>4$, in which effects upto second order are confounded only with third or higher order effects. Here, if all the elements are different from zero, the resultant design will contain 80 points by taking half-replicates of the point-sets of C_5. But if one or more elements are zero then obviously the full factorial is to be taken.

As there are two types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ ($i \neq j$), the relation (B) gives

$$32\,(a^4+b^4+c^4+d^4+e^4) = 3\left\{32(a^2b^2+b^2c^2+c^2d^2+d^2e^2+e^2a^2)\right\}$$

$$= 3\left\{32(a^2c^2+b^2d^2+c^2e^2+d^2a^2+b^2e^2)\right\}$$

.......(24)

Let $a^2 = u\,e^2$, $b^2 = v\,e^2$, $c^2 = s\,e^2$, and $d^2 = t\,e^2$, then (24) gives

$$u^2+v^2+s^2+t^2+1 = 3\,(u\,v+v\,s+s\,t+t+u) \quad ....(25)$$

$$u\,v+v\,s+s\,t+t+u = u\,s+v\,t+u\,t+s+v \quad .....(26)$$

These two equations (25) and (26) in four unknown variables v, u, s, and t will furnish infite positive solutions for (u,v,s,t). For instance, when u=0, s = 1, v = 1.83396 and t = 6.02299. Similarly when u=0, s = 2, v = 6.716340 and t = [illegible].269017. To meet the desirable property of getting designs with lesser number of experimental points, we present three different designs with 40 experimental points.

Design No.1:

$$u = 0$$
$$v = 1.422080$$
$$s = 1.369220$$
$$t = 0$$

Design No.2:

$$u = 0$$
$$v = 0.296810$$
$$s = 0$$
$$t = 0.422090$$

Design No.3:

$$u = 0$$
$$v = 0.703162$$
$$s = 0$$
$$t = 2.368842$$

Designs with six factors:-

Let (a , d , b , d , c , d) be a point set then the cyclical group C_6 is

$$(a, d, b, d, c, d),$$
$$(d, b, d, c, d, a),$$
$$(b, d, c, d, a, d),$$
$$(d, c, d, a, d, b),$$
$$(c, d, a, d, b, d),$$
$$(d, a, d, b, d, c).$$

By taking half replicates of the point sets of C_6, the resultant design will have 196 points. There being two types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ ($i \neq j$), the relation (B) gives

$$32\,(a^4 + b^4 + c^4 + 3d^4) = 3\left[\,32\left\{a^2b^2 + b^2c^2 + c^2a^2 + 3(d^2)^2\right\}\right]$$

$$= 3\left[\,32(\,2\,a^2d^2 + 2\,b^2d^2 + 2\,c^2d^2)\,\right] \qquad \text{....(27)}$$

Putting $a^2 = s\,d^2$, $b^2 = t\,d^2$, and $c^2 = u\,d^2$, the equation (27) gives

$$u^2 + s^2 + t^2 + 3 = 6(\,u + s + t\,) \qquad \text{............ (28)}$$

$$u\,s + s\,t + u\,t + 3 = 2\,(\,u + s + t\,) \qquad \text{.......... (29)}$$

These two equations (28) and (29) in three unknowns u, s, and t will furnish infinite series of rotatable designs for each positive solution of (u , s , t). We will describe the geometrical procedure to assess quickly and easily the solutions for u, s, and t.

Changing the origin of (28) and (29) to (1, 1, 1), i.e.

(30).. $u = u'+1$, $s = s' + 1$, $t = t' + 1$, the equations (28) and (29) reduce to

$$u'^2 + s'^2 + t'^2 - 4\,(\,u' + s' + t'\,) - 12 = 0 \qquad \text{.... (31)}$$

$$u'\,s' + s'\,t' + t'\,u' = 0 \qquad \text{........................ (32)}$$

The equation (31) represents a sphere having centre (2,2,2) and radius equal to $2\sqrt{6}$ and the equation (32) represents a cone having axes as the generators. The equations to any generator of (32), whose direction cosines are l,m,n, are

$$u'/l = s'/m = t'/n = r \qquad \text{......(33)}$$

where $lm + mn + nl = 0$ and $l^2 + m^2 + n^2 = 1$

Any point on this generator (33) whose distance from origin is r, has co-ordinates $u' = lr$, $s' = mr$, $t' = nr$, and if it is to lie on the sphere (31), then

$$r^2 (l^2 + m^2 + n^2) - 4r(l + m + n) - 12 = 0 \quad \ldots\ldots (34)$$

Now $(l + m + n)^2 = l^2 + m^2 + n^2$ as $lm + mn + nl = 0$

$= 1$

Therefore $l + m + n = \pm 1$. So the equation (34) reduces to

$$r^2 \mp 4r - 12 = 0 \quad \ldots\ldots\ldots (35)$$

For $l + m + n = 1$, we get $r = -2, +6$ and $l + m + n = -1$, we get $r = +2, -6$.

Now $u' + s' + t' = r(l + m + n)$. For $l + m + n = 1$ and $r = 6$, it reduces to $u' + s' + t' = 6$ .... (36)

and $l + m + n = -1$ and $r = 2$, it reduces to

$$u' + s' + t' = -2 \quad \ldots\ldots\ldots\ldots\ldots\ldots (37)$$

For $r = -2$ and $l + m + n = 1$, and for $r = -6$ and $l + m + n = -1$, we will get the same two equations (36) and (37).

Thus, to find the points of intersection of a sphere (31) and a cone (32) is equivalent to find the points of intersection of a plane (36 or 37) and a cone (32) whose equations are

$$\left.\begin{aligned} u' + s' + t' &= 6 \\ u's' + s't' + u't' &= 0 \end{aligned}\right\} \quad \ldots\ldots\ldots\ldots (38)$$

$$\left.\begin{aligned} u' + s' + t' &= -2 \\ u's' + s't' + u't' &= 0 \end{aligned}\right\} \quad \ldots\ldots\ldots\ldots (39)$$

For instance,

By assigning any specified value to u', the solutions for s' and t' can easily be obtained from (38) and (39). Choose those sets of values of (u',s',t') which will give positive values for (u , s , t) using the equation (30). For instance, let u' = 0 then from (38) we get s' = 0, t' = 6 or s' = 6, t' = 0. Using (30) we get two designs in 192 non-central points having solutions for u , s, and t as:

Design 1:	Design 2:
$u = 1$	$u = 1$
$s = 1$	$s = 7$
$t = 7$	$t = 1$

Those two designs are not different since ultimately they give the same design matrix.

Unfortunately, because of the large number of moments to be balanced when selecting design points, the desirable achievements of getting designs with lessor number of experimental points is rarely possible to assess with this method with more than five factors. Thus some of the designs to be presented are useful only when large number of design points is allowable.

When either one of u , s, and t is zero, the resultant design will have 96 experimental points with the solutions for u, s, and t as:

Design 1:	Design 2:	Design 3:
$u = 0$	$u = (9 + \sqrt{21})/2$	$u = (9 - \sqrt{21})/2$
$s = (9 + \sqrt{21})/2$	$s = (9 - \sqrt{21})/2$	$s = 0$
$t = (9 - \sqrt{21})/2$	$t = 0$	$t = (9 + \sqrt{21})/2$

These three designs are not different because they give ultimately the same design matrix.

<u>Designs with seven factors:-</u>

Let (0 , 0 , a , b , c , d , e) be a point set, then the cyclical group C_7 is

(0 , 0 , a , b , c , d , e) ,
(0 , a , b , c , d , e , 0) ,
(a , b , c , d , e , 0 , 0) ,
(b , c , d , e , 0 , 0 , a) ,
(c , d , e , 0 , 0 , a , b) ,
(d , e , 0 , 0 , a , b , c) ,
(e , 0 , 0 , a , b , c , d) .

By taking half replicates of the point sets of C_7, the resultant designs will have 112 points when none of the elements a , b , c , d , e is zero. But if one or more elements are zero, obviously the full factorial is to be taken.

There being three types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ (i ≠ j), the relation (B) gives

$$16(a + b + c + d + e) = 3 \left| 16(a^2b^2+ b^2c^2+ c^2d^2+ d^2e^2+ e^2a^2 \right.$$

$$= 3 \left| 16(a^2c^2+ b^2d^2+ c^2e^2) \right|$$

$$= 3 \left| 16(a^2d^2+ b^2e^2+ e^2a^2) \right|$$

......(40)

Putting $b^2= u\ a^2$, $c^2= v\ a^2$, $d^2= s\ a^2$ and $e^2= t\ a^2$, the equations

(40) reduce to

$$u^2 + v^2 + s^2 + t^2 + 1 = 3\,(u + u\,v + v\,s + s\,t) \quad \ldots\ldots \quad (41)$$

$$u + u\,v + v\,s + s\,t = v + u\,s + v\,t \quad \ldots\ldots\ldots\ldots \quad (42)$$

$$v + u\,s + v\,t = s + t + u\,t \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (43)$$

These three equations (41), (42), and (43) in four unknowns u,v,s,t will furnish infinite series of rotatable designs for each positive solution of (u,v,s,t). To get the solutions for (u,v,s,t) is quite difficult and will be extremely difficult with more than seven factors.

Designs with k factors:-

We derived designs upto six factors and noticed that the solution for the unknowns (involved in the equations) presents dif iculty with seven factors. Again, if we proceed with more than seven factors, it is evident that with the present method, it will be rather extremely difficult but not impossible to evolve new designs. However, we will outline the general procedure for construction of designs and later we will see what sort of modification will simplify this procedure.

Let the point set $(x_1\,,\,x_2\,\ldots\ldots,\,x_k)$ be the generator of the cyclical group C_k. Note that all the elements are nonzero. Let $(1/2^p \times 2^k)$ be the appropriate $1/2^p$ fractional replicate of the full factorial so that no main effects and two factor interactions are confounded. Then the total number of points in the design is $k\,(1/2^p \times 2^k)$, as there being k point sets.

When all the k elements in the point set $(x_1, x_2, \ldots, x_k)$ are different from each other then the total types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ $(i \neq j)$ will be $k/2$ or $(k-1)/2$ for even or odd k, the number of factors. This is quite obvious. The relation (B) will give $k/2$ or $(k-1)/2$ equations in $(k-1)$ unknowns for even or odd k. The particular cases of this, are the designs presented for $k = 4, 5,$ and 7.

It is interesting to note that the number of equations depends on the distinctness and spacing of the elements in the initial point set. That is, by a judicious selection of the initial point set, the total number of equations can be reduced considerably. Fortunately, we could investigate a point set for even number of factors which reduces considerably the total number of equations obtained through the relation (B).

Designs with even number of factors:-

Let the point set $(x_1, x, x_2, x, \ldots, x_k, x)$ be the generator of the cyclical group C_{2k} where the (k+1) elements x, $x_1, x_2, \ldots, x_k$ are nonzero and different from each other. Note that the element x is placed alternatively at the even places. The total types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ $(i \neq j)$ will be $(2k + 4)/4 = (k + 2)/2$ or $(2k + 2)/4 = (k + 1)/2$ for even or odd k. This is evident since there will be only one type of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ $(i \neq j)$ at a jump of odd steps from x_1 which is of the form

$$\left\{ 1/(1/2^p) \times 2^k \right\} \left| 2\left(x_1^2 x^2 + x_2^2 x^2 + \ldots + x_k^2 x^2 \right) \right|$$

While there will be $k/2$ or $(k-1)/2$ types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ $(i \neq j)$

at jumps of even steps, for even or odd k. For instance, with 8 factors, let (a , e , b , e , c,e , d , e) be the point set then $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ at jump of steps 1,3,5 and 7 is

$$\left| 2\ (a^2e^2 + b^2e^2 + c^2e^2 + d^2e^2) \right| \quad \ldots\ldots(44)$$

While the other two types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ at jumps of steps 2 and 4 are

$$\left| (a^2b^2 + b^2c^2 + c^2d^2 + d^2a^2 + 4\ e^4) \right| \ldots\ldots\ldots \quad (45)$$

and

$$\left| 2\ (a^2c^2 + b^2d^2 + 2\ e^4) \right| \quad \ldots\ldots \quad (46)$$

These three (44) and (45) and (46) are the only types of $\sum_{u=1}^{N} x_{iu}^2\ x_{ju}^2$ while the others will be identical with one of them.

The total types of $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ ($i \neq j$) will be $(k + 2)/2$ or $(k + 1)/2$ for even or odd k. Therefore, the relation (B) will give $(k + 2)/2$ or $(k + 1)/2$ equations in k unknowns for even or odd k. Thus the reduction in the total number of equations as compared to the previous method is $k - (2k + 4)/4 = (k - 2)/2$ or $(k-1) - (2k + 2)/4 = (k - 1)/2$ for even or odd k. The particular case of this approach is the designs presented for $k = 6$.

THIRD ORDER ROTATABLE DESIGNS

A necessary and sufficient condition due to Box and Hunter (1957), for "rotatibility" of order d of a design, has been presented in the previous chapter. They studied the requirements and properties of second order rotatable designs. In a recent paper, Gardiner et al (1959) extended the criterion of rotatibility to experimental designs for estimating response surfaces by third order polynomial equations. They constructed third order rotatable designs by examining regular and semi-regular geometrical figures. Such designs permit a response surface to be fitted easily and provide spherical information contours. A third order rotatable design aids the fitting of a third order (i.e. cubic) surface.

Let k be the number of independent variables or factors, and let $x_{1u}, x_{2u}, \ldots, x_{ku}$ be the levels of these factors for the uth experimental point in the k-dimensional factor space, $(u = 1, 2, \ldots, N)$. Let η_u be the expectation of the response at the uth experimental point. It is assumed that the response surface may be approximated by a third degree polynomial, within the range of interest, that is,

$$\eta_u = \beta_0 x_{ou} + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i\leq j=1}^{k} \beta_{ij} x_{iu} x_{ju} + \sum_{i\leq j\leq l=1}^{k} \beta_{ijl} x_{iu} x_{ju} x_{lu} \qquad \ldots.(47)$$

This set of N points is said to form a rotatable design of third order in k factors if the following relations hold;

$$(A) \quad \sum_{u=1}^{N} x_{1u}^2 = \sum_{u=1}^{N} x_{2u}^2 = \ldots\ldots = \sum_{u=1}^{N} x_{ku}^2 = \lambda_2 N \ (\lambda_2 = 1)$$

(B) $\sum_{u=1}^{N} x_{1u}^{4} = \sum_{u=1}^{N} x_{2u}^{4} = \ldots\ldots\ldots = \sum_{u=1}^{N} x_{ku}^{4} = 3 \sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2}$

$$= 3\lambda_4 N \quad (i \neq j)$$

(C)

(C_1) $\sum_{u=1}^{N} x_{1u}^{6} = \sum_{u=1}^{N} x_{2u}^{6} = \ldots\ldots = \sum_{u=1}^{N} x_{ku}^{6} = 5\sum_{u=1}^{N} (x_{iu}^{4} x_{ju}^{2})$

$$= 15\lambda_6 N \quad (i \neq j)$$

(C_2) $\sum_{u=1}^{N} x_{iu}^{4} x_{ju}^{2} = 3 \sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2} x_{lu}^{2} \quad (i \neq j \neq l)$

(D)

(D_1) $\lambda_4 > k/_{k+2}$,

(D_2) $\lambda_6 > \frac{k+2}{k+4} \lambda_4^2$,

and all other sums of powers and products upto and including order six are zero. The relations (D_1) and (D_2) ensure the estimation of the terms involved in the third degree equation (47). The criterion of rotatibility for a third order design is characterized mathematically by relations (A), (B), and (C) with their attendant restrictions, the relations (D_1) and (D_2).

The following are the desirable properties of an experimental design of order d, as advanced by Box and Hunter (1957).

(i) The design should allow the approximating polynomial of degree d (tentatively assumed to be representationally adequate) to be estimated with satisfactory accuracy within the region of interest.

(ii) It should allow a check to be made on the adequacy of the assumed polynomial equation.

(iii) It should not contain excessively large number of experimental points.

(iv) It should lend itself to "blocking" so that systematic effects due to differences in experimental material or enviornment can be readily eliminated.

In this chapter, we are chiefly concerned to satisfy the properties (iii) and (iv) so that (i) and (ii) are simultaneously satisfied.

Arrangement of the designs in blocks:-

A major difficulty in any experimental programme requiring a large number of trials is the maintenance of a steady experimental enviourment. Experimental results are frequently biased by such factors as time trends, heterogenous raw material, differences between shifts of workers, etc. Of course, the biasing effects of such sources of variation can be reduced by ensuring that all the experimental trials are run in a random order. Moreover, the variation due to some factors can be eliminated, or much reduced, by dividing the design programme into sub-sets or blocks, each block comprising the experiments run on a given shift or using a particular batch of raw material. To reduce the biasing effect of other unidentified factors, the experiments are then randomly run within the block.

However, the control of different enviourmental conditions is not only the reason for wanting to block an experimental design. In attempting to explore the response pattern as an unknown function of several independent variables, an experimenter's strategy generates sequences of experiments that fall naturally into separate blocks. Suppose a third order rotatable design is split into two blocks such that each block is a complete second order rotatable design. Then for example, an experimenter's first step is usually to approximate the response function using a second order polynomial. If the second order polynomial is used for this purpose, the experimenter can determine whether the second order polynomial is adequate as a representation of the unknown function by noting any evidence of lack of fit. If second order polynomial is observed inadequate, the experimental design is then usually augmented by the second block to permit the estimation of the coefficients in a third order polynomial (47). Thus the experimental programme progresses sequentially, using blocks of experimental points, each block being separately appraised to provide information for the next step.

We shall discuss how the designs may be performed in orthogonal blocking arrangements. Let n_1 be the number of points in the first block and n_2 be the number of points in the second block. Let δ_1 be the effect of first block, δ_2 the effect of second block, and let $z_{wu} = 1$, if the uth observation occurs in the wth block, $w = 1,2$ and $z_{wu} = 0$ otherwise. On the usual assumption, that the effect of carrying out a particular trial in one block rather than another is merely to change the expected value of the response by a fixed amount which depends only on the particular blocks involved, such arrangements insure that the estimated coefficients of the polynomial are completely independent of the block differences and their standard errors depend on the within-block variance only. Then the expectation of the uth observation can be written

$$\eta_u = \beta_0 x_{0u} + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i\leq j=1}^{k} \beta_{ij} x_{iu}x_{ju} + \sum_{i\leq j\leq l=1}^{k} \beta_{ijl} x_{iu}x_{ju}x_{lu}$$

$$+ \sum_{w} \delta_w (z_{wu} - \bar{z}_w) \quad \ldots\ldots\ldots \quad (48)$$

in which $\bar{z}_w = \sum_{u=1}^{N} z_{wu} / N$ and $N = n_1 + n_2$.

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

$$\sum_u (z_{wu} - \bar{z}_w) = 0 \quad \ldots\ldots\ldots \quad (49)$$

$$\sum_u (z_{wu} - \bar{z}_w)\, x_{iu} = 0 \quad \ldots\ldots\ldots \quad (50)$$

$$\sum_u (z_{wu} - \bar{z}_w)\, x_{iu}x_{ju} = 0 \quad \ldots\ldots\ldots \quad (51)$$

$$\sum_u (z_{wu} - \bar{z}_w)\, x_{iu}x_{ju}x_{lu} = 0 \quad \ldots\ldots\ldots \quad (52)$$

for $w = 1,2$ and $i,j,l = 1,2,\ldots\ldots,k$. (49) is satisfied by the definition of $\bar{z}_w$ while (50), (51), and (52) are satisfied with one exception, by the fact that $(z_{wu} - \bar{z}_w)$ is constant within blocks and each block contains rotatable arrangement of points. The exception is in (51) when $i = j$. For this case if n_{10} = the number of points at the centre in the first block, and n_{20} = the number of points at the centre in the second block, (51) becomes

$$\sum_{u=1}^{n_1} x_{iu}^2 \Big/ \sum_{u=n_1+1}^{n_2} x_{iu}^2 = (n_1 + n_{10})/(n_2 + n_{20}) \quad \ldots\ldots\ldots \quad (53)$$

where the summations in the numerator and denominator is for those values of u in the first block and second block respectively.

Suppose a second degree polynomial is fitted with the help of block 1 having $(n_1 + n_{10})$ experimental points. In analysis of variance, the sum of squares of deviations from the fitted second degree polynomial contains two sources of variation, (i) experimental error, (ii) and "lack of fit". To test for the adequacy of the fitted polynomial, the estimate of experimental error is needed. Sometimes provision for an estimate of experimental error is available from previous experiments or can be obtained from repeated observations. To compare the mean square for "lack of fit", the estimate of experimental error mean square can be provided from repeated n_{10} observations at the centre of the design and is given by

$$1/\ (n_{10}-1) \quad \sum_{t=1}^{n_{10}} \left(y_{to} - \bar{y}_o \right)^2$$

where y_{to} is the tth repeated observation at the centre of the design and $\bar{y}_o$ is the mean of the observations at the centre.

Gardiner et al (1959) derived sequential third order rotatable designs upto four factors. No attempt was made by them to explore response surfaces with more than four factors, chiefly because the approach pursued required excessively large number of experimental points. We are presenting sequential third order rotatable designs upto eleven factors. Even with three and four factors, these designs contain small number of experimental points as compared to the designs of Gardiner et al (1959). We are also presenting a few non-sequential third order rotatable designs with considerably small number of experimental points.

Let $(x_1, x_2, \ldots, x_k)$ be a point set in k dimensions and let P_k be the symmetric group of order k, that is, the group with the elements of P_k, provided all the elements are nonzero and distinct. The point set $(x_1, x_2, \ldots\ldots, x_k)$

[illegible] point set in k dimensions with, say, r elements of a and (k − r) elements of b, with $1 \leqslant r < (k + 1)/2$. Then the symmetrical group P_k will give C_r^k point sets by operating upon $(a, a, \ldots\ldots, a, b, b, \ldots\ldots, b)$. The total number of points is $C_r^k \times 2^k$ when a and b are nonzero. Gardiner et al (1959) called this figure with $C_r^k \times 2^k$ points in k-dimentions as "truncated cube (r)". For example the "truncated cube (1)" in k dimensions is given by the following point sets:

$$
\begin{array}{l}
(a, a, \ldots\ldots, a, b), \\
(a, a, \ldots\ldots, b, a), \\
\vdots \\
(b, a, \ldots\ldots, a, a),
\end{array}
$$

where a occurs (k − 1) times and b occurs only once. The total number of points in "truncated cube (1)" is $k \times 2^k$. The well known k-dimensional octahedron, is the figure formed by 2k points, given by

$$
\begin{array}{l}
(\pm a, 0, \ldots\ldots, 0), \\
(0, \pm a, \ldots\ldots, 0), \\
\vdots \\
(0, 0, \ldots\ldots, \pm a).
\end{array}
$$

Non-sequential third order rotatable design in two factors:-

Gardiner et al (1959) discovered third order rotatable designs in two factors by locating seven or more experimental points on each of two or more concentric circles of different nonzero radii. A third order rotatable design is obtained in 16 points starting with point set $(a, \sqrt{2}\, a)$ which has unequally spaced points on a circle with radius $\sqrt{5}\, a$. This design contains

(i) 8 points of point set $(a, \sqrt{2}\, a)$ given by

$$(\pm a, \pm \sqrt{2}\, a),$$

and $(\pm \sqrt{2}\, a, \pm a)$,

(ii) 4 points of point set $(\sqrt{3.336568}\, a, 0)$ given by

$$(\pm \sqrt{3.336568}\, a, 0),$$

and $(0, \pm \sqrt{3.336568}\, a)$,

(iii) 4 points of point set $(\sqrt{1.693313}\, a, 0)$ given by

$$(\pm \sqrt{1.693313}\, a, 0),$$

and $(0, \pm \sqrt{1.693313}\, a)$.

The parameters λ_4 and λ_6 for this design are given below for various numbers of points added at the centre of the design. The values of a^2 are also given so as to satisfy the scaling convention $\sum_{u=1}^{N} x_{iu}^2 = N$, the total number of experimental points. Also given are the values of $4/6\ \lambda_4^2$, which in accordance with the relation (D_2) must always be exceeded by λ_6.

No. of centre-points added (1)	N, total No. of points. (2)	λ_4 (3)	λ_6 (4)	$\frac{4}{6}\lambda_4^2$ (5)	a^2 (6)
0	16	.5261	.1908	.1845	.7253024
1	17	.5589	.2154	.2083	.7706338
2	18	.5918	.2415	.2335	.8159652
4	20	.6576	.2981	.2883	.9066280
6	22	.7233	.3607	.3488	.9972908

This table provides a basis for the selection of a more useful design in the sense that with what differences the relations (D_1) and (D_2) are satisfied. For instance, if the relation (D_2) is very close to an equality, that is, the difference between columns (4) and (5) is very small, then the linear and cubic coefficients are very poorly estimated, (Gardiner et al (1959)).

Non-sequential third order rotatable design in three factors:-

A third order rotatable design in three factors may be formed from the points of the following point sets,

(i) 24 points of the point set $(a, a, \sqrt{0.127017}\,a)$ given by

$$(\pm a, \pm a, \pm\sqrt{0.127017}\,a),$$

$$(\pm a, \pm\sqrt{0.127017}\,a, \pm a),$$

and $$(\pm\sqrt{0.127017}\,a, \pm a, \pm a),$$

(ii) 6 points of the point set $(\sqrt{2.363435}\,a, 0, 0)$ given by

$$(\pm\sqrt{2.363435}\,a, 0, 0)$$

$(0 , 0, \pm \sqrt{2.363435}\ a),$

and $(0 , \pm \sqrt{2.363435}\ a, 0).$

(iii) 6 points of the point set $(\sqrt{1.182393}\ a, 0, 0)$ given by

$(\pm \sqrt{1.182393}\ a , 0 , 0),$

$(0 , \pm \sqrt{1.182393}\ a, 0),$

and $(0 , 0 , \pm \sqrt{1.182393}\ a).$

(i) is a "truncated cube (1)" while (ii) and (iii) are octahedra of different radii. The total number of points in the design is 36. The parameters λ_4 and λ_6 for this design are given below for various numbers of points added at the centre of the design. The values of a^2 are also given so that $\sum_{u=1}^{N} x_{iu}^2 = N$. Also given are the values of $5/7\ \lambda_4^2$, which, in accordance with the relation (D_2) must always be exceeded by λ_6.

No. of centre points added	N, the total number of points.	λ_4	λ_6	$\frac{5}{7}\lambda_4^2$	a^2
0	36	.6214	.2820	.2758	1.493293
1	37	.6387	.2979	.2914	1.534773
2	38	.6559	.3142	.3073	1.576254
3	39	.6732	.3309	.3237	1.617734
4	40	.6905	.3481	.3405	1.659215
6	42	.7250	.3838	.3754	1.742175
9	45	.7768	.4406	.4310	1.866616

Third order rotatable design in three factors (Sequential):-

The practically useful design is the one which can be performed sequentially. Consider the sequential design as being performed in two blocks, the first block permits the estimation of the coefficients in the second order rotatable design and forms a nucleus for the third order rotatable design. If the second order polynomial is inadequate then the set of points comprising the second block is added to the points of the first block and a third order polynomial is fitted.

To fit the design into sequential programming, we take the following two blocks where each block constitutes a second order rotatable design.

Block 1:

(i) 12 points of the point set ($\sqrt{2}$ a, $\sqrt{2}$ a, 0) given by

$$(\pm\sqrt{2}\, a , \pm\sqrt{2}\, a , 0),$$

$$(\pm\sqrt{2}\, a , 0 , \pm\sqrt{2}\, a),$$

and $(0 , \pm\sqrt{2}\, a , \pm\sqrt{2}\, a)$,

(ii) 6 points of the point set ($2^{\frac{3}{4}}$ a, 0 , 0) given by

$$(\pm 2^{\frac{3}{4}} a, 0 , 0),$$

$$(0 , \pm 2^{\frac{3}{4}} a , 0),$$

and $(0 , 0 , \pm 2^{\frac{3}{4}} a)$,

plus n_{10}, the requisite number of centre points.

Total number of points in block 1 = 18 + n_{10}.

Block 2:

(i) 8 points of the point set (a,a,a) given by

$(\pm a, \pm a, \pm a)$.

(ii) 8 points by replicating the above point set (i)

(iii) 6 points of the point set ($\sqrt{3.818662}$ a ,0 , 0) given by

$(\pm \sqrt{3.818662}\, a, 0, 0)$,

$(0, \pm \sqrt{3.818662}\, a, 0)$,

and $(0, 0, \pm \sqrt{3.818662}\, a)$,

(iv) 6 points of the point set ($\sqrt{1.190709}$ a, 0 , 0) given by

$(\pm \sqrt{1.190709}\, a, 0, 0)$,

$(0, \pm \sqrt{1.190709}\, a, 0)$,

and $(0, 0, \pm \sqrt{1.190709}\, a)$,

plus n_{20}, the requisite number of centre points.
Total number of points in block 2 = 28 + n_{20}.

The equation (53) which determines n_{10} and n_{20} for orthogonal blocking is

$$21.656856/26.018742 = (18 + n_{10})/(28 + n_{20})$$

Or $n_{10} = .8324\, n_{20} + 5.3060$ ....(54)

The number of centre points in blocks, n_{10} and n_{20}, so as to satisfy the equation (54) is shown below. The total number of points N and other design parameters are also given including the values of a^2 so as to satisfy $\sum x_{iu}^2 = N$. The number of non central points in the design is 18 + 28 = 46.

n_{10}	n_{20}	N	λ_4	λ_6	$\frac{5}{7}\lambda_4^2$	a^2
5	0	51	.7180	.3840	.3682	1.0697296
6	1	53	.7462	.4147	.3977	1.1116798
7	2	55	.7743	.4466	.4283	1.1536299
8	3	57	.8025	.4797	.4600	1.1955801
9	4	59	.8306	.5140	.4928	1.2375303

Sequential third order rotatable designs in four factors:-

With k = 4, four sequential third order rotatable designs have been obtained. These four designs have 72, 112, 72 and 120 noncentral experimental points respectively.

Design with 72 points:

A sequential third order rotatable design may be formed from the points of the following three point sets.

(1) $C_2^4 \times 2^2 = 24$ points of the point set $(\sqrt[3]{4}\, a, \sqrt[3]{4}\, a, 0, 0)$

(known as "truncated cube (2) ") given by

$(\pm \sqrt[3]{4}\, a , \pm \sqrt[3]{4}\, a , 0 , 0)$,

$(\pm \sqrt[3]{4}\, a , 0 , 0, \pm \sqrt[3]{4}\, a)$,

$(\pm \sqrt[3]{4}\, a , 0 , \pm \sqrt[3]{4}\, a , 0)$,

$(0, \pm \sqrt[3]{4}\, a , \pm \sqrt[3]{4}\, a , 0)$,

$(0 , \pm \sqrt[3]{4}\, a , 0 , \pm \sqrt[3]{4}\, a)$, and $(0 , 0 , \pm \sqrt[3]{4}\, a , \pm \sqrt[3]{4}\, a)$,

(ii) 32 points of doubly replicated point set (a , a , a , a) (i.e. a cube) given by $(\pm a, \pm a, \pm a, \pm a)$.

(iii) 16 points of doubly replicated point set $(2 a, 0, 0, 0)$ (i.e. a octahedron) given by

$(\pm 2 a , 0 , 0 , 0)$,

$(0 , \pm 2 a , 0 , 0)$,

$(0, 0, \pm 2 a , 0)$,

and $(0, 0 , 0, \pm 2 a)$.

By double replication of a point set, we mean twice an observation being made at each point of that point set. For sequential programming, the first block consists of a set of points of point set (i), plus n_{10} the requisite number of centre points, while the second block consists of a set of points of point sets (ii) and (iii), plus n_{20} the requisite number of centre points. The total number of points in the first block and second block are $24 + n_{10}$ and $48 + n_{20}$.

The equation (53) for orthogonal blocking to determine n_{10} and n_{20}, is given by

$$30.2301052 / 48 = (24 + n_{10}) / (48 + n_{20})$$

Or $$n_{10} = .6299\, n_{20} + 6.2381 \qquad \text{.........} (55)$$

Given below are the values of the parameters λ_4 , λ_6 and n_{10} , n_{20} to satisfy the equation (55). Also given are the values of a^2 so that $\sum x_{iu}^2 = N$, the total number of points.

n_{10}	n_{20}	N	λ_4	λ_6	$\frac{6}{8}\lambda_4^2$	a^2
6	0	78	.7314	.4065	.4012	0.9969567
7	1	80	.7502	.4276	.4220	1.0225190
8	3	83	.7783	.4603	.4543	1.0608691
10	6	88	.8252	.5174	.5107	1.1247716

Designs with 112, 72, and 120 points:

It was intended to present third order rotatable design in four factors starting with the point set (a,a,a,b), known as "truncated cube (1)". It has been found that the following point sets may form an infinite series of third order rotatable designs.

(i) $C_1^4 \times 2^4 = 64$ points of the point set (a,a,a,b) given by

(± a , ± a , ± a , ± b),

(± a , ± a , ± b , ± a),

(± a , ± b , ± a , ± a),

and (± b , ± a , ± a , ± a),

(ii) $C_2^4 \times 2^2 = 24$ points of the point set (c,c,0,0),

(iii) 8 points of the point set (d , 0 , 0 , 0),

(iv) 8 points of the point set (e , 0 , 0 , 0),

(v) 8 points of the point set (f , 0 , 0 , 0),

(vi) 8 points of the point set (g , 0 , 0 , 0).

The generation of points for the above point sets has been illustrated in the previous design as well as in the introduction of this chapter. The values of a , b , c , d, e , f and g are to be chosen so as to satisfy the relations (A), (B), (C), and (D). The relations (B), (C_1), and (C_2) give the following three equations.

$$48 a^4 + 16 b^4 + 12 c^4 + 2 (d^4 + e^4 + f^4 + g^4) = 3 (32 a^2 b^2 + 32 a^4 + 4 c^4) \quad \ldots\ldots\ldots (56)$$

$$48 a^6 + 16 b^6 + 12 c^6 + 2 (d^6 + e^6 + f^6 + g^6) = 5 (16 a^4 b^2 + 16 a^2 b^4 + 32 a^6 + 4 c^6) \quad \ldots\ldots(57)$$

$$16 a^4 b^2 + 16 a^2 b^4 + 32 a^6 + 4 c^6 = 3 (48 a^4 b^2 + 16 a^6) \quad \ldots\ldots(58)$$

Put $b^2 = p a^2$, $c^2 = q a^2$, $d^2 = u a^2$, $e^2 = v a^2$, $f^2 = s a^2$, and $g^2 = t a^2$, then the above three equations (56), (57), and (58) reduce to

$$u^2 + v^2 + s^2 + t^2 = 24 + 48 p - 8 p^2 \quad \ldots\ldots\ldots (59)$$

$$8 q^3 - 2 (u^3 + v^3 + s^3 + t^3) = 16 p^3 - 80 (p + p^2) - 112 \quad \ldots\ldots (60)$$

$$q^3 = 4 + 32 p - 4 p^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots (61)$$

By substituting the values of q^3, from (61), in (6), we get two equations in terms of p,u,v,s and t, namely,

$$u^2 + v^2 + s^2 + t^2 = 24 + 48\,p - 8\,p^2 \qquad \ldots\ldots(62)$$

$$u^3 + v^3 + s^3 + t^3 = 72 + 168\,p + 24\,p^2 - 8\,p^3 \qquad \ldots\ldots(63)$$

By assigning a specified positive value to p, the value of q can be obtained from (61) while the values of u,v,s, and t are to be got from (62) and (63). Assign that specified value to p, which brings positive solutions for q , u , v , s , and t. The purpose of taking last four point sets (iii), (iv), (v), and (vi) (octahedra) is to get positive solutions for u, v , s , and t. Take minimum number of such point sets which can supply positive solution for u, v, s, and t. For instance, let p = 0, then the equations (61), (62) and (63) reduce to

$$q^3 = 4 \qquad \ldots\ldots(64)$$

$$u^2 + v^2 + s^2 + t^2 = 24 \qquad \ldots\ldots(65)$$

$$u^3 + v^3 + s^3 + t^3 = 72 \qquad \ldots\ldots(66)$$

It can be seen that by taking only two point sets (d,0,0,0) and (c, 0, 0, 0), the positive solutions for u and v is not possible. But by adding the points of the point set (f,0,0,0), it is possible to get the positive solutions for u,v, and s. The solutions for q,u,v, and s are

$$q^3 = 4$$

$$u = 2$$

$$v = 3.4324565$$

$$s = 2.8667477$$

and obviously $t = 0$

Thus, the resultant design in 112 noncentral experimental points can be fitted into sequential programming by taking a set of points of point set (ii), plus n_{10} the requisite number of centre points in the first block. The second block consists of points obtained from the point sets (i), (iii), (iv), and (v), plus n_{20} the requisite number of centre points. The total number of points in the first block and the second block are $24 + n_{10}$ and $88 + n_{20}$ respectively.

The equation (53) which expresses the orthogonal blocking is

$$19.0488132 / 64.5984084 = (24 + n_{10}) / (88 + n_{20})$$

Or $n_{10} = .2948\, n_{20} + 1.9494$ ....(67)

The values of n_{10}, n_{20}, λ_6, λ_4 and $6/8\ \lambda_4^2$ are given below. Also given are the values of a^2 so as to satisfy $\Sigma\, x_{iu}^2 = N$, the total number of points.

n_{10}	n_{20}	N	λ_4	λ_6	$\frac{6}{8}\lambda_4^2$	a^2
2	0	114	.6856	.3553	.3525	1.362866
2	1	115	.6916	.3615	.3587	1.374821
3	4	119	.7157	.3871	.3841	1.422641

In the above design with 112 points, we noticed that the points of the point set (a,a,a,0) is doubly replicated. Of course, it is possible to derive design with single replication of the point set (a,a,a,0) having 32 points, in conjuction with point sets (ii), (iii), and (iv). The solutions for q, u, and v are

$$q^3 = 2$$

$$u = 3.247411$$

$$v = 1.205952$$

and obviously $s = 0$, $t = 0$.

The resultant design contains 72 non-central points.

Another design is obtained in 120 points by putting $p = 1$, in (61), (62), and (63). The resultant three equations are

$$q^3 = 32$$

$$u^2 + v^2 + s^2 + t^2 = 64$$

$$u^3 + v^3 + s^3 + t^3 = 256$$

The solutions for u , v , s and t are

$$u = v = s = t = 4.$$

For two stages of experimentation, the first block consists of the points of point set (ii) plus n_{10}, the requisite number of centre points and the second block comprises of points of point set (i) and quadruplicated point set (2 a,0,0,0) plus n_{20}, the requisite number of centre points. The point set (i) is nothing but a quadruplicated point set (a,a,a,a),(i.e. a cube). The total number of points in the first block and second block are $24 + n_{10}$ and $96 + n_{20}$ respectively.

The equation (53) which expresses the orthogonal blocking is point sets (ii), (iii), and (iv). The solutions for q, u, and v are

$$q^3 = 2$$
$$u = 3.247411$$
$$v = 1.205952$$

and obviously $s = 0, \quad t = 0$.

The resultant design contains 72 non-central points.

Another design is obtained in 120 points by putting p = 1, in (61), (62), and (63). The resultant three equations are

$$q^3 = 32$$
$$u^2 + v^2 + s^2 + t^2 = 64$$
$$u^3 + v^3 + s^3 + t^3 = 256$$

The solutions for u, v, s and t are

$$u = v = s = t = 4.$$

For two stages of experimentation, the first block consists of the points of point set (ii) plus n_{10}, the requisite number of centre points and the second block comprises of points of point set (i) and quadruplicated point set (2 a,0,0,0) plus n_{20}, the requisite number of centre points. The point set (i) is nothing but a quadruplicated point set (a,a,a,a),(i.e. a cube). The total number of points in the first block and second block are $24 + n_{10}$ and $96 + n_{20}$ respectively.

The equation (53) which expresses the orthogonal blocking is

$$38.097624 / 96 = (24 + n_{10}) / (96 + n_{20})$$

Or $n_{20} = 2.5198\ n_{10} - 35.5238$ .... (68)

Below are given the values of n_{10}, n_{20}, λ_4, λ_6, $6/8\ \lambda_4^2$ and a^2 so that $\sum x_{in}^2 = N$.

n_{10}	n_{20}	N	λ_4	λ_6	$\frac{6}{8}\lambda_4^2$	a^2
14	0	134	.7774	.4766	.4532	0.9992720
15	2	137	.7948	.4918	.4737	1.0216437
16	5	141	.8179	.5552	.5018	1.0514728
17	7	144	.8354	.5503	.5233	1.0738445

Sequential third order rotatable design in five factors:-

A third order rotatable design in five factors may be performed sequentially in the following two blocks.

Block 1.

(i) 32 points of the point set (a,a,a,a,a) given by

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

(ii) 10 points of the point set $(2^{5/4} a, 0, 0, 0, 0)$ given by

$(\pm 2^{5/4} a, 0, 0, 0, 0)$,

$(0, \pm 2^{5/4} a, 0, 0, 0),$

$(0, 0, \pm 2^{5/4} a, 0, 0),$

$(0, 0, 0, \pm 2^{5/4} a, 0),$

and $(0, 0, 0, 0, \pm 2^{5/4} a).$

Plus n_{10} the requisite number of centre points. The total number of points in block 1 = $42 + n_{10}$.

Block 2.

(i) $C_3^5 \times 2^3 = 80$ points of the point set $(2^{\frac{1}{2}}a, 2^{\frac{1}{2}}a, 2^{\frac{1}{2}}a, 0, 0)$ given by

$(\pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, 0, 0),$

$(\pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, 0, \pm 2^{\frac{1}{2}}a, 0),$

$(\pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, 0, 0, \pm 2^{\frac{1}{2}}a),$

$(\pm 2^{\frac{1}{2}}a, 0, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, 0),$

$(\pm 2^{\frac{1}{2}}a, 0, \pm 2^{\frac{1}{2}}a, 0, \pm 2^{\frac{1}{2}}a),$

$(\pm 2^{\frac{1}{2}}a, 0, 0, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a),$

$(0, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, 0),$

$(0, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, 0, \pm 2^{\frac{1}{2}}a),$

$(0, \pm 2^{\frac{1}{2}}a, 0, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a),$

and $(0, 0, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a, \pm 2^{\frac{1}{2}}a).$

(ii) $C_2^5 \times 2^2 = 40$ points of the point set $(2^{2/3} a, 2^{2/3} a, 0, 0, 0)$, developable as described above,

(iii) 10 points of the point set $(\sqrt{5.8693939}\, a,0,0,0,0)$, developable as described in point set (ii) of block 1

(iv) 10 points of the point set $(\sqrt{.9225051}\, a,0,0,0,0)$, plus n_{20}, the requisite number of centre points.

The total number of points in the block 2 = $140 + n_{20}$.

The resultant design contains 182 non-central experimental points while the values of n_{10} and n_{20} are to be chosen so as to satisfy the condition for orthogonal blocking (52). Again, the scaling factor a, is chosen so that $\sum x_{iu}^2 = N$.

<u>Sequential third order rotatable design in six factors:-</u>

A sequential third order rotatable design in six factors consists in performing experiments in the following two blocks.

Block 1.

(i) 64 points of the point set (a,a,a,a,a,a)

(ii) 12 points of the point set $(2 \times 2^{\frac{1}{4}} a, 0,0,0,0,0)$, plus n_{10}, the requisite number of centre points.

The total number of points in block 1 = $76 + n_{10}$.

Block 2.

(i) $C_3^6 \times 2^3 = 160$ points of the point set $(4^{1/3} a, 4^{1/3} a, 4^{1/3} a, 0,0,0)$ (i.e. known as "truncated cube(3)"),

(ii) 24 points of the doubly replicated point set

$$(2^{\frac{1}{2}}a,0,0,0,0,0,0)$$

plus n_{20}, the requisite number of centre points.

The total number of points in block 2 = 184 + n_{20}.

The resultant design contains 260 non-central points and the values of n_{10}, n_{20} are to be determined from the orthogonal blocking condition (53). The value of a, the scaling factor, is chosen so that $\sum x_{iu}^2 = N$, the total number of experimental points.

To reduce the size of the experiment, a suitable fractional replicate can replace the full factorial. Considerable savings were demonstrated by Box and Hunter (1957) in the case of second order rotatable designs by the use of fractional replication for $k > 4$. Since with $k > 4$, the main effects and two factor interactions are confounded only with third or higher order effects when fractional replication is used. But for a third order rotatable design, we must have atleast seven factors, to make use of fractional replication. Since with $k > 7$, the effects upto order three are confounded only with fourth or higher order effects. The half replicate of point set (a,a,...,a) in k factors is the half replicate of the 2^k design with levels + a and - a. We will use the usual factorial notation $\frac{1}{2}\, 2^k$ to denote the half replicate of a point set (a,a,.......,a) which confounds effects upto order three with fourth or higher order effects.

Sequential third order rotatable design in seven factors:-

A sequential third order rotatable design in seven factors may be performed in two stages of experimentation by taking the following two blocks.

Block 1.

(i) $\frac{1}{2}\, 2^7 = 64$ points of the half replicated point set (a, a, a, a, a, a, a),

(ii) 14 points of the point set $(\sqrt{7.542072}\, a, 0, 0, 0, 0, 0, 0)$,

(iii) 14 points of the point set $(\sqrt{2.667288}\, a, 0, 0, 0, 0, 0, 0)$,

plus n_{10}, the requisite number of centre points.

The total number of points in the block 1 = 92 + n_{10}.

Block 2.

(i) $C_3^7 \times 2^3 = 280$ points of the point set $(2^{\frac{1}{2}} a, 2^{\frac{1}{2}} a, 2^{\frac{1}{2}} a, 0, 0, 0, 0)$, known as "truncated cube (4)"),

plus n_{20}, the requisite number of centre points.

The total number of points in block 2 = 280 + n_{20}.

The resultant design contains 372 non-central points and the values of n_{10}, n_{20} are to be determined so as to satisfy the condition of orthogonal blocking (53). Chose a, the scaling factor so that $\Sigma x_{iu}^2 = N$.

Sequential third order rotatable design in seven or more factors:-

Of greater interest are those point sets which may form sequential third order rotatable designs in seven factors and may be extended to more than seven factors. In doing so, it was found that the following point sets constitute sequential third order rotatable designs upto eleven factors.

(i) $\frac{1}{2}2^k = 2^{k-1}$ points of the half replicated point set $(a, a, \ldots\ldots\ldots, a)$,

(ii) $\frac{1}{2}2^k = 2^{k-1}$ points of the half replicated point set $(b, b, \ldots\ldots\ldots, b)$

(iii) $C_3^k \times 2^3$ = points of the point set $(c, c, c, 0, 0, \ldots, 0)$, where c occurs 3 times and zero occurs $(k-3)$ times,

(iv) 2 k points of the point set $(d, 0, 0, \ldots\ldots, 0)$,

(v) 2 k points of the point set $(e, 0, 0, \ldots\ldots, 0)$,

(vi) 2 k points of the point set $(f, 0, 0, \ldots\ldots, 0)$,

(vii) 2 k points of the point set $(2^{(k-1)/4} a, 0, 0, \ldots\ldots, 0)$.

For a design to be performed sequentially, the first block consists of a set of points of the point sets (i) and (vii) while the second blocks contains a set of points of the point sets (ii), (iii), (iv), (v), and (vi).

The moments of the design upto order six are given below.

$$\Sigma x_i^2 = 2^{k-1}(a^2 + b^2) + 2(2^{(k-1)/2} a^2 + d^2 + e^2 + f^2) + C_2^{k-1} \times 2^3 c^2$$

$$\Sigma x_i^4 = 2^{k-1}(a^4 + b^4) + 2(2^{k-1} a^4 + d^4 + e^4 + f^4) + C_2^{k-1} \times 2^3 c^4$$

$$\Sigma x_i^2 x_j^2 = 2^{k-1}(a^4 + b^4) + (k-2)\; 2^3 c^4$$

$$\sum x_i^6 = 2^{k-1}(a^6+b^6) + 2(2^{3(k-1)/2}a^6 + d^6 + e^6 + f^6) + C_2^{k-1}\, 2^3 c^6$$

$$\sum x_i^2 x_j^4 = 2^{k-1}(a^6+b^6) + (k-2)\, 2^3 c^6$$

$$\sum x_i^2 x_j^2 x_k^2 = 2^{k-1}(a^6+b^6) + 2^3 c^6$$

and all other sums of powers and products upto and including order six are zero. The values of a, b, c, d, e, and f are so chosen that the relationships (A), (B), (C), and (D) are satisfied.

The relationships (B), (C_1), and (C_2) give

$$2^{k-1}(a^4+b^4) + 2(2^{k-1}a^4 + d^4 + e^4 + f^4) + C_2^{k-1}\, 2^3 c^4$$
$$= 3\left[2^{k-1}(a^4+b^4) + (k-2)\, 2^3 c^4\right] \quad \ldots\ldots\ldots\ldots(69)$$

$$\text{or } (d^4+e^4+f^4) = 2^{k-1}b^4 + 2(k-2)(7-k)c^4 \quad \ldots(69)$$

$$2^{k-1}(a^6+b^6) + 2(2^{3(k-1)/2}a^6 + d^6 + e^6 + f^6) + C_2^{k-1}\, 2^3 c^6$$
$$= 5\left[2^{k-1}(a^6+b^6) + (k-2)\, 2^3 c^6\right] \quad \ldots\ldots\ldots\ldots(70)$$

$$\text{and } 2^{k-1}(a^6+b^6) + (k-2)\, 2^3 c^6 = 3\left[2^{k-1}(a^6+b^6) + 2^3 c^6\right]$$

$$\text{or } c^6 = 2^{k-3}(a^6+b^6)/(k-5) \quad \ldots\ldots\ (71)$$

Substituting the value of c^6 from (71) in (70) and after simplyfing, we have

$$d^6 + e^6 + f^6 = 2^{k-1} \left[2 (a^6 + b^6) + (a^6 + b^6)/(k-5) \left\{ 5(k-2) - (k-1)(k-2)/2 \right\} - 2^{(k-1)/2} a^6 \right] \quad \ldots\ldots(72)$$

Let $b^2 = p\, a^2$, $c^2 = q\, a^2$, $d^2 = u\, a^2$, $e^2 = v\, a^2$, and $f^2 = s\, a^2$, then the equations (69), (72) and (71) reduce to

$$u^2 + v^2 + s^2 = 2^{k-1} p^2 + 2 (k-2)(7-k)\, q^2 \quad \ldots\ldots (73)$$

$$u^3 + v^3 + s^3 = 2^{k-1} \left[2 (1 + p^3) + (1+p^3)/(k-5) \left\{ 5 (k-2) - (k-1)(k-2)/2 \right\} - 2^{(k-1)/2} \right] \quad \ldots.(74)$$

and $$q^3 = 2^{k-3} (1 + p^3)/(k-5) \quad \ldots\ldots\ldots\ldots (75)$$

For a sequential third order rotatable design in k factors, the positive solutions for p,q,u,v, and s are so chosen that the three equations (73), (74), and (75) are satisfied. Again the scaling factor, a , is chosen so that $\sum x_{iu}^2 = N$, the total number of experimental points.

<u>An infinite series of sequential third order rotatable designs in seven factors:-</u>

With k = 7 , an infinite series of sequential third order rotatable designs has been obtained. Putting k = 7 in (73), (74), and (75), we get

$$u^2 + v^2 + s^2 = 2^6 p^2 \quad \ldots\ldots (76)$$

$$u^3 + v^3 + s^3 = 2^6 \left[7 (1+p^3) - 8 \right] \quad \ldots.(77)$$

and $q^3 = 2^4 (1 + p^3) /2 = 8 (1 + p^3)$ ..... (78)

The purpose of taking three point sets of the type (a' , 0 , 0 ....,0),(i.e. octohedra), in the second block is to get positive solutions for u,v, and s for positive values of p and q. We put s = 0, since it is possible to achieve positive solutions for u and v for positive values of p and q. By putting s = 0, (76), (77) give

$$u^2 + v^2 = 2^6 p^2 \qquad = A \text{ (say)} \qquad .... (79)$$

$$u^3 + v^3 = 2^6 \left\{ 7 (1+ p^3) - 8 \right\} \qquad = B \text{ (say)} ...(80)$$

Where A and B have positive values.

According to Das (1960), the positive solutions for u and v are possible if

$$A^3/2 \leqslant B^2 \leqslant A^3$$

$$\text{Or } 2^{12} \times 32 p^6 \leqslant 2^{12}(49 p^6 - 14 p^3 + 1) \leqslant 2^{12} \times 64 p^6$$

$$\text{or } 0 \leqslant 2^{12} (17 p^6 - 14 p^3 + 1) \leqslant 2^{12} \times 32 p^6 \quad ... (81)$$

There will be infinite values of p which will be satisfying the condition (81) and for each such value of p, we will get a rotatable design. For instance, the values of p^3 which satisfy the left hand equality of (81) are given by

$$17 p^6 - 14 p^3 + 1 = 0$$

$$\text{or } p^3 = (7 \pm 32^{\frac{1}{2}})/ 17$$

For $p^3 = (7 + 32^{\frac{1}{2}})/17$, the solutions for u and v are same and are given by

$u = v = 5.127048.$

The resultant design contains 450 non-central experimental points with the values of p,q,u,v, and s given by

$$p^3 = (7 + 32^{\frac{1}{2}})/17$$

$$q^3 = (24 + 32^{\frac{1}{2}}) 8 / 17$$

$$u = v = 5.127048 \quad \text{and} \quad s = 0.$$

For $p^3 = (7 - 32^{\frac{1}{2}}) / 17$, we get negative value of B in (80) and thus the positive solutions for u and v can not be obtained.

Sequential third order rotatable designs from eight to eleven factors:-

It is now evident that the derivation of sequential third order rotatable designs in more than seven factors can be sought by assigning the positive specified values to p,q,u,v, and s, so that the equations (73), (74), and (75) are satisfied. Below is given the table: 4, showing the values of p^3, q^3, u, v, and s, for k = 8,9,10, and 11. Also given are the total number of points in each block and the resultant design. The values of n_{10} and n_{20} are to be determined so as to satisfy the condition for orthogonal blocking (53). The designs presented are not exhaustive but they are simply illustrative.

Table No. 4: The values of p^3, q^3, u, v and s for k = 8,9,10,11

Number of factors k	The number of experimental points in block 1.	The number of experimental points in block 2.	Total number of experimental points N	p^3	q^3	u	v	s
8	$144 + n_{10}$	$608 + n_{20}$	$752 + n_{10}+n_{20}$	8	96	15.0050688	5.9377388	0
9	$274 + n_{10}$	$964 + n_{20}$	$1238 + n_{10}+n_{20}$	5	96	11.4266036	5.6619408	0
10	$532 + n_{10}$	$1512 + n_{20}$	$2044 + n_{10}+n_{20}$	12	$2^7 \times 2.6$	19.1371124	3.6032760	0
11	$1046 + n_{10}$	$2410 + n_{20}$	$3456 + n_{10}+n_{20}$	27	$\frac{2^{10} \times 7}{3}$	24.1828710	11.5089848	18.8000000

S U M M A R Y

Of major importance to statistical designs of experiments involving quantitative variables or factors is the detection and description of the functional relationship between two or more variables - the relationship such as exists between yield or response on one hand and the levels of different quantitative variables on the other. An empirical investigation of such a relationship requires in taking observations at predetermined levels of the controllable variables, i.e. an experimental design must be selected prior to experimentation.

An attempt has been made first to study such response surfaces from the data collected on the usual factorial experiments in agriculture. A method has been evolved for fitting a second order (i.e. a quadratic) surface by expressing the different coefficients involved in this surface as functions of main effects and two factor interactions using data from complete, confounded, and fractionally replicated designs of 3^k series. The approach adopted is quite general but for clarity and appreciation, the discussion has been restricted to designs of 3^k series. A numerical example for a 3^2 factorial is also given.

Box and Hunter (1957) advanced the criterion of "rotatibility" to experimental designs for fitting response surfaces. Such designs permit a response surface to be fitted easily and provide spherical information contours. A second

order rotatable design aids the fitting of second order (i.e. a quadratic) surface. Draper (1960) obtained infinite series of second order rotatable designs in four or more factors. These designs contain excessively large number of experimental points. It has been possible, through the present investigation to obtain infinite series of second order rotatable designs in four, five, six, and seven factors with considerably small number of experimental points. A general method for obtaining such designs for any even number of factors has also been indicated.

Gardiner et al (1959) extended the criterion of rotatibility to experimental design for fitting a third order (i.e. a cubic) surface. They derived sequential third order rotatable designs upto four factors. No attempt was made by them to obtain designs in five and six factors, chiefly because the approach pursued required excessively large number of experimental points. It has been possible, through the present investigation, to obtain sequential third order rotatable designs upto eleven factors. These designs possess the desirable property of having small number of experimental points. Non-sequential third order rotatable designs in two and three factors are also derived.

R E F E R E N C E S

1. Bose, R.C., and Draper, Norman. R. (1959) Second order rotatable designs in three dimensions, Ann. Math. Stat. Vol.30

2. Box, G.E.P. (1952) Multi-factor designs of first order, Biometrika Vol. 39.

3. Box, G.E.P. (1954) The exploration and exploitation of response surfaces: Some general considerations and examples, Biometrics Vol.10.

4. Box, G.E.P., and Hunter, J.S. (1954) A confidence region for the solution of a set of simultaneous equations with an application to experimental design, Biometrika Vol.41.

5. Box, G.E.P., and Hunter, J.S. (1957) Multi-factor experimental designs for exploring response surfaces, Ann. Math.Stat Vol. 28.

6. Box, G.E.P., and Wilson, K.B. (1951) On the experimental attainment of optimum conditions, Jour. Roy. Stat. Soc. (B) Vol.13.

7. Box, G.E.P., and Youle, P.V. (1955) The exploration and exploitation of response surfaces: An example of the link between the fitted surface and the basic mechanism of the system, Biometrics Vol. 11.

8. Box, G.E.P., and Draper, Norman.R. (1959) A basis for the selection of a response surface design, Jour. Amer. Stat. Asso. Vol. 54

9.	Cochran, W.G., and Cox, G.M.	(1957)	Experimental Designs, John Wiley and Sons, New York.
10.	Das, M.N.	(1960)	Construction of rotatable designs from factorial designs (Unpublished).
11.	Davies, O.L.	(1956)	The Design and Analysis of Industrial Experiments, Hafner Publishing Co., New York.
12.	Draper, Norman.R.	(1960)	Second order rotatable designs in four or more dimensions, Ann. Math. Stat. Vol. 31.
13.	Folks, John Leroy.	(1959)	Comparision of designs for exploration of response relationships, Jour. Amer. Stat. Asso. Vol. 54.
14.	Gardiner, D.A., Grandage, A.H.E., and Hader, R.J.	(1959)	Third order rotatable designs for exploring response surfaces, Ann. Math. Stat. vol. 30
15.	Hartley, H.O.	(1959)	Smallest composite designs for quadratic response surfaces, Biometrics Vol.15.
16.	Plackett, R.L.	(1951)	Discussion to the paper "On the experimental attainment of optimum conditions", by Box and Wilson, Jour. Roy. Stat. Soc. (B) Vol.13.
17.	Plackett, R.L., and Burman, J.P.	(1946)	The design of multifactorial experiments, Biometrika Vol. 33.

18. Yates, F. (1937) The design and analysis of factorial experiments. Tech. Communication No. 35, Imperial Bureau of Soil Sci., Harpenden, England.

19. (1959) Fourth Annual Report. Studies on the green manuring of crops - Mysore, Agricultural Research Station, Mandya. Indian Council of Agricultural Research.