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DESIGNS FOR FITTING RESPONSE SURFACES IN AGRICULTURAL EXPERIMENTS

Rajender Parsad
R.Srivastava
and
P.K.Batra

INDIAN AGRICULTURAL STATISTICS RESEARCH INSTITUTE (ICAR)
LIBRARY AVENUE: NEW DELHI – 110 012
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PREFACE

Response surface methodology is used (i) to determine and to quantify the relationship between the response and the levels of quantitative factors and (ii) to obtain optimum combinations of levels of various quantitative factors. To meet these objectives, the data from the experiments involving quantitative factors can be utilized for fitting the response surfaces over the region of interest. Response surfaces besides inferring on the twin purposes can also provide information on the rate of change of the response variable and can help in studying the interactions between quantitative factors.

Response surface methodology has been extensively used in industrial experimentation but appear to be not so popular in experiments pertaining to agricultural, horticultural and allied sciences. This may be due to the fact that the experimental situations in agricultural sciences are different from those in industrial experiments. Broadly five distinctions *viz.* (i) time and factor range (ii) factor levels (iii) blocking (iv) accuracy of observations' (v) shape of response surface are identified.

Considering all these points, it may be desirable that the agricultural experiments should be more robust, less model dependent, should accommodate more flexible system of blocking and should have equispaced factor levels in more combinations in comparison to industrial experiments.

Keeping in view the importance and relevance of response surface methodology in agricultural research this study entitled *Designs for fitting Response Surfaces in Agricultural Experiments* was undertaken to develop response surface designs both for response optimization and slope estimation when factors are with equispaced levels and to prepare their catalogue. It also aimed at obtaining response surface designs for qualititative-cum-quantitave factors, to study the robustness aspects of response surface designs against single missing observation and to develop a computer software for the analysis of designs obtained and catalogued.

In this investigation, response surface designs for both symmetric and asymmetric factorial experiments when the factors are at equispaced doses have been obtained both for response optimization and slope estimation. A new criterion in terms of second order moments and mixed fourth order moments is also introduced. This criterion helps in minimizing the variance of the estimated response to a reasonable extent. The response surface designs developed for qualitative-cum-quantitative experiments can be used to take into account the effect that the various levels of qualitative factors have on the relationship of quantitative factors with response. The designs obtained for slope estimation may be useful for obtaining reliable yardsticks of various inputs. These designs can also be used to estimate the rate of change of biological populations, rate of change of chemical reactions, etc. Catalogues of designs with number of factors (v) and number of design points (N) satisfying $3 \le v \le 10$ and $N \le 500$ have been prepared for the benefit of the users. The catalogue of second order rotatable designs with orthogonal blocking is quite useful for the agricultural experiments that require control of variability in the experimental units. The computer software "Response" developed and codes written using Statistical Analysis System (SAS) and Statistical Package for Social Sciences (SPSS) will be quite useful for fitting of response surfaces in agricultural experiments. The results would also be useful to the practicing statisticians in various ICAR institutes and State Agricultural Universities who are engaged in advisory services in the form of suggesting appropriate designs to the experimenters.

One of the significant features of the study is that some of the designs obtained during the present investigation have actually been used in the National Agricultural Research System. The experimental situations along with the designs used are also given for the benefit of the users. The results would also be immensely useful to the students and scientists engaged in carrying out research and teaching in the experimental designs.

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Rajender Parsad
R.Srivastava
and
P.K.Batra

CONTENTS

I	**Introduction**		**1 - 6**
	1.1	Introduction	1
	1.2	Objectives	6
	1.3	Practical/ Scientific Utility	6
II	**Response Surface Methodology**		**7 - 33**
	2.1	Introduction	7
	2.2	The Quadratic Response Surface	8
	2.3	Determining the Co-ordinates of the Stationary Point of a Quadratic Response Surface	11
	2.4	The Canonical Equation of a Second Order Response System	12
	2.5	Exploration of the Response Surface in the Vicinity of Stationary Point	13
	2.6	Ridge Analysis	16
	2.7	Response Surface Models without Intercept Term	16
	2.8	Development of Computer Software	20
	2.9	Empirical Illustrations	24
III	**Response Surface Designs**		**34 –104**
	3.1	Introduction	34
	3.2	First Order Response Surface Designs	37
	3.3	Second Order Response Surface Designs for Response Optimization	40
	3.4	Designs for Slope Estimation	78
	3.5	Blocking in Second Order Response Surface Designs	86
IV	**Robustness Against One Missing Observation**		**105 - 123**
	4.1	Introduction	105
	4.2	Robustness of Response Surface Designs against Single Missing Observation	107
	4.3	Robustness of Modified and/or Rotatable Second Order Response Surface Designs	110
V	**Response Surface Designs for Qualitative Cum Quantitative Factors**		**124 - 139**
	5.1	Introduction	124
	5.2	Inclusion of Terms Involving Qualitative Factor in the Model	126
	5.3	Designs Considerations in First Order Response Surfaces	127
	5.4	Designs for Fitting Second Order Response Surfaces	128
VI	**Extension of Research Findings**		**140 - 141**
	SUMMARY		**142 – 144**
	REFERENCES		**145 - 148**

CHAPTER I

INTRODUCTION

1.1. Introduction

The subject of Design of Experiments deals with the statistical methodology required for making inferences about the treatments effects on the basis of responses (univariate or multivariate) collected through the planned experiments. To deal with the evolution and analysis of methods for probing into mechanism of a system of variables, the experiments involving several factors simultaneously are being conducted in agricultural, horticultural and allied sciences. Data from experiments with levels or level combinations of one or more factors as treatments are normally investigated to compare level effects of the factors and also their interactions. Though such investigations are useful to have objective assessment of the effects of the levels actually tried in the experiment, this seems to be inadequate, especially when the factors are quantitative in nature and cannot throw much light on the possible effect(s) of the intervening levels or their combinations. In such situations, it is more realistic and informative to carry out investigations with twin purposes:

a) To determine and to quantify the relationship between the response and the settings of experimental factors.
b) To find the settings of the experimental factor(s) that produces the best value or the best set of values of the response(s).

If all the factors are quantitative in nature, it is natural to think the response as a function of the factor levels and data from quantitative factorial experiments can be used to fit the response surface over the region of interest. Response surfaces besides inferring about the twin purposes as mentioned above also provide information about the rate of change of a response variable. They can also indicate the interactions between the quantitative treatment factors. The special class of designed experiments for fitting response surfaces is called response surface designs. A good response surface design should possess the properties *viz.* detectability of lack of fit, the ability to sequentially build up designs of increasing order and the use of a relatively modest, if not minimum, number of design points.

Designed experiments for fitting response surfaces are used extensively in industrial experimentation but appear to be not so popular in research areas in agricultural and horticultural sciences. Response surface methodology and associated design theory were developed in an industrial context and limitations and opportunities of industrial experimentation are so different from those in agricultural experimentation that the designs appropriate in one area appear to be inappropriate in the other. The books by Box and Draper (1987), Myers and Montgomery (1995) and Khuri and Cornell (1996) discuss the aspects of experimental designs with emphasis on the industrial context. Two excellent reviews on the topic are by Hill and Hunter (1966) and Myers, Khuri and Carter (1989). Several concepts *viz*. rotatability, partial rotatability, slope rotatability, orthogonal blocking, etc. have been studied in detail. In most of the literature, the orientation is generally based on industrial experiments and they lack in understanding the problems relating to agricultural experimentation. Before stating the problems of agricultural experiments, it will not be out of place to state some situations in agricultural research scenario, where response surface methodology can be usefully employed.

Example 1.1: The over-use of nitrogen (N) relative to Phosphorus (P) and Potassium (K) concerns both the agronomic and environmental perspective. Phosphatic and Potassic fertilizers have been in short supply and farmers have been more steadily adopting the use of nitrogenous fertilizers because of the impressive virtual response. There is evidence that soil P and K levels are declining. The technique of obtaining individual optimum doses for the N, P and K through separate response curves may also be responsible for unbalanced fertilizer use. Hence, determining the optimum and balanced dose of N, P and K for different crops has been an important issue. This optimum and balanced dose should be recommended to farmers in terms of doses from the different sources and not in terms of the values of N, P and K alone, as the optimum combination may vary from source to source. However, in actual practice the values of N, P and K are given in terms of kg/ha rather than the combined doses alongwith the source of the fertilizers.

Example 1.2: [Adhikary and Panda, 1983]. In agronomy or various other fields of experimentation where several factors influence the response(s), various type of natural grouping exists in practice where experimentation is not possible if the grouping is ignored. Table 1 shows the type of grouping of manures applied to various cereals in the Eastern region in India.

Table 1

Manure group	Type of manure		Crop	Operability region (usual range of application/hectare)
Inorganic	i)	N	Rice	40 to 120 kg
			Wheat	60 to 100 kg
			Jute	40 to 80 kg
			Potato	120 to 180 kg
	ii)	P	Rice	40 to 60 kg
			Wheat	40 to 60 kg
			Jute	40 to 60 kg
			Potato	120 to 180 kg
	iii)	K	Rice	40 to 120 kg
			Wheat	60 to 100 kg
			Jute	40 to 80 kg
			Potato	120 to 180 kg
Organic	i)	FYM	Rice	
	ii)	Compost	Wheat	4 to 10 tonnes
			Potato	
Physical Factors (which can be controlled) affecting the yield	i)	Temperature	For all cereals	18^0C to 36^0C
	ii)	Water Content	-do-	12 to 75 acre inches
	iii)	Salinity	-do-	2-6 m.mhos/cm (E.C.)
	iv)	pH	-do-	6 to 7.5

Again each of the inorganic fertilizers may be obtained from different sources with differential effects. Thus the type of grouping shown in Table 2 is also important with respect to the availability of manures from various sources.

Table 2

Type of manure		**Source**
Nitrogen	i)	Ammonia
	ii)	Urea
	iii)	Cynamide
Phosphorus	i)	Rock Phosphate
	ii)	Super Phosphate
	iii)	Basic Slog
Potassium	i)	Murate of Potash
	ii)	Sulphate of Potash
	iii)	Potassium Nitrate

The grouping exhibited in Table 2 is important because it is well known that all sources of nitrogen may not be equally responsive to all sources of phosphorus even if their nitrogen content remains the same. Further, there are some restrictions in making choice of fertilizer sources e.g. ammonia cannot be used with rock phosphate, urea with sodium nitrate or potassium nitrate, ammonium sulphate/ammonium nitrite with super phosphate, super phosphate with lime, etc.

Example 1.3: Yardsticks (a measure of the average increase in production per unit input of a given improvement measure) of many fertilizers, manures, pesticides for various crops are being obtained and used by planners and administrators in the formulation of policies relating to manufacture/ import/ subsidy of fertilizers, pesticides, development of irrigation projects, etc.

The yardsticks have been obtained from the various factorial experiments. However, these will be more reliable and have desirable statistical properties, if response surface designs for slope estimation are used.

Example 1.4: In the usual fertilizer trials the response or yield of a crop not only depends on various doses of fertilizers but also on other factors like source of fertilizer, method of application of fertilizer, variety of crop, etc. That is, there may be several qualitative factors in the experiments. Such experiments involving qualitative and quantitative factors are called qualitative-cum-quantitative experiments. The response surface designs for quantitative-cum-qualitative factors may be useful for these situations.

Example 1.5: For value addition to the agriculture produce, food-processing experiments are being conducted. In these experiments, the major objective of the experimenter is to obtain the optimum combination of levels of several factors that are required for the product. To be specific, suppose that an experiment related to osmotic dehydration of the banana slices is to be conducted to obtain the optimum combination of levels of concentration of sugar solution,

solution to sample ratio and temperature of osmosis. The levels of the various factors are the following

	Factors	Levels
1.	Concentration of sugar solution	40%, 50%, 60%, 70% and 80%
2.	Solution to sample ratio	1:1, 3:1, 5:1, 7:1and 9:1
3.	Temperature of osmosis	25^0C, 35^0C, 45^0C, 55^0C and 65^0C

In this situation, response surface designs for 3 factors each at five equispaced levels can be used.

In the above situations, the response surface methodology can be very useful. Although a lot of literature on rotatable, group divisible, slope rotatable response surface designs is available for industrial experiments, yet their adoption in agricultural experiments has been very limited. Hardly have these designs been adopted in agricultural experiments. Edmondson (1991) listed the differences between agricultural or horticultural experiments and the industrial experiments. The major distinctions are outlined as follows:

i) **Time and factor range:** Industrial experiments may be completed in a few days or weeks, while an agricultural experiment may run for a year or more. Industrial experiments may be sequential and there may be good prior information about a particular region of interest in the factor space. Agricultural experiments often must be examined in a more general region of factor space and the results of a single experiment may have to be stand-alone.

ii) **Factor levels:** The levels of individual quantitative factors usually can be controlled and manipulated in industrial experiments but treatment factor levels in agriculture may be difficult to control. For this reason, unequally spaced factor levels and numerous levels of a factor are undesirable in agricultural experimentation.

iii) **Block designs:** In some areas of agricultural and horticultural research, the use of elaborate blocking systems to control environmental variability may be essential. It may also be necessary to incorporate one or more levels of splitting of experimental plots or units. Industrial response surface designs usually provide only very simple block structure and are inflexible for more complex designs.

iv) **Accuracy of observations:** Industrial experiments usually give reliable and accurate observations. Agricultural experiments may give observations, which are much less trustworthy. Entire plot observations may be "lost", the natural background variability may be high and because treatments may be complex and applied over a long period, mistakes and blunders, which may not be reported, are common.

v) **Shape of response surface:** Agricultural and biological systems may be less understood than industrial systems. A simple quadratic response function over the region of interest may not provide a good approximation and for this reason designs for fitting response surfaces in agricultural experiments must provide both estimate the coefficients and test the "goodness of fit" of an assumed quadratic response surface.

Taken together, these points mean that relative to the industrial experiments the agricultural experiments must be less model dependent and should accommodate a more flexible system of blocking. The level of factors may be equispaced as desired by the experimenter mainly due to the fact that there is a considerable practical ease in handling the doses. The rotatable designs available in literature are such that the dose ranges for different factors in terms of coded doses are equal for all the factors in a design. In practice, however, it often happens that the factors included in the experiment do not have the same dose range in terms of original units. Thus a design, which is rotatable in terms of the coded doses, ceases to be rotatable when brought to actual doses, if the actual dose range happens to be different for different factors. This is due to the fact that there are unequal changes in scales of different factors. Except an attempt by Dey (1969) not much work has been done to obtain response surface designs for these experimental situations. Analysis of data using response surface designs may be a stumbling block in the adoption of these designs in agricultural experimentation.

The statistical software packages like Statistical Analysis System (SAS), Statistical Package for Social Sciences (SPSS), Design Expert, Statistica, etc. can be usefully employed for the analysis of data. However, these softwares may be cost prohibitive, therefore, development of a computer software that is capable of analyzing the data from response surface designs needs attention.

Most of the literature on response surface designs is available for symmetrical factorial experiments but in agricultural and horticultural experiments, various factors have unequal number of levels. Except some attempts by Ramachander (1963), Mehta and Das (1968) and Dey (1969) not much work has been done on response surface designs for asymmetrical factorials and no work seems to have been done for response surface designs for slope estimation for equispaced levels and unequal dose ranges for symmetrical factorials and asymmetrical factorials.

The designs for fitting response surfaces generally require many experimental runs. Moreover, a rotatable design may lose efficiency or even become a singular design and therefore, fitting of a response surface may become impossible when some observations are lost. Therefore, the robustness aspects of these designs against loss of data is of importance. The problem of missing values in response surfaces was first investigated by Draper (1961) followed by McKee and Kshirsagar (1982). Srivastava, Gupta and Dey (1991) have studied the robustness aspects of second order rotatable response surface designs (SORD) obtained through central composite designs on the basis of loss of information pertaining to loss of single treatment combination. However, to study the effect of a single missing observation of SORD in general remains an open problem.

A survey of experiments stored under the project Agricultural Field Experiments Information System of IASRI, reveals that many qualitative-cum-quantitative experiments are being conducted with an aim to obtain optimum combination of levels of various quantitative factors and interaction of qualitative and quantitative factors. A beginning has been made by Draper and John (1988) to obtain response surface designs for quantitative and qualitative variables. They have considered the case when there are 2-quantitative factors and one or two qualitative factors only. Some methods of construction of response surface designs for qualitative and quantitative factors have also been obtained by Wu and Ding (1998) and Aggrawal and Bansal (1998). The experiments with quantitative factors are usually conducted with only three levels mainly due to the large size of the experiment. However, if the response surface designs are used, then more levels for each of the factors can be accommodated and still the design can be conducted in fewer runs. The designs available in the literature for such situations are scattered in the form of Ph.D. theses and in journals. These are not easily accessible to research workers/practicing statisticians. Keeping in view the importance of response surface methodology in agricultural experimentation, the broad objectives of the present investigation are:

1.2. Objectives

1. To obtain response surface designs for response optimization and slope estimation when various factors are with equispaced levels and/or have unequal dose ranges for both symmetrical as well as asymmetrical factorials.
2. To obtain response surface designs for qualitative-cum-quantitative factors.
3. To study the robustness aspects of response surface designs against non-availability of data on some point(s).
4. To prepare a catalogue of response surface designs suitable for agricultural experiments.
5. To develop computer software for the analysis of the designs obtained and catalogued.

1.3 Practical / Scientific Utility

The response surface designs developed for factorial experiments with equispaced doses with a flexibility in choosing the levels of each of the factors can be used by agricultural and horticultural research workers, food technologists, etc. where the existing response surface designs cannot be used. The response surface designs for qualitative-cum-quantitative experiments can be used to take into account the effect that the various levels of qualitative factors have on the relationship of quantitative factors with response. The designs obtained for slope estimation may be useful for obtaining reliable composite/ individual yardsticks of various inputs. These designs can also be used to estimate the rate of change of biological populations, rate of change of chemical reactions, etc. All the designs are readily available in the catalogues and hence, the users will have an easy access to the designs. The catalogue of second order rotatable designs with orthogonal blocking is quite useful for the agricultural experiments that require control of variability in the experimental units. The computer software developed and codes written using Statistical Analysis System (SAS) and Statistical Package for Social Sciences (SPSS) will be quite useful for fitting of response surfaces in agricultural experiments. The results would also be useful to the practicing statisticians in various ICAR institutes and State Agricultural Universities who are engaged in advisory services in the form of suggesting appropriate designs to the experimenters. Some designs obtained during the present investigation have actually been used in the National Agricultural Research System. The experimental situations along with the designs used are also given for the benefit of the users. The results would also be immensely useful to the students and scientists engaged in carrying out research and teaching in the experimental designs. The results obtained would form a basis for developing this subject further.

CHAPTER II

RESPONSE SURFACE METHODOLOGY

2.1. Introduction

Response surface methodology is useful for factorial experiments with v quantitative factors that are under taken so as to determine the combination of levels of factors at which each of the quantitative factors must be set in order to optimize the response in some sense. Let there be v independent variables denoted by $x_1, x_2, ..., x_v$ and the response variable be y and there are N observations. To meet the objectives, we postulate that the response as a function of input factors, as

$$y_u = \varphi(x_{1u}, x_{2u}, ..., x_{vu}) + e_u \tag{2.1.1}$$

where $u = 1,2,\ldots, N$ represents the N observations and x_{iu} is the level of the i^{th} factor in the u^{th} treatment combination, $i = 1,2,\ldots,v$; $u = 1,2,\ldots, N$. Let N points (treatment combinations) chosen from all possible treatment combinations be denoted by

$$\begin{matrix} x_{11} & x_{21} & \cdots & x_{i1} & \cdots & x_{v1} \\ x_{12} & x_{22} & \cdots & x_{i2} & \cdots & x_{v2} \\ \vdots & \vdots & \cdots & \vdots & \cdots & \vdots \\ x_{1u} & x_{2u} & \cdots & x_{iu} & \cdots & x_{vu} \\ \vdots & \vdots & \cdots & \vdots & \cdots & \vdots \\ x_{1N} & x_{2N} & \cdots & x_{iN} & \cdots & x_{vN} \end{matrix}$$

and y_u denote the response obtained from u^{th} treatment combination. The function φ describes the form in which the response and the input variables are related and e_u is the random error associated with the u^{th} observation such that random errors e_u

(i) have zero mean {E (e_u) = 0} and common variance σ^2
(ii) are mutually independent and
(iii) are normally distributed.

The assumption (iii) is required for tests of significance and confidence interval estimation procedures.

Knowledge of function φ gives a complete summary of the results of the experiment and also enables us to predict the response for values of x_{iu}, that have not been included in the experiment. If the function φ is known then using methods of calculus, one may obtain the values of $x_1, x_2, ..., x_v$ which give the optimum (say, maximum or minimum) response. In practice, the mathematical form of φ is not known; we, therefore, often approximate it, within the experimental region, by a polynomial of suitable degree in variables, x_{iu}. The adequacy of the fitted polynomial is tested through the usual analysis of variance. Polynomials which adequately represent the true dose-response relationship are called **Response Surfaces** and the designs that allow the fitting of response surfaces and provide a measure for testing their adequacy are called **response surface designs**.

If the function φ in (2.1.1) is a polynomial of degree one in x_{iu}'s *i.e.*

$$y_u = \beta_0 + \beta_1 x_{1u} + \beta_2 x_{2u} + \ldots + \beta_v x_{vu} + e_u \ , \tag{2.1.2}$$

we call it a first-order (linear) response surface in $x_1, x_2, \ldots, x_v$. If (2.1.1) takes the form

$$y_u = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} + \sum_{i=1}^{v} \beta_{ii} x_{iu}^2 + \sum_{i=1}^{v-1} \sum_{i'=i+1}^{v} \beta_{ii'} x_{iu} x_{i'u} + e_u \ , \tag{2.1.3}$$

we call it a second-order (quadratic) response surface. In the sequel we discuss the quadratic response surface in detail. The fitting of first order response surfaces is a particular case of the fitting of quadratic response surface and will be discussed in Note 2.2.1.

2.2 The Quadratic Response Surface

The general form of a quadratic (second-degree) response surface is

$$\begin{aligned} y_u = \beta_0 &+ \beta_1 x_{1u} + \beta_2 x_{2u} + \ldots + \beta_v x_{vu} + \beta_{11} x_{1u}^2 + \beta_{22} x_{2u}^2 + \ldots + \beta_{vv} x_{vu}^2 + \\ &\beta_{12} x_{1u} x_{2u} + \beta_{13} x_{1u} x_{3u} + \ldots + \beta_{v-1,v} x_{v-1,u} x_{vu} + e_u \end{aligned} \tag{2.2.1}$$

A general linear model can represent the quadratic response surface (2.2.1) and is given by

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e} \tag{2.2.2}$$

where **y** = $\begin{bmatrix} y_1 & y_2 & \ldots & y_N \end{bmatrix}'$ is an $N \times 1$ vector of observations, **X** is $N \times [(v+1)(v+2)/2]$ matrix of independent (explanatory) variables and their functions; $N > [(v+1)(v+2)/2]$ and is given by

$$\begin{bmatrix} 1 & x_{11} & \cdots & x_{v1} & x_{11}^2 & \cdots & x_{v1}^2 & x_{11}x_{21} & x_{11}x_{31} & \cdots & x_{v-2,1}x_{v-1,1} & x_{v-1,1}x_{v,1} \\ 1 & x_{12} & \cdots & x_{v2} & x_{12}^2 & \cdots & x_{v2}^2 & x_{12}x_{22} & x_{12}x_{32} & \cdots & x_{v-2,2}x_{v-1,2} & x_{v-1,2}x_{v,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & \cdots & x_{vN} & x_{1N}^2 & \cdots & x_{vN}^2 & x_{1N}x_{2N} & x_{1N}x_{3N} & \cdots & x_{v-2,N}x_{v-1,N} & x_{v-1,N}x_{v,N} \end{bmatrix}$$

$\boldsymbol{\beta}$ = $\left(\beta_0 \ \beta_1 \cdots \beta_v \ \beta_{11} \ \beta_{22} \cdots \beta_{vv} \ \beta_{12} \ \beta_{13} \cdots \beta_{v-1,v}\right)'$ is a $[(v+1)(v+2)/2] \times 1$ vector of unknown parameters and **e** = $\left(e_1 \ e_2 \cdots e_N\right)'$ is a $N \times 1$ vector of random errors distributed as $\mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_N)$.

Using the procedure of ordinary least squares that minimizes the sum of squares due to random errors, the normal equations for estimating $\boldsymbol{\beta}$'s are

$$\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{y} \tag{2.2.3}$$

and the ordinary least squares estimates of $\boldsymbol{\beta}$'s are

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \tag{2.2.4}$$

The variance-covariance matrix of estimates of parameters is

$$\mathbf{V}(\mathbf{b}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1} \tag{2.2.5}$$

where σ^2 is the error variance. The estimated response at u^{th} point $\mathbf{x}'_u$ *i.e.*, the u^{th} row of **X,** is

$$\begin{aligned}\hat{y}_u &= b_0 + b_1x_{1u} + b_2x_{2u} + \ldots + b_vx_{vu} + b_{11}x_{1u}^2 + b_{22}x_{2u}^2 + \ldots + b_{vv}x_{vu}^2 + \\ &\quad b_{12}x_{1u}x_{2u} + b_{13}x_{1u}x_{3u} + \ldots + b_{v-1,v}x_{v-1,u}x_{vu}.\end{aligned} \tag{2.2.6}$$

Variance of the predicted response is given by

$$\text{Var}(\hat{y}_u) = \sigma^2\mathbf{x}'_u(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_u \tag{2.2.7}$$

The u^{th} residual (the difference between the u^{th} observed response value and corresponding predicted value) $r_u = y_u - \hat{y}_u$, $u = 1, 2, \ldots, N$. The error variance is estimated by

$$\hat{\sigma}^2 = \frac{\sum_{u=1}^{N} r_u^2}{N - q_1} = \frac{(\mathbf{y} - \mathbf{Xb})'(\mathbf{y} - \mathbf{Xb})}{N - q_1}$$

$$\hat{\sigma}^2 = \frac{\mathbf{y}'\mathbf{y} - \mathbf{b}'\mathbf{X}'\mathbf{y}}{N - q_1} = \frac{SSE}{N - q_1}, \tag{2.2.8}$$

where SSE is the residual sum of squares and $q_1 = (v+1)(v+2)/2$. Let $\bar{y}$ be the mean of y_u's and $\hat{y}_u$ the estimated value of y_u from the fitted model, then, Analysis of Variance (ANOVA) Table for fitting model (2.2.1) is given as follows:

ANOVA

Sources of Variation	**Degrees of freedom**	**Sum of Squares**	**Mean Squares**	**F-Ratio**
Regression (fitted Model)	$q_1 - 1$	$SSR = \sum_{u=1}^{N}(\hat{y}_u - \bar{y})^2 = \mathbf{b}'\mathbf{X}'\mathbf{y} - \frac{(\mathbf{1}'\mathbf{y})^2}{N}$	MSR= $\frac{SSR}{q_1 - 1}$	$\frac{MSR}{MSE}$
Error	$N - q_1$	$SSE = \sum_{u=1}^{N}(y_u - \hat{y}_u)^2 = \mathbf{y}'\mathbf{y} - \mathbf{b}'\mathbf{X}'\mathbf{y}$	MSE= $\frac{SSE}{N - q_1}$	
Total	$N - 1$	$SST = \sum_{u=1}^{N}(y_u - \bar{y})^2 = \mathbf{y}'\mathbf{y} - \frac{(\mathbf{1}'\mathbf{y})^2}{N}$		

The above ANOVA is useful for testing the null hypothesis H_0: all values of $\beta_i, \beta_{ii}, \beta_{ii'}$ (excluding β_0) are zero against the alternative hypothesis H_1: at least one of the $\beta_i, \beta_{ii}, \beta_{ii'}$ (excluding β_0) is not zero. The ratio of MSR to MSE follows an F-distribution with

$q_1 - 1$ and $N - q_1$ degrees of freedom. If $F_{cal} > F_{\alpha,(q_1-1),(N-q_1)}$ then the null hypothesis is rejected at α% level of significance. The rejection of the null hypothesis in ANOVA leads to infer that at least one of the parameters in the null hypothesis is non-zero.

Sometimes the experimenter may be interested in making some specified comparisons. In such cases, we may proceed as follows:

For testing H_0 : **Aβ=L** against H_1 : **Aβ≠L,** where **A** is a matrix of rank Z and **L** is $Z \times 1$ vector, The following F-test can be used with Z and $N - q_1$ degrees of freedom.

$$F_{H_0} = \frac{(\mathbf{Ab} - \mathbf{L})(\mathbf{A}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{A}')^{-1}(\mathbf{Ab} - \mathbf{L})/Z}{MSE}. \tag{2.2.9}$$

Lack of Fit Test

Sometimes, the experimenter may be interested in testing whether the fitted model describes the behavior of the response over the experimental ranges of the factors. The adequacy of the fitted model can be tested using the test of lack of fit, if there are repeated observations for responses on the same values of independent variables. The F-statistic that can be used for this purpose is

$$F = \frac{SS_{LOF} / (N' - q_1)}{SS_{PE} / (N - N')} \tag{2.2.10}$$

where N is the total number of observations, N' is the number of distinct treatments. SS_{PE} (sum of squares due to pure error) has been calculated in the following manner: denote the l^{th} observation at the u^{th} design point by y_{lu}, where $l = 1, \ldots, r_u (\geq 1), u = 1, \ldots.. N'$. Define $\bar{y}_u$ to be average of r_u observations at the u^{th} design point. Then, the sum of squares for pure error is

$$SS_{PE} = \sum_{u=1}^{N'} \sum_{l=1}^{r_u} (y_{lu} - \bar{y}_u)^2 \tag{2.2.11}$$

The sum of squares due to lack of fit (SS_{LOF}) = SSE - SS_{PE}

The model is said to be a good fit if the test of lack of fit is non-significant. The statistics *viz.* *R*-Square (coefficient of determination) and adjusted R-square (adjusted coefficient of determination) can also be used as indicators for the adequacy of fit.

$$R^2 = SSR / SSE$$

$$R_A^2 = 1 - \frac{\text{Total degrees of freedom}}{\text{Error degrees of freedom}}(1 - R^2).$$

Note 2.2.1: In case of a first order response surface (2.1.2), **X** in (2.2.2) is $N \times (v+1)$ matrix of independent (explanatory) variables and is given by

$$\begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{v1} \\ 1 & x_{12} & x_{22} & \cdots & x_{v2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & \cdots & x_{vN} \end{bmatrix}$$

$\boldsymbol{\beta} = (\beta_0\ \beta_1 \cdots \beta_v)'$ is a $(v+1)\times 1$ vector of unknown parameters and $\mathbf{e} = (e_1\ e_2 \cdots e_N)'$ is a $N \times 1$ vector of random errors distributed as $\mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_N)$. The procedure of fitting the first order response surface (2.1.2) and testing of hypothesis remains the same as described for quadratic response surface except for change of **X** matrix and $\boldsymbol{\beta}$-vector. First order response surface is the first step in developing an empirical model through a sequential experimentation. Once the first order response surface is fitted, the contour lines are drawn by joining the points that produce the same value of predicted response. In such experiments, the starting conditions would often not be very close to maximum. Thus, the experimenter often first needs some preliminary procedure, to bring him to a suitable point where the second degree equation can most gainfully be employed. One such procedure is the 'steepest ascent' method.

In the sequel, we describe the procedure of determining the optimum settings of inputs in a quadratic response surface.

2.3. Determining the Co-ordinates of the Stationary Point of a Quadratic Response Surface

A near stationary region is defined as a region where the surface slopes along the *v* variable axes are small as compared to the estimate of experimental error. The stationary point of a near stationary region is the point at which the slope of the response surface is zero when taken in all the directions. The coordinates of the stationary point $\mathbf{x}_0 = (x_{01}, x_{02}, ..., x_{0v})'$ are obtained by differentiating the estimated response surface (2.3.1) with respect to each x_i and equating the derivatives to zero and solving the resulting equations

$$\hat{y}(\mathbf{x}) = b_0 + \sum_{i=1}^{v} b_i x_i + \sum_{i=1}^{v} b_{ii} x_i^2 + \sum_{i=1}^{v-1} \sum_{i'=i+1}^{v} b_{ii'} x_i x_{i'} \tag{2.3.1}$$

In matrix notation (2.3.1) can be written as

$$\hat{y}(\mathbf{x}) = b_0 + \mathbf{x}'\mathbf{b}_L + \mathbf{x}'\mathbf{B}\mathbf{x} \tag{2.3.2}$$

where $\mathbf{x} = (x_1, x_2, ..., x_v)'$, $\mathbf{b}_L = (b_1, b_2, ..., b_v)'$
and

$$\mathbf{B} = \begin{bmatrix} b_{11} & b_{12}/2 & \dots & b_{1v}/2 \\ b_{12}/2 & b_{22} & \dots & b_{2v}/2 \\ \dots & \dots & \dots & \dots \\ b_{1v}/2 & b_{2v}/2 & \dots & b_{vv} \end{bmatrix}$$

From (2.3.2), we get

$$\frac{\partial \hat{y}(\mathbf{x})}{\partial \mathbf{x}} = \mathbf{b}_L + 2\mathbf{B}\mathbf{x} \tag{2.3.3}$$

The stationary point $\mathbf{x}_0$ is obtained by equating (2.3.3) to zero and solving for $\mathbf{x}$, *i.e.*

$$\mathbf{x}_0 = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b}_L \tag{2.3.4}$$

The elements of vector $\mathbf{x}_0$ do not tell us anything about the nature of the response surface at the stationary point. The elements of $\mathbf{x}_0$ might represent the point at which the fitted surface attains a maximum or a minimum or where the fitted surface comes together in the form of a minimax or saddle point. However, the predicted response value denoted by $\hat{y}_0$, is obtained by substituting $\mathbf{x}_0$ for $\mathbf{x}$ in (2.3.2).

$$\hat{y}_0 = b_0 + \frac{\mathbf{X}_0'\mathbf{b}_L}{2}$$

To find the nature of the surface at the stationary point we examine the second order derivative of $\hat{y}(\mathbf{x})$. From (2.3.3), we get

$$\frac{\partial^2 \hat{y}(\mathbf{x})}{\partial \mathbf{x}^2} = 2\mathbf{B} \qquad \text{(since } \mathbf{B} \text{ is symmetric).}$$

The stationary point is a maximum, minimum or a saddle point according as the matrix **B** is negative definite, positive definite or indefinite. The nature of the response surface in the neighborhood of the stationary point, can be described in a greater detail if the response surface is expressed in canonical form.

2.4. The Canonical Equation of a Second Order Response Surface

Here we shift the origin to $\mathbf{x}_0$ and define the intermediate variables $(z_1, \ldots, z_v)' = (x_1 - x_{01}, \ldots, x_v - x_{0v})'$ or $\mathbf{z} = \mathbf{x} - \mathbf{x}_0$. The second order response equation (2.3.2) in term of z_i is

$$\begin{aligned}\hat{y}(\mathbf{z}) &= b_0 + (\mathbf{z} + \mathbf{x}_0)'\mathbf{b}_L + (\mathbf{z} + \mathbf{x}_0)'\mathbf{B}(\mathbf{z} + \mathbf{x}_0) \\ &= \hat{y}_0 + \mathbf{z}'\mathbf{B}\mathbf{z}\end{aligned} \tag{2.4.1}$$

In the intermediate variables, the predicted response is a linear function of the estimate of the response at the stationary point, $\hat{y}_0$, plus a quadratic form in the values of z_i.

To obtain the canonical form of the predicted response equation, we define a set of variables, $\mathbf{W} = (W_1, W_2, \cdots, W_v)'$ as

$$\mathbf{W} = \mathbf{M}'\mathbf{z} \tag{2.4.2}$$

where **M** is a $v \times v$ orthogonal matrix whose columns are the eigenvectors of the matrix **B**. Thus $\mathbf{M}^{-1} = \mathbf{M}'$ and $(\mathbf{M}')^{-1} = \mathbf{M}$. The matrix **M** has the property of diagonalysing **B**, *i.e.*, $\mathbf{M}'\mathbf{B}\mathbf{M} = \operatorname{diag}(\lambda_1, \lambda_2, \cdots, \lambda_v)$, where $\lambda_1, \lambda_2, ..., \lambda_v$ are the corresponding eigenvalues of **B**. The axes associated with the variables $W_1, W_2, \cdots, W_v$ are called the principal axes of the response system. The transformation in (2.4.2) is a rotation of z_i axes to form the W_i axes.

$$\mathbf{z}'\mathbf{B}\mathbf{z} = \mathbf{W}'\mathbf{M}'\mathbf{B}\mathbf{M}\mathbf{W} = \lambda_1 W_1^2 + \cdots + \lambda_v W_v^2 .$$

The eigenvalues of **B** are real (since the matrix **B** is a real symmetric matrix) and are the coefficients of the W_i^2 terms in the canonical equation

$$\hat{y} = \hat{y}_0 + \sum_{i=1}^{v} \lambda_i W_i^2 \qquad (2.4.3)$$

If the eigenvalues of **B** are

(i) all negative, then at stationary point, the surface has a maximum
(ii) all positive, then at stationary point the surface has a minimum
(iii) of mixed signs, i.e. some are positive and others are negative, then stationary point is a saddle point of the fitted surface.

The above analysis can be achieved by using the Statistical Packages like SAS. PROC RSREG fits a second order response surface and locates the coordinates of the stationary point, predicted response at the stationary point and gives the eigenvalues $\lambda_1, \lambda_2, ..., \lambda_v$ and the corresponding eigenvectors. It also helps in determining whether the stationary point is a point of maxima, minima or is a saddle point. The lack of fit of a second order response surface can also be tested using LACKFIT option under model statement in PROC RSREG. The steps of PROC RSREG are as given below:

```
PROC RSREG;
MODEL RESPONSE = <List of input variables>/LACKFIT NOCODE;
RUN;
```

2.5 Exploration of the Response Surface in the Vicinity of Stationary Point

The estimated response increases upon moving away from the stationary point along W_i if corresponding λ_i is positive and decreases upon moving away from stationary point along W_i if corresponding λ_i is negative. The estimated response does not change in value in the direction of the axis associated with W_i if the corresponding λ_i is zero (or very close to zero). The magnitude of λ_i indicates how quickly the response changes in the direction of axis associated with W_i variable. If the stationary point is minimax point and is inside the region of experimentation, then it is desirable to explore the response surface in the vicinity of stationary point and to determine the combinations of inputs for a given response. To achieve this, the W_i *'s* corresponding to negative λ_i's are set to zero. Now, the values of the W_i *'s* corresponding to positive λ_i's are generated.

To be clearer, let two of the $\lambda_i's$ denoted by λ_1 and λ_2 be positive. Then, a restricted canonical equation can be written as

$$Y_{des} = \hat{y}_0 + \lambda_1 W_1^2 + \lambda_2 W_2^2$$

where Y_{des} denotes the desired response.

If $Y_{des} - \hat{y}_0$ is denoted by difference of the desired and predicted response, then

$$\text{Difference} = \lambda_1 W_1^2 + \lambda_2 W_2^2$$

$$\Rightarrow \quad \frac{W_1^2}{a^2} + \frac{W_2^2}{b^2} = 1$$

where $a^2 = \lambda_1/\text{Difference}$, $b^2 = \lambda_2/\text{Difference}$

This equation represents an ellipse. The semi-length of its W_1-axis is *a*. Therefore, any chosen value for W_1 must have an absolute value less than or equal to the semi-length of W_1-axis. W_1 should be so generated that it falls inside the interval (-*a*, *a*). Once the W_1 is generated, W_2 can be obtained as

$$W_2 = \left[\frac{(\text{Difference} - \lambda_1 W_1^2)}{\lambda_2} \right]^{1/2}.$$

Once the $W_i\ 's$ are known, we would like to express W_i in terms of x_i 's. This can be achieved by $\mathbf{x} = \mathbf{MW} + \mathbf{x}_0$. The above relationship can easily be obtained by using (2.4.3). One can write a customized SAS code using PROC IML for carrying out such analysis.

For illustration, let us assume that we get $\lambda_1, \lambda_2, \lambda_3$ and λ_4 as 0.009811, -0.000003805, –0.000058, –0.000288. As λ_2, λ_3 and λ_4 are negative, therefore, take $W_2 = W_3 = W_4 = 0$. Let

M = {0.8931648 –0.046490 –0.021043 0.446825,
–0.3678540 0.364152 –0.404116 0.7541662,
0.1801135 0.929149 0.1993512 –0.253969,
–0.1857390 –0.043750 0.8924721 0.4087548 };

denote the matrix of eigenvectors. Let the estimated response at the stationary point be 2784.797kg/ha. Let the desired response be Y_{des} =3000kg/ha. Therefore, let W_1, obtained from the equation is sqrt (difference/0.00981)=AX1, say. To obtain various different sets of many values of W_1, generate a random variable, u, which follows uniform distribution and multiply this value with $2u-1$ such that W_1 lies within the interval, (-AX1, AX1). Now to get a combination of $x_i's$ that produces the desired response obtain $\mathbf{x} = \mathbf{MW} + \mathbf{x}_0$.

```
PROC IML;
W=J(4,1,0);
Ydes=3000;
W2=0;
W3=0;
W4=0;
Dif=Ydes-2784.7972;
Ax1=Sqrt(dif/.009811);
u= uniform(0);
W1= ax1*(2*u-1); print w1;
w[1,] = W1;
w[2,] = 0;
w[3,] = 0;
w[4,] = 0;
m = {0.8931648  -0.04649     -0.021043    0.446825,
     -0.367854     0.3641522 -0.404116    0.7541662,
      0.1801135   0.929149    0.1993512  -0.253969,
     -0.185739   -0.04375      0.8924721    0.4087548 };

xest = {1874.0833,5767.5836, 12638.21, 3163.2204};
x = m*w+xest;
print x;
run;
```

The above analysis can also be performed using SPSS. To carry out the analysis in SPSS. Prepare the Data file. In the data file generate the squares of the variables and their cross products. From the Menus Choose **Analyze → Regression →Linear**. Further, Call eigen (matrix whose eigenvalues and eigenvectors, matrix of eigenvectors, matrix of eigenvalues are required) can be used for performing canonical analysis, if one has used the regression analysis for response surface fitting using any of the statistical software packages commonly available. The syntax for obtaining the eigenvectors and eigenvalues is

```
matrix.
compute A = {1,2,3;2,4,5;3,5,6}.
CALL EIGEN (A,B,C).
Print a.
Print b.
Print c.
end matrix.
```

Here B and C are respectively the matrices of eigenvectors and eigenvalues resectively.

For exploration of the response surface in the vicinity of saddle point, the following code in SPSS has been developed:

```
matrix.
compute ydes = {3000}.
compute dif = {ydes-2784.7972}.
compute ax1 = sqrt(dif/.009811).
compute u = uniform(1,1).
compute w1 = ax1*(2*u-1).
```

```
compute w = {w1;0;0;0}.
compute m = {0.8931,-0.0464,-0.0210,0.4468;-0.3678,0.3641,-0.4041,0.7541;0.1801,0.9291,0.1993,-
0.2539;
-0.1857,-0.0437,0.8924,0.4087}.

compute mprime = transpos(m).
compute xest = {1874.0833;5767.5836;12638.21;3163.2204}.
compute x = m*w+xest.
print u.
print w.
print x.
end matrix.
```

2.6 Ridge Analysis

During the analysis of a fitted response surface, if the stationary point is well within the experimental region, the canonical analysis performed is sufficient. In some experimental situations, it is possible that the location of the stationary point is not inside the experimental region. In such cases, the ridge analysis may be helpful to search for the region of optimum response. The method of ridge analysis computes the estimated ridge of the optimum response for increasing radii from the center of the original design. This analysis is performed to answer the question that there is not a unique optimum of the response surface within the range of the experimentation, in which direction should further searching be done in order to locate the optimum. The following statements of SAS may be used for performing the ridge analysis

```
PROC  RSREG;
model dependent (variable<list = independent variables>)
ridge max:
run:
```

For mathematical details on the ridge analysis, a reference may be made to Khuri and Cornell (1996).

2.7 Response Surface Models without Intercept Term

The above discussion relates to the situations, where the intercept β_0, the expected value of the response variable, when the input variables takes the value zero. Also in some situations, however, it is expected that there is no output when input vector is zero. To deal with such situations one has to use a no-intercept model. If in (2.1.2) and (2.1.3), β_0 is excluded then we get response surfaces (first order and second order respectively) without intercept. In that case, the new vector of unknown parameters $\boldsymbol{\beta}$ is of the order $v \times 1$ for first order response surface and of the order $[v(v+3)/2] \times 1$ for second order response surface. $\mathbf{X}$ is $N \times v$ matrix for first order and $N \times v(v+3)/2$ for the second order response surface and is obtained by excluding the column of ones from the $\mathbf{X}$ as defined in (2.1.1). General procedure of analysis of the model fitting remains the same for both with and without intercept models. Therefore, the response surface fitting without intercept terms can be done as per procedure of section 2.2. The analysis of variance table for a response surface without intercept term is

ANOVA of a Response Surface (with no intercept)

Sources of Variation	Degrees of freedom	Sum of Squares	Mean Squares	F-Ratio
Regression (fitted Model)	q_2	$\text{SSR} = \sum_{u=1}^{N} \hat{y}_u^2 = \mathbf{b}'\mathbf{X}'\mathbf{y}$	$\text{MSR}=\frac{\text{SSR}}{q_2}$	$\frac{\text{MSR}}{\text{MSE}}$
Error	$N-q_2$	$\text{SSE} = \sum_{u=1}^{N} (\hat{y}_u - y_u)^2 = \mathbf{y}'\mathbf{y} - \mathbf{b}'\mathbf{X}'\mathbf{y}$	$\text{MSE}=\frac{\text{SSE}}{N-q_2}$	
Total	N	$\text{SST} = \sum_{u=1}^{N} y_u^2 = \mathbf{y}'\mathbf{y}$		

The test procedure is same as that of with intercept models except that there are $q_2 + 1 = q_1$ parameters in the with intercept models and no-intercept models have only q_2 parameters, therefore, degrees of freedom for Regression are same in both ANOVA tables with or without intercept terms. Specific comparisons can also be made as per (2.2.9).

For a quadratic response surface without intercept term $q_2 = v(v+3)/2 = q_1 - 1$. The estimated response at u^{th} point in case of a second order response surface is

$$\begin{aligned}\hat{y}_u &= b_1 x_{1u} + b_2 x_{2u} + \ldots + b_v x_{vu} + b_{11} x_{1u}^2 + b_{22} x_{2u}^2 + \ldots + b_{vv} x_{vu}^2 + \\ &\quad b_{12} x_{1u} x_{2u} + b_{13} x_{1u} x_{3u} + \ldots + b_{v-1,v} x_{v-1,u} x_{vu}.\end{aligned} \tag{2.7.1}$$

Note 2.7.1: For without intercept models, the R^2 statistic is based on the uncorrected regression and uncorrected total sum of squares. Therefore, the value of R^2 statistic will be much larger than those for the model with intercept term that are based on corrected regression and corrected total sum of squares. Therefore, one has to be careful in the choice of R^2 statistic while comparing the no-intercept models with models containing the intercept term. For such comparisons, it is desirable that the R^2 statistic based on the corrected regression and corrected total sum of squares is used. Other statistic like mean square error or mean absolute error ($\sum |y - \hat{y}| / N$ may be used for such comparisons. The most commonly used softwares for performing the regression analysis are MS-EXCEL, SPSS or SAS, etc. However, one has to be very cautious in the use of these softwares for the fittng of response surfaces without intercept. In MS-EXCEL, the regression option under data analysis in the tools menu gives corrected sum of squares due to regression, corrected total sum of squares and R^2 based on these sum of squares but the degrees of freedom for regression is 'q_1' instead of 'q_2'. Therefore, necessary corrections are required to be made in the adjusted R^2 etc. If one uses SPSS or PROC REG of SAS version 6.12 with no-intercept using NOINT option or Restrict Intercept=0, one gets uncorrected total and regression sums of squares. Therefore, one has to adjust the regression (total) sum of squares and their respective degrees of freedoms, R^2, adjusted R^2 etc., appropriately.

The determination of co-ordinates of the stationary point and the canonical analysis for the no-intercept quadratic response surface models can be performed on the similar steps of with intercept quadratic response surface by excluding β_0 from the model. However, PROC RSREG of SAS fits a quadratic response surface with intercept only. To fit a second order response surface without intercept some extra efforts are required that are described in the sequel

Stepwise Procedure of Fitting of Response Surface Designs Using PROC IML of SAS

To fit a second order response surface without intercept PROC REG of SAS for polynomial fitting can be used. For this first we have to generate the square and cross product terms from the input variables. The steps of PROC REG are given as below:

```
PROC REG;
MODEL Response = < List of input variables, List of Square of the input variables, list of the product of input variables taken two at a time>/NOINT;
RUN:
```

Further customized SAS code using PROC IML can be written for determining the co-ordinates of the stationary point, predicted response at stationary point and canonical equation of second order response surface.

One can also write a customized SAS Code for fitting a complete quadratic response surface with intercept = 0, determining the stationary point and for performing the canonical analysis. The procedure is described in the sequel.

Let there be four input variables denoted by x1,x2,x3 and x4 and response is yield, then the following SAS code is to be used for the analysis.

/* SAS Code for fitting of a no-intercept second order response surface */

```
data abc;
input x1 x2 x3 x4 yield;
/*Generation of the square and cross product terms */
x5=x1*x1;
x6=x2*x2;
x7=x3*x3;
x8=x4*x4;
x9=x1*x2;
x10=x1*x3;
x11=x1*x4;
x12=x2*x3;
x13=x2*x4;
x14=x3*x4;
/* enter the data to be analyzed */
cards;
………….
```

```
…………
…………
;
proc print;
run;
/* Invoke PROC IML and create the X and Y matrices */
/* Use variables X1, X2, … ,X14 */;
proc iml;
use chkdat8;
read all var{'x1', 'x2', 'x3', 'x4', 'x5', 'x6', 'x7', 'x8', 'x9', 'x10', 'x11',
 'x12', 'x13', 'x14'} into X;
read all var{'yield'} into Y;
/* Define the number of observations (N) as number of rows of X */;
N=nrow(X);
/* Define the Number of variables (g) as the number of columns of X */
g=ncol(X);
/* Compute C, the inverse of X’X */
C=inv(X`*X);
/* Obtain the vector of estimated coefficients as BHAT */
BHAT = C*X`*Y;
/* Comput Estimated response, YEST */
YEST = X*BHAT;
/* Obtain the residuals, e , error sum of squares, SSE and error mean square, MSE */
e=Y-Yest;
SSE=e`*e;
DFE=N-g;
MSE=SSE/DFE;
/*  Compute the dispersion matrix of the estimates, DISPMAT */
DISPMAT=MSE@C;
/* Compute Regression Sum of Squares, SSR, Mean Squares due to regression, MSR */
SSR=bhat`*X`*Y;
DFR=g;
MSR=SSR/DFR;
/*  Compute total sum of squares, SST*/
SST=Y`*Y;
TDF=N;
```

/* Compute corresponding F-ratio, R^2, R_A^2 and standard error of the estimated response, SE*/

```
F=MSR/MSE;
RSQ=ssr/sst;
RSQA=1-(TDF*SSE)/(DFE*SST);
SE=SQRT(MSE);
/* Obtain the vector of estimated coefficients of linear terms, b1 */
b1=bhat[1,1]//bhat[2,1]//bhat[3,1]//bhat[4,1];
b2=bhat[5,1]//0.5*bhat[9,1]//0.5*bhat[10,1]//0.5*bhat[11,1];
b3=0.5*bhat[9,1]//bhat[6,1]//0.5*bhat[12,1]//0.5*bhat[13,1];
b4=0.5*bhat[10,1]//0.5*bhat[12,1]//bhat[7,1]//0.5*bhat[14,1];
b5=0.5*bhat[11,1]//0.5*bhat[13,1]//0.5*bhat[14,1]//bhat[8,1];
/* Obtain the matrix coefficients corresponding to squares and cross product terms, b */
B=b2||b3||b4||b5;
```

/* Compute $\mathbf{B}^{-1}$, binv */

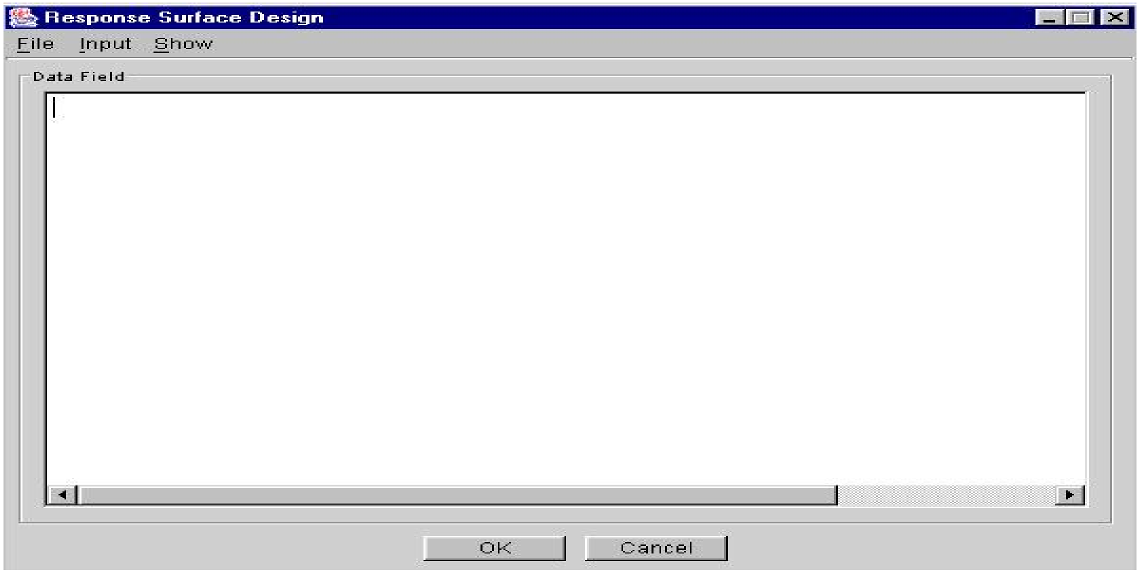
```
Binv=inv(B);
/* Obtain eigenvalues and eigenvectors of B beig, eigvec */
beig=eigval(B);
beigvec=eigvec(B);
/* Compute the stationary point, B-1b/2*/
xest=(-0.5)@(Binv*b1);
/* Compute the estimated response at the stationary point */
Yxest=(0.5)@(xest`*b1);
/* Print the Various Statistic obtained */
print bhat, dispmat, rsq, rsqa, se, dfr, ssr, msr, f, dfe, sse, mse, tdf,sst B, beig,
beigvec, xest,yxest;
run;
```

If one wants to use the above for the fitting of second order response surface with intercept, then one more additional statement as

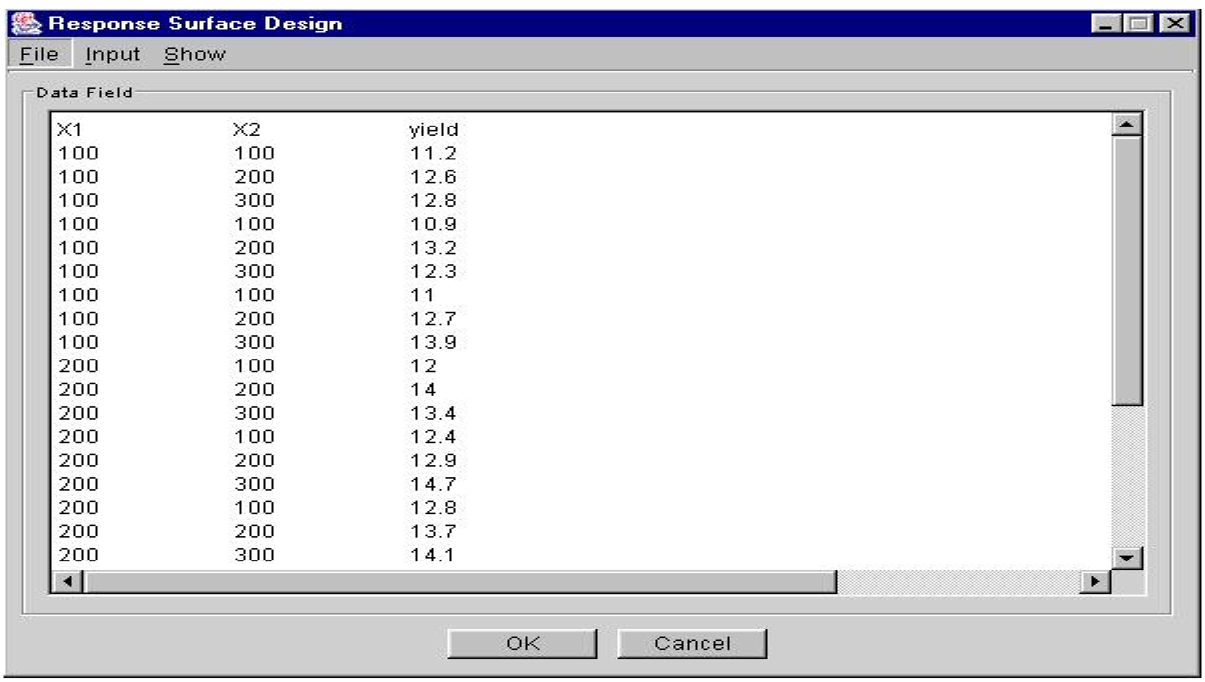
U = j(n,1,1)||x; /*add column of ones to X*/ after the statement n=nrow(x) and change the TDF as N-1.

2.8. Development of Computer Software

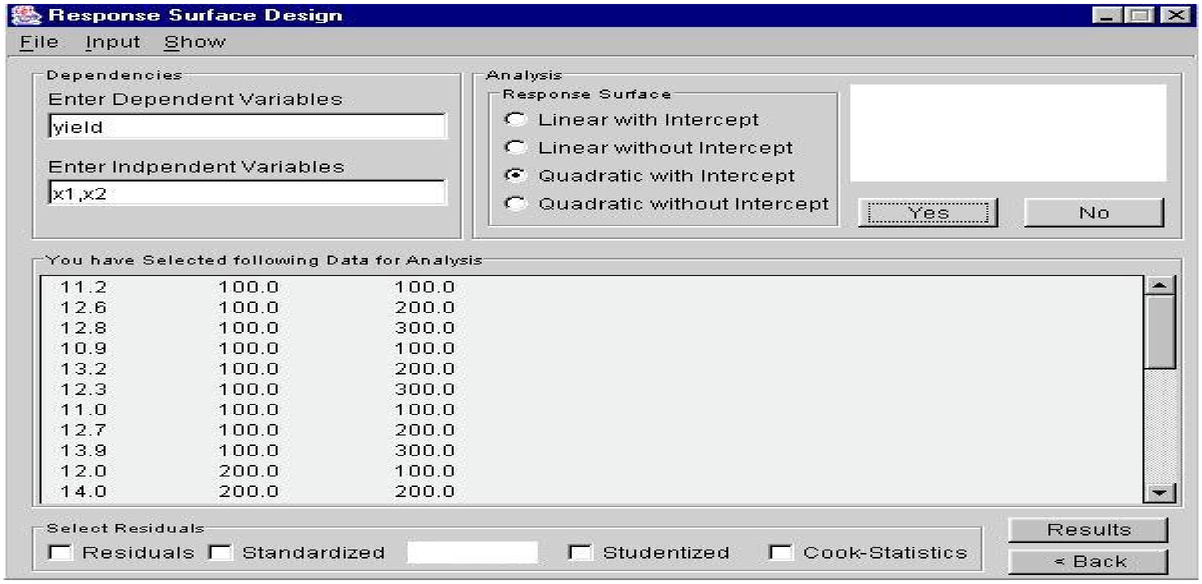
The statistical software packages like Statistical Analysis System (SAS), Statistical Package for Social Sciences (SPSS), Design Expert, Statistica, etc. can be usefully employed for the analysis of data. However, these software may be cost prohibitive, therefore, development of a computer software that is capable of analyzing the data from response surface designs needs attention. A menu driven, user friendly computer software for the response surface fitting has been developed. The software is capable of fitting linear and quadratic response surfaces both with and without intercept. It also determines the co-ordinates of the stationary point and performs canonical analysis for the quadratic response surfaces. Exploration of the response surface in the vicinity of the stationary point is also possible from the software. Further, it can generate 3-dimensional surface plots and contour plots. The software is also capable of obtaining the estimated responses, residuals, standardized and studentized residuals and Cook's statistic. studentized residuals and Cook's statistic can be used for detection of outlier(s), if any, in the data. The software has been developed using JAVA. The software requires a data file in ASCII. The different values may be separated by one or more blank spaces, tab or commas. One can also take the data from MS-EXCEL worksheet. After installing, when we run the software following screen appears:



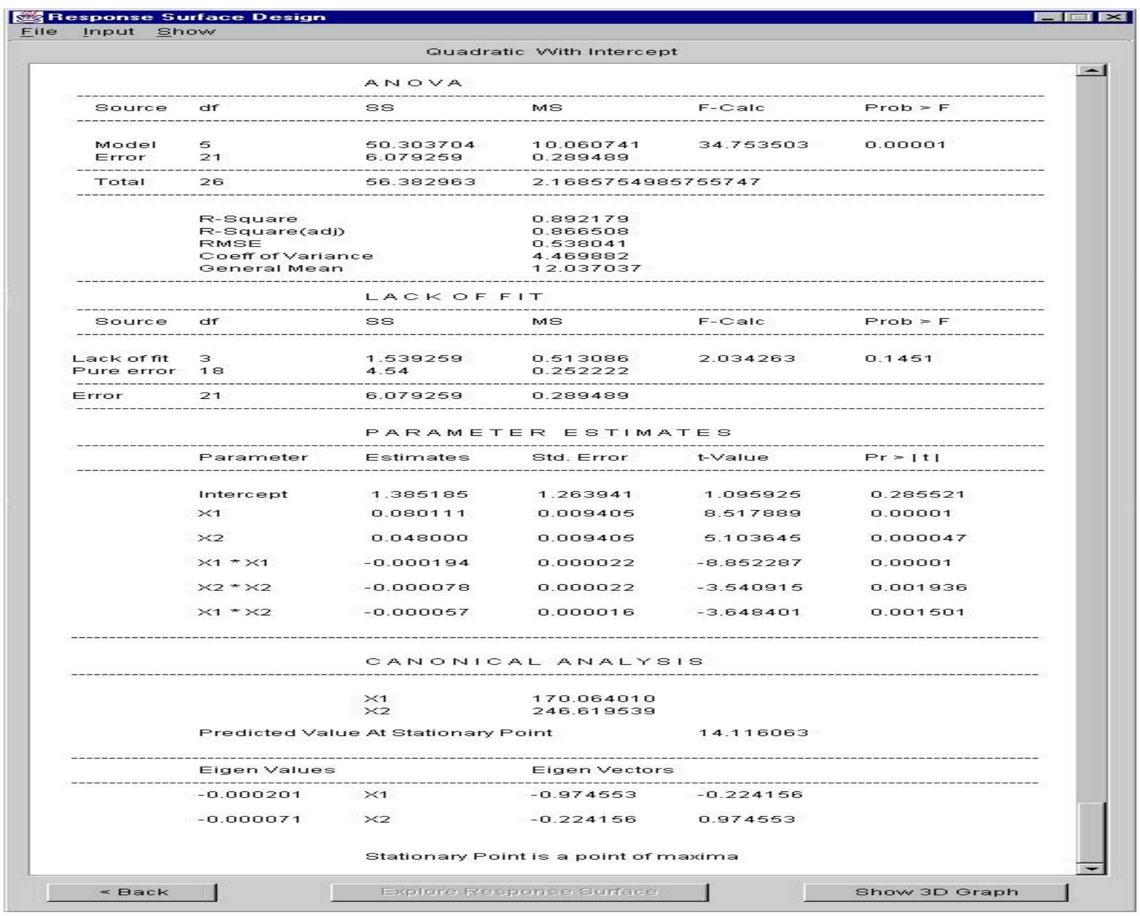
One can open the ASCII data file or may paste the data from an EXCEL Worksheet. The view of data is as given below:



Once the data is entered, Press OK button, for performing the analysis. Click on OK button gives the following screen:



This screen requires that the dependent variable and independent variables may be entered. Once the variables are entered then one may select one of the options (i) Linear with intercept, (ii) Linear without intercept, (iii) Quadratic with Intercept and (iv) Quadratic Without intercept. On clicking on Results one gets:



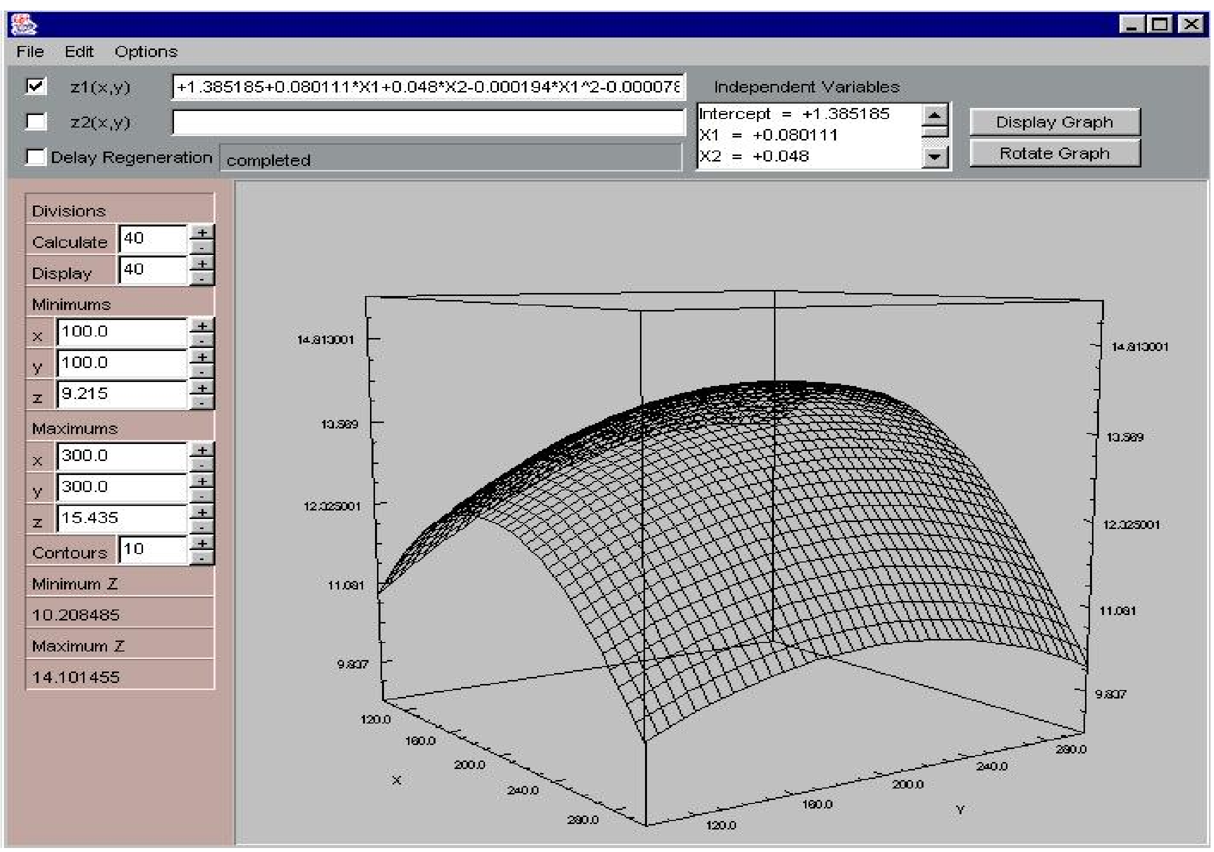
To get the residuals, standardized residuals, Cook's Statistics, one has to check the appropriate boxes.

Residuals Result

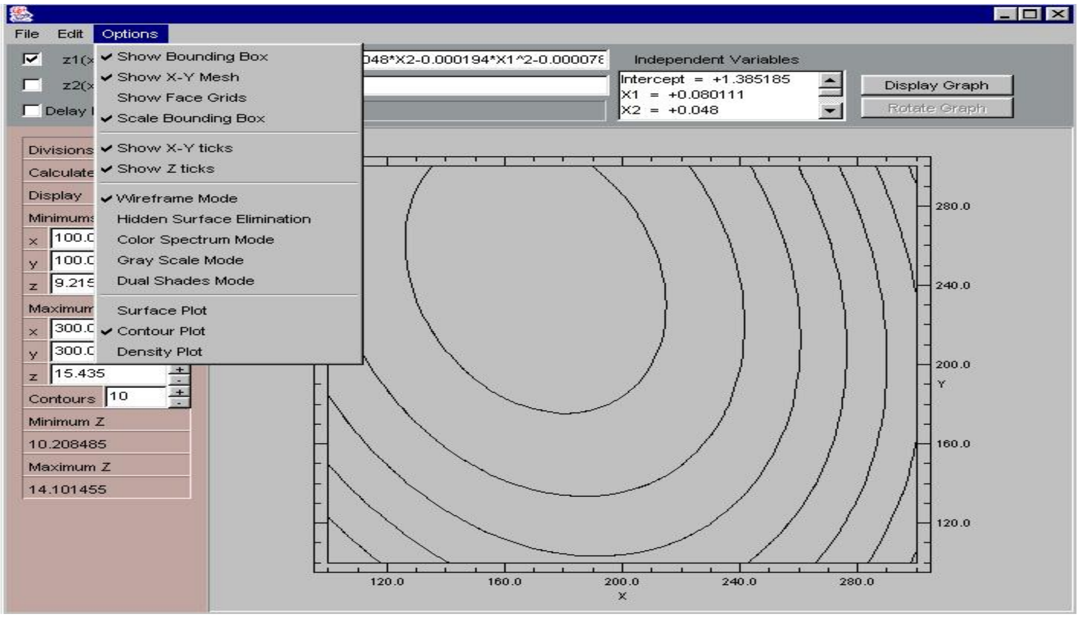
Original Y's	Predicted	Residuals	Standard	Var. Residu...	Student	Cook-Stats
11.2	10.907407	0.292593	0.543811	0.24759	0.588026	0.021155
12.6	12.807407	-0.207407	-0.385486	0.261313	-0.405736	0.006236
12.8	13.151852	-0.351852	-0.653949	0.24759	-0.70712	0.030592
10.9	10.907407	-0.007407	-0.013767	0.24759	-0.014887	1.4E-5
13.2	12.807407	0.392593	0.72967	0.261313	0.768001	0.022342
12.3	13.151852	-0.851852	-1.583246	0.24759	-1.711976	0.179314
11.0	10.907407	0.092593	0.172092	0.24759	0.186084	0.002119
12.7	12.807407	-0.107407	-0.199627	0.261313	-0.210113	0.001672
13.9	13.151852	0.748148	1.390503	0.24759	1.503561	0.138313
12.0	12.518519	-0.518519	-0.963715	0.261313	-1.014341	0.038973
14.0	13.851852	0.148148	0.275347	0.261313	0.289812	0.003181
13.4	13.62963	-0.22963	-0.426788	0.261313	-0.449208	0.007643
12.4	12.518519	-0.118519	-0.220278	0.261313	-0.231849	0.002036
12.9	13.851852	-0.951852	-1.769105	0.261313	-1.86204	0.131333
14.7	13.62963	1.07037	1.989383	0.261313	2.093889	0.166075
12.8	12.518519	0.281481	0.52316	0.261313	0.550642	0.011485
13.7	13.851852	-0.151852	-0.282231	0.261313	-0.297057	0.003343
14.1	13.62963	0.47037	0.874227	0.261313	0.920152	0.032071
10.9	10.240741	0.659259	1.225295	0.24759	1.32492	0.107399
11.3	11.007407	0.292593	0.543811	0.261313	0.572378	0.01241
10.2	10.218519	-0.018519	-0.034418	0.24759	-0.037217	8.5E-5
9.8	10.240741	-0.440741	-0.819158	0.24759	-0.885761	0.048001

Save Print Close

If one clicks on the 3-D graph, one gets



If one clicks at the options and the contour plot, following screen appears:



The software is also capable of exploration of the response surface, when the stationary point is a saddle point and lies within the experimental region.

2.9. Empirical Illustrations

Example 2.9.1: Consider an experiment that was conducted to investigate the effects of three fertilizer ingredients on the yield of a crop under fields conditions using a second order rotatable design. The fertilizer ingredients and actual amount applied were nitrogen (N), from 0.89 to 2.83 kg/plot; phosphoric acid (P_2O_5) from 0.265 to 1.336 kg/plot; and potash (K_2O), from 0.27 to 1.89 kg/plot. The response of interest is the average yield in kg per plot. The levels of nitrogen, phosphoric acid and potash are coded, and the coded variables are defined as

X_1=(N-1.629)/0.716, X_2=(P_2O_5-0.796)/0.311, X_3=(K_2O -1.089)/0.482

The values 1.629, 0.796 and 1.089 kg/plot represent the centres of the values for nitrogen, phosphoric acid and potash, respectively. Five levels of each variable are used in the experimental design. The coded and measured levels for the variables are listed as

			Levels of x_I		
	-1.682	**-1.000**	**0.000**	**+1.000**	**+1.682**
N	0.425	0.913	1.629	2.345	2.833
P_2O_5	0.266	0.481	0.796	1.111	1.326
K_2O	0.278	0.607	1.089	1.571	1.899

Six center point replications were run in order to obtain an estimate of the experimental error variance. The complete second order model to be fitted to yield values is

$$Y = \beta_0 + \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{3} \beta_{ii} x_i^2 + \sum_{i=1}^{2} \sum_{i'=2}^{3} \beta_{ii'} x_i x_{i'} + e$$

The following table list the design settings of x_1, x_2 and x_3 and the observed values at 15 design points N, P_2O_5, K_2O and yield are in kg.

Table 2.9.1: Central Composite Rotatable Design Settings in the Coded Variables x_1, x_2 and x_3, the original variables N, P_2O_5, K_2O and the Average Yield of a Crop at Each Setting

x_1	x_2	x_3	**N**	**P_2O_5**	**K_2O**	**Yield**
-1	-1	-1	0.913	0.481	0.607	5.076
1	-1	-1	2.345	0.481	0.607	3.798
-1	1	-1	0.913	1.111	0.607	3.798
1	1	-1	2.345	1.111	0.607	3.469
-1	-1	1	0.913	0.481	1.571	4.023
1	-1	1	2.345	0.481	1.571	4.905
-1	1	1	0.913	1.111	1.571	5.287
1	1	1	2.345	1.111	1.571	4.963
-1.682	0	0	0.425	0.796	1.089	3.541
1.682	0	0	2.833	0.796	1.089	3.541
0	-1.682	0	1.629	0.266	1.089	5.436
0	1.682	0	1.629	1.326	1.089	4.977
0	0	-1.682	1.629	0.796	0.278	3.591
0	0	1.682	1.629	0.796	1.899	4.693
0	0	0	1.629	0.796	1.089	4.563
0	0	0	1.629	0.796	1.089	4.599
0	0	0	1.629	0.796	1.089	4.599
0	0	0	1.629	0.796	1.089	4.275
0	0	0	1.629	0.796	1.089	5.188
0	0	0	1.629	0.796	1.089	4.959

```
OPTIONS LINESIZE = 72;
DATA RP;
INPUT N P K YIELD;
CARDS;
….
….
….
;

PROC RSREG;
MODEL YIELD = N P K /LACKFIT NOCODE;
RUN;
```

Response Surface for Variable YIELD

Response Mean	4.464050
Root MSE	0.356424
R-Square	0.8440
Coef. of Variation	7.9843

Regression	d.f.	Sum of Squares	R-Square	F-Ratio	Prob > F
Linear	3	1.914067	0.2350	5.022	0.0223
Quadratic	3	3.293541	0.4044	8.642	0.0040
Crossproduct	3	1.666539	0.2046	4.373	0.0327
Total Regression	9	6.874147	0.8440	6.012	0.0049

Regression	d.f.	Sum of Squares	R-Square	F-Ratio	Prob > F
Lack of Fit	5	0.745407	0.149081	1.420	0.3549
Pure Error	5	0.524973	0.104995		
Total Error	10	1.270380	0.127038		

Parameter	D.F.	Estimate	Std Error	T-ratio	Prob > |T|
INTERCEPT	1	6.084180	1.543975	3.941	0.0028
N	1	1.558870	0.854546	1.824	0.0981
P	1	-6.009301	2.001253	-3.003	0.0133
K	1	-0.897830	1.266909	-0.709	0.4947
N*N	1	-0.738716	0.183184	-4.033	0.0024
P*N	1	-0.142436	0.558725	-0.255	0.8039
P*P	1	2.116594	0.945550	2.238	0.0491
K*N	1	0.784166	0.365142	2.148	0.0573
K*P	1	2.411414	0.829973	2.905	0.0157
K*K	1	-0.714584	0.404233	-1.768	0.1075

Factor	D.F.	Sum of Squares	Mean Squares	F-Ratio	Prob > F
N	4	2.740664	0.685166	5.393	0.0141
P	4	1.799019	0.449755	3.540	0.0477
K	4	3.807069	0.951767	7.492	0.0047

d.f. denotes degree of freedom

Canonical Analysis of Response Surface

Factor	Critical Value
N	1.758160
P	0.656278
K	1.443790

Predicted value at stationary point 4.834526

	Eigenvectors		
Eigenvalues	N	P	K
2.561918	0.021051	0.937448	0.347487
-0.504592	0.857206	-0.195800	0.476298
-1.394032	-0.514543	-0.287842	0.807708

Stationary point is a saddle point.

The eigenvalues obtained are λ_1, λ_2 and λ_3 as 2.561918, -0.504592, -1.394032. As λ_2 and λ_3 are negative, therefore, take $W_2 = W_3 = 0$. Let

M = {0.021051 0.857206 -0.514543,
0.937448 -0.195800 -0.287842,
0.34787 0.476298 0.807708};

denotes the matrix of eigenvectors. The estimated response at the stationary points be 4.834526 kg/plot. Let the desired response be Y_{des} =5.0 kg/plot. Therefore, let W_1, obtained from the equation is sqrt (difference/2.561918)=AX1, say. To obtain various different sets of many values of W_1, generate a random variable, u, which follows uniform distribution and multiply this value with $2u-1$ such that W_1 lies within the interval, (-AX1, AX1). Now to get a combination of $x_i's$ that produces the desired response obtain $\mathbf{x} = \mathbf{M} * \mathbf{W} + \mathbf{x_0}$.

```
PROC IML;
W=J(3,1,0);
Ydes=5.0;
W2=0;
W3=0;
Dif=Ydes - 4.834526;
Ax1=Sqrt(dif/2.561918);
u= uniform(0);
W1= ax1*(2*u-1); print w1;
w[1,] = w1;
w[2,] = 0;
w[3,] = 0;
m = {0.021051  0.857206    -0.514543,
     0.937448  -0.195800   -0.287842,
     0.34787    0.476298    0.807708};
xest = {1.758160, 0.656278, 1.443790};
x = m*W+xest;
print x;
run;
```

Combinations of N, P, K estimated to produce 5.0 kg/plot of Beans.

Y	N	P	K
5.0	1.760	0.730	1.471
	1.762	0.815	1.503
	1.754	0.460	1.371

One can select a practically feasible combination of N, P and K.

Example 2.9.2: This example is a real life example and is a consequence of the advisory services provided to All India Co-ordinated Research Project on Energy Requirement in Agricultural Sector. The SAS code developed for fitting of second order response surfaces without intercept and exploration of the response surface in the vicinity of stationary point developed in this investigation, has been used. The data on energy usage in agricultural production system is being collected from the farmers of the selected villages in different agro-climatic zones under the All India Co-ordinated Research Project on Energy Requirement in Agricultural Sector. The information is collected on uses of Human Labour (human), Animal labour (animal), Diesel, Electricity (elect), Seed Rate (seed), Farmyard Manure (FYM), Fertilizer (fert), Chemicals (chem), Machinery (mach), etc. These are then converted into Mega Joule / hectare (MJ/ha) using internationally accepted conversion factors. The energy usages are also available on agricultural operations like tillage (till), sowing, bund making (bm), fertilizer application (fa), harvesting (ht), threshing (th), transplanting (trans), transportation (tport), etc. Adding the energy levels from different sources generates the total energy used for crop production that forms another factor in the study. The data available on yields are converted into kg per hectare basis. As of now, the data is available on yield (kg/ha or MJ/ha), energy used (MJ/ha) from various sources and total energy used (MJ/ha). For illustration purposes, we use the data on wheat collected from Sihoda (M.P.) is as given below:

NO	HUMAN	ANIMAL	DIESEL	ELECT	SEED	FYM	FERT	CHEM	MACH	Yield
1	754	0	2207	2011	1513	0	3199	22	309	2353
2	754	0	1598	2199	1544	0	6337	0	239	2595
3	900	0	1572	2660	1384	0	4371	12	246	2883
4	596	0	1534	2023	1362	0	2688	0	271	2409
5	809	0	1534	1794	1526	0	4982	10	235	2965
6	836	0	1534	1486	1251	0	4172	0	359	3459
7	879	0	2148	2865	1038	0	6143	14	342	4236
8	956	0	1745	2872	1068	0	3162	7	273	2689
9	843	0	1653	2052	1550	0	5857	4	265	2817
10	706	0	1567	2185	1640	0	4568	0	238	2551
11	767	0	1560	2551	1744	0	5449	0	287	3089
12	692	0	1598	2199	1589	0	6105	0	269	2548
13	922	0	1446	2436	1397	0	4790	10	294	2566
14	667	0	1480	1782	1529	0	2829	0	231	2081
15	765	0	1534	1847	1725	0	5375	12	240	2712
16	773	0	1520	2092	1669	0	5280	7	259	2337
17	842	0	1972	2388	1494	0	5169	0	285	2330
18	654	0	1395	1447	1453	0	4884	0	195	2224
19	974	0	1861	2870	1434	0	5141	7	272	2991
20	894	0	2096	2375	1453	0	4523	65	321	3058
21	753	0	1632	1684	1546	0	4575	0	250	2734
22	932	0	1490	1810	1557	0	4628	0	257	3177
23	823	0	1673	2015	1981	0	5864	13	291	3055
24	788	0	1678	2474	1476	0	3974	15	270	2934
25	806	0	1697	2272	1695	0	4839	0	249	2636
26	293	0	1278	1034	1453	0	2150	0	167	1853
27	670	0	1104	1639	1321	0	6399	6	204	2134
28	833	0	1832	2228	1513	0	5375	12	275	2759
29	705	0	1583	1990	1297	0	5931	6	239	2647

30	961	0	1809	2746	1651	0	6515	15	290	2770
31	703	0	1476	1892	1302	0	4057	12	235	2331
32	684	0	1628	1883	1583	0	2756	13	236	2534

The data according to agricultural operation wise is

Yield	Total	TILL	sow	BM	IRRIGN	WEED	FA	SPRY	HARV	THRSH	TPort
2824	9782	1270	486	11	1918	0	7	0	362	421	55
3231	14352	1069	436	15	2749	0	15	0	368	470	112
3020	10270	1081	472	16	2524	0	3	0	460	611	94
2718	10502	1111	567	54	2097	0	5	0	390	489	31
2404	10309	1051	459	459	2159	0	3	0	294	456	52
2471	13596	1111	567	5	2316	0	2	0	292	364	44
2965	11919	1353	516	15	3081	0	10	0	339	524	102
2965	10556	1389	567	141	2097	0	10	0	336	611	102
3000	13315	993	405	14	2553	0	14	0	331	436	104
3198	10713	1144	500	17	2672	0	3	0	487	647	100
2976	10782	1010	625	54	1862	0	11	0	412	542	53
2762	11002	1047	500	77	2562	0	6	0	377	499	68
2589	13490	1072	540	5	2175	0	9	0	329	322	51
2677	11145	1407	574	16	2718	0	8	0	313	479	91
3089	11481	1259	567	294	2207	0	10	0	308	530	36
3343	10414	1144	500	17	2316	0	6	0	487	575	103
2696	10896	1010	625	54	1796	0	11	0	395	531	35
2353	10015	1240	590	590	1884	0	12	0	317	578	69
2595	12671	1185	567	9	2207	0	6	0	291	468	58
2883	11145	1173	540	23	2739	0	12	0	306	475	111
2409	8474	1111	567	30	1713	0	10	0	321	616	58
2965	10890	1114	567	31	1817	0	6	0	385	407	46
3459	9638	1112	567	5	1784	0	6	0	428	201	252
4236	13429	1270	566	22	2699	0	11	0	446	653	567
2689	10083	1229	416	12	3232	0	7	0	255	391	303
2817	12224	1207	606	20	2024	0	13	0	375	489	81
2551	10904	1255	456	19	2262	0	6	0	275	359	62
3089	12358	691	567	10	2458	0	15	0	336	611	477
2548	12452	1222	533	37	2014	0	18	0	354	562	18
2566	11295	1143	436	26	2228	0	9	0	406	752	97
2081	8518	1097	523	0	1766	0	6	0	286	419	64
2712	11498	1116	571	34	1842	0	15	0	301	445	63
2337	11600	1126	536	16	2051	0	5	0	314	528	68
2330	12150	1191	405	567	2374	0	8	0	343	520	80
2224	10028	1232	286	5	1485	0	12	0	222	392	58
2991	12559	1297	724	21	2980	0	13	0	343	498	102
3058	11727	1176	571	558	2316	0	12	0	321	635	97
2734	10440	1182	603	8	1606	0	6	0	378	487	49

3177	10674	633	487	6	2157	0	6	0	480	311	591
3055	12660	1212	618	29	1830	0	7	0	377	631	99
2934	10675	1302	531	18	2565	0	9	0	271	458	54
2636	11558	1389	459	20	2383	0	10	0	279	409	77
1853	6375	832	567	7	952	0	5	0	158	222	29
2134	11343	692	515	54	1579	0	9	0	258	444	66
2759	12068	1363	402	230	2170	0	6	0	342	606	50
2647	11751	1191	540	9	2045	0	6	0	301	384	42
2770	13987	1335	625	18	2808	0	7	0	350	563	100
2331	9677	1080	535	17	1864	0	5	0	317	439	50
2534	8783	1264	509	30	1912	0	9	0	268	402	37

The one of the objectives of AICRP on Energy Requirement in Agricultural Sector is to obtain the optimum values of the various sources for maximum productivity.

To obtain the optimum energy levels for different sources like human energy, animal energy, diesel energy, electrical energy, FYM energy, fertilizer energy, machinery, irrigation, etc. to maximize the yield, a first thing that comes to mind is to use the response surface methodology. Further, one can easily see that the seed rate is one of the variables and if seed rate is zero then the yield will be zero. Therefore, the fitting of response surfaces without intercept is recommended. In this situation, the number of the energy sources is generally 9. Therefore, the number of observations required for a second order response surface without intercept is >45, to have at least one degree of freedom for error. However, if in some situations, one or two of these energy sources may not exist, still we require a large number of points. It is pertinent to carry out the response surface fitting separately for the different categories. The choice of categorization of farmers would normally depend upon the purpose of analysis. The simplest categorization can be made on the basis of land holding. Categorization of the farmers on the basis of irrigated or rainfed, electricity use or non-use, bullock or tractor use, based on productivity levels like low ($\leq$ 2000 Kg/ha), medium (2000 - 3250 Kg/ha), high ($\geq$ 3250 Kg/ha), etc. or based on the ratio of total energy to yield (energy-yield ratio) like good (< 3.50), average (3.50 - 4.00), poor (4.00 - 5.00), very poor $\geq$ 5.00 was also suggested. As the recommendations have to be made separately for different categories of farmers, therefore, the response surface fitting has to be done separately for each categories of farmers. In most of the cases, it is not possible to fit a complete second order response surface in most of the situations.

Therefore, we thought to utilize the data on energy usage at the time of different agricultural operations. These energy levels can be grouped into three or four variables, based on the agricultural operations, viz. $x1$ =*seed+ sowing +transportation;* $x2$ = *irrigation + weeding + tillage;* $x3$ =*fertilizer application (fa) +fertilizer (fert)+chemical (chem)+ farm yard manure (fym) + spray* and $x4$ = *harvesting (ht) + threshing (th).* As no output is expected when no energy is supplied to the system, we fit a second order response surface using $x1$, $x2$, $x3$ and $x4$ with no intercept. We obtain the co-ordinates of the secondary point, estimated response at the stationary point, canonical equation of the second order response surface, etc. If the stationary point is a saddle point, obtain the combination of levels of $x1$, $x2$, $x3$ and $x4$ that give a desired yield.

The above analysis can be performed using the SAS code given in Section 2.8.

Results of Second order Response surface fitting for small farmers are:

Analysis of Variance

Source	d.f.	Sum of Squares	Mean Squares	F-Ratio	Pr > F
Model	14	236554231.25	16896730.80	94.022	0.0001
Error	18	3234795.75	179710.875		
UnCorrected Total	**32**	239789027.00			

Root MSE	Yield Mean	CV	R^2	Adj-R^2
423.92319	2701.78125	15.69051	0.9865	0.9760

Parameter Estimates

Variable	d.f.	Parameter Estimate	Standard Error	t Value	Pr > |t|
X1	1	2.089288	3.12722135	0.668	0.5125
X2	1	1.566736	2.16844994	0.723	0.4793
X3	1	0.681377	1.24496477	0.547	0.5909
X4	1	-12.130016	11.3907506	-1.065	0.3010
X1*x1	1	-0.000723	0.00144548	-0.500	0.6231
X2*x2	1	-0.000159	0.00030916	-0.513	0.6144
X3*x3	1	-0.000078043	0.00006903	-1.131	0.2731
X4*x4	1	0.001419	0.00422387	0.336	.7409
X1*x2	1	-0.000288	0.00081362	-0.354	0.7271
X1*x3	1	-0.000049902	0.00072818	-0.069	0.9461
X1*x4	1	0.003320	0.00486338	0.683	0.5036
X2*x3	1	-0.000024840	0.00019162	-0.130	0.8983
X2*x4	1	0.000555	0.00217111	0.256	0.8012
X3*x4	1	0.000336	0.00090729	0.371	0.7153

The co-ordinates of the stationary point are:

X1	X2	X3	X4
1993.717	3905.9324	4497.6676	645.86875

Predicted yield at the Stationary Point is: 2757.611 Kg/ha.

$$\mathbf{B} = \begin{bmatrix} -0.000723 & -0.000144 & -0.000025 & 0.0016598 \\ -0.000144 & -0.000159 & -0.000012 & 0.0002774 \\ 0.000025 & -0.000012 & -0.000078 & 0.0001681 \\ 0.0016598 & 0.0002774 & 0.0001681 & 0.0014186 \end{bmatrix}$$

The vector of coefficients of linear terms is given by

$$\mathbf{b} = \begin{bmatrix} 2.089288 \\ 1.566736 \\ 0.681377 \\ -12.130016 \end{bmatrix}$$

Stationary Point

X1 1993.717
X2 3905.9324
X3 4497.6676
X4 645.86875

Estimated Response At Stationary Point : 2757.611 kg/ha

Eigenvalue	X1	X2	X3	X4
0.0023429	0.4712988	0.06986	0.0557161	0.8774353
-0.000078	-0.065601	-0.103409	0.9922808	-0.019539
-0.000127	-0.189451	0.9776132	0.0897149	0.0182272
-0.001679	0.8588844	0.1694065	0.0650058	-0.47895

Nature of the Stationary Point: Saddle Point. The stationary point lies within the range.

Exploration of the Response surface in the vicinity of the Stationary Point

In the above example the $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are 0.0023429, –0.000078, –0.000127 and –0.001679. As λ_2, λ_3 *and* λ_4 are negative, therefore, take $W_2 = W_3 = W_4 = 0$. The estimated response at the stationary points is 2757.611 kg/ha. Let the desired response Y_{des} =3000kg/ha. Therefore, let W_1, obtained from the equation is sqrt(difference/0.00981)=AX1, say. To obtain various different sets of many values of W_1, generate a random variable, u, which follows uniform distribution and multiply this value with $2u-1$ such that W_1 lies within the interval, (-AX1, AX1). Now to get a combination of $x_i's$ that produces the desired response obtain

$$\mathbf{x} = \mathbf{M} * \mathbf{W} + \mathbf{x_0}.$$

```
proc iml;
W=J(4,1,0);
Ydes=3000;
W2=0;
W3=0;
W4=0;
Dif=Ydes-2757.611;
Ax1=Sqrt(dif/.0023429);
u=uniform(0);
```

```
W1=ax1*(2*u-1); print w1;
w[1,]=w1;
w[2,]=0;
w[3,]=0;
w[4,]=0;
m={0.4712988 -0.065601 -0.189451 0.8588844,
   0.06986 -0.103409 0.9776132 0.1694065,
   0.0557161 0.9922808 0.0897149 0.0650058,
   0.8774353 -0.019539 0.0182272  -0.47895};
xest={1993.717,3905.9324, 4497.6676, 645.86875};
x=m*W+xest;
print x;
run;
```

Combinations of X1, X2, X3 and X4 estimated to produce 3000 kg/hectare of yield

X1	X2	X3	X4
1869.538	3887.526	4482.987	414.6801
1890.511	3890.634	4485.467	453.7267
1855.407	3885.431	4481.317	388.3714
1942.944	3898.406	4491.665	551.3433
2130.328	3926.182	4513.818	900.203
1870.913	3887.729	4483.15	417.24
1846.295	3884.08	4480.24	371.408
1851.315	3884.824	4480.833	380.7532

Depending upon the practical importance and availability of resources, one may choose one of these combinations.

CHAPTER III

RESPONSE SURFACE DESIGNS

3.1 Introduction

As discussed in Chapter II, the response surface methodology is a collection of statistical techniques for modelling and analysis of problems in which response(s) are influenced by several variables. This helps in finding the relationship between response(s) and variables, and determining the optimal conditions of variables that optimize the response(s). Fitting of response surfaces to unorganized data although now feasible with the availability of high-speed computers yet involves complex computations and control of precision of estimates of response at desired points is not possible. An alternative is to use the preplanned combinations of input variables and generate the data through appropriate designs. Several series of such designs are available in the literature. Data from factorial experiments with quantitative and equispaced factor levels can be used for fitting such relations conveniently. Box and Wilson (1951) and Box and Hunter (1957) introduced a series of response surface designs with the property that the variances of estimates of response at points equidistant from the centre of the design are all equal. They called these designs as rotatable designs. Considerable research activities followed the introduction of these designs though mainly for construction of designs. For an excellent review on this subject a reference may be made to the text books by Box and Draper (1987), Khuri and Cornell (1996) and Myers and Montgomery (1995) besides two excellent reviews by Hill and Hunter (1966) and Myers, Khuri and Carter (1989). Very little work exists in literature to obtain further series of response surface designs particularly when the levels are equidistant. Another area that has received little attention is the investigation of the more flexible asymmetrical response surface designs. Some useful references on this aspect are Ramchander (1963), Mehta and Das (1968), Draper and Stoneman (1968) and Dey (1969). All the methods of construction obtained in the above investigations, are for situations with unequispaced factor levels. Dey (1969) gave methods of construction of both rotatable and non-rotatable designs when levels of factors are equispaced or have unequidose ranges. The non-rotatable type of designs have a special feature that a part of the design retains the property of rotatability and as such these designs have been called as partially rotatable designs. A direct and straight forward method of construction of asymmetrical rotatable designs is also given. But the method yields response surface designs when some factors are at three levels and others are at five levels.

In this Chapter we introduce some series of response surface designs for both symmetrical and asymmetrical factorial experiments when the various factors are at equispaced levels that provide estimates of response at specific points with a reasonably high precision. A new criterion in terms of second order moments and mixed fourth order moments is also introduced. This criterion helps in minimizing the variance of the estimated response to a reasonable extent. In section 3.2 we discuss about the first order response surface designs. Section 3.3 is devoted to second order response surface designs for response optimization. Catalogues of the designs with number of factor (v) and number of design points (N) satisfying $3 \le v \le 10$ and $N \le 500$.

The above discussion relates to the experiments, where the experimenter is interested in determining the optimum combination of inputs for response optimization. In some situations, however, the experimenter is more interested in rate of change of response rather than the absolute response. If the difference in responses at points close together in the factor space are involved, that is the estimation of the local slope of the response surface is of interest. Researchers have taken up the problem of designs for estimating the slope of a response surface with different approaches following the pioneering work of Atkinson (1970). Atkinson (1970) used the least squares estimates of the coefficients in a first order polynomial model to estimate the slope of a response surface. A criterion was developed for designing experiments to estimate the slope with minimum mean squared error when the true response is quadratic. However, the problem is related only to single factor, *i.e.*, it is the problem of fitting curves. Ott and Mendenhall (1972) showed that the problem of estimation of the slope of the second order model bears some similarity to the problem of estimating expected response for the first order linear model. The estimated response $\hat{y}$ possesses a variance that varies with the independent variable. However, works related to estimating the estimated response were confined to two point designs, *i.e.*, designs for which all observations are taken at only two settings of the independent variable. In contrast, estimation of the slope of a second order model requires a minimum of three settings of the independent variables in order to estimate the three parameters of the model.

Murty and Studden (1972) discussed the problem of estimating the slope of a polynomial regression at a fixed point of experimental region such that

a) The variance of the least square estimate of the slope at the fixed point is minimum and
b) The average variance of the least square estimate of the slope is minimum

Slope rotatability and minimax criterion have been studied at length for obtaining designs for estimating the slope of a response surface. Hader and Park (1978) were the first to introduce the criterion of slope rotatability analogues to the criterion of rotatability. For a slope rotatable response surface design the variance of the partial derivative of the estimated response is constant at a constant distance from the origin of the design. Hader and Park (1978) examined the slope rotatability aspects of response surface designs obtainable through central composite designs. Gupta (1989) examined the slope rotatability aspects of designs obtained through BIB designs. Anjaneyulu, Dattatreya Rao and Narsimham (1995) introduced third order slope rotatable designs and obtained them through doubly balanced incomplete block designs. Park (1987) has extended the work of slope rotatability over axial directions to the class of slope rotatable designs over all directions. Further, Park and Kim (1992) introduced measures that quantify the amount of slope rotatability over axial directions in a given response surface design, Jang and Park (1993) gave a measure for evaluating slope rotatability over all directions in a response surface design. This measure is used to form slope variance dispersion graph evaluating the overall slope estimation capability of an experimental design throughout the region of interest.

Huda and Mukerjee (1984) and Mukerjee and Huda (1985) made the study of optimal designs for obtaining response surface designs for slope estimation. Huda and Mukerjee (1984) obtained design by minimising the variance of the difference maximized over all pairs of the points. For estimating the slope of a response surface, Mukerjee and Huda (1985) obtained 'minimax' second and third order designs. These designs are obtained by minimizing the variance of the estimated slope maximized overall points in the factor space. However, as is well known, a theoretically optimal design, may not be often implementable, because the mass distribution may have irrational weights. It, therefore, becomes important to study the performance of the discrete (exact) designs as compared to the possibly hypothetical theoretically optimal designs. A study of this kind was made by Huda (1987) with respect to minimax central composite designs for estimating the slope of a second order response surface design. However, the most of these studies are biased towards industrial experimentation and none of these give designs for slope estimation when the levels are equispaced, which is a common feature of agricultural experiments. An effort has been made to obtain slope rotatable designs for the situations in which various factors have equispaced doses and are presented in Section 3.4.

Further, in agricultural experiments, the use of elaborate blocking systems is essential to control environmental variability. Orthogonal blocking aspects of second order response surface designs have been discussed in Section 3.5.

Before proceeding further, we discuss some preliminaries regarding coding of levels of factors in response surface designs.

A design for fitting response surface consists of a number of suitable combinations of levels of several input factors. We shall use v for number of factors and N for number of combinations in the design each factor having a constant number of levels.

Users of such designs, usually provide range of real physical level for each factor under investigation with the origin of levels at zero for most factors. Designs, on the other hand, are usually constructed using coded levels and not the physical levels. The level codes are obtained as below.

First shift the origin of the levels of each factor at or near the middle of the range of the factor. This level generally corresponds to the approximate optimum level of the factor. The code for the changed origin is taken as zero.

Further level codes of a factor are taken in pairs like km and $-km$ one on each side of the changed origin where k is a positive constant and m is a scaling constant for the factor. The values of k have been so taken that the physical doses corresponding to the maximum value of k remain within the range. Such pairs of codes have been called equidistant (from the origin) codes.

The physical levels can be obtained from the above level codes as discussed below. Let $M_{\min}$ and $M_{\max}$ denote the minimum and maximum physical levels of a factor. The level codes corresponding to these physical levels are denoted by $-km$ and km. Treating the values of a physical level and the corresponding coded level as the co-ordinates of a point, the different points from possible physical levels within the range lie on a straight line. Taking the equation of the line as

$$Y=A+BX$$

and with the points $(M_{\min}, -km)$ and $(M_{\max}, km)$ on the line it is found that

$$A=(M_{\min}+M_{\max})/2 \text{ and } \quad B=(M_{\max}-M_{\min})/km.$$

Thus, the equation of the line is known. Now, given any level code, the corresponding physical level is obtained from Y by substituting the code value for X in the equation of the line.

A combination of level codes is called a design point. The combination with 0 code for each factor is called a center point. We initiate the discussion with first order response surface designs in the sequel

3.2 First Order Response Surface Designs

Let there be v factors each at s levels. The N-design points are chosen out of s^v total treatment combinations. If x_{iu} denotes the level of the i^{th} factor in the u^{th} treatment combination, then the matrix $\mathbf{X}$ for a first order response surface is given by

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{i1} & \cdots & x_{v1} \\ 1 & x_{12} & x_{22} & \cdots & x_{i2} & \cdots & x_{v2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1u} & x_{2u} & \cdots & x_{iu} & \cdots & x_{vu} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & \cdots & x_{iN} & \cdots & x_{vN} \end{bmatrix}$$

The first order response surface to be fitted is as given in (2.1.2)

$$y_u = \beta_0 + \beta_1 x_{1u} + \beta_2 x_{2u} + \ldots + \beta_v x_{vu} + e_u . \tag{3.2.1}$$

$$E(e_u) = 0;\ \ Cov(e_u, e_{u'}) = \begin{cases} \sigma^2 & \text{if } u = u' \\ 0 & \text{if } u \neq u' \end{cases}$$

The model in (3.2.1) can be written as

$$\mathbf{y} = \mathbf{X\beta} + \mathbf{e} \tag{3.2.2}$$

where $\mathbf{y}$ = $\begin{bmatrix} y_1 & y_2 & \ldots & y_N \end{bmatrix}'$ is an $N \times 1$ vector of observations, $\mathbf{X}$ is $N \times (v+1)$ matrix of independent (explanatory) variables and their functions; $\boldsymbol{\beta}$ = $\left(\beta_0\ \beta_1 \cdots \beta_v\right)'$ = $(\beta_0, \boldsymbol{\theta}')'$ is a $(v+1)\times 1$ vector of unknown parameters and $\mathbf{e}$ = $\left(e_1\ e_2 \cdots e_N\right)'$ is a $N \times 1$ vector of random errors distributed as $\mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_N)$.

Using the procedure of ordinary least squares that minimizes the sum of squares due to random errors, the normal equations for estimating $\boldsymbol{\beta}$'s are

$$\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{y} \tag{3.2.3}$$

and the ordinary least squares estimates of $\boldsymbol{\beta}$'s are

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \tag{3.2.4}$$

Here $$\mathbf{X}'\mathbf{X} = \begin{bmatrix} N & \sum_{u=1}^{N} x_{1u} & \sum_{u=1}^{N} x_{2u} & \cdots & \sum_{u=1}^{N} x_{iu} & \cdots & \sum_{u=1}^{N} x_{vu} \\ \sum_{u=1}^{N} x_{1u} & \sum_{u=1}^{N} x_{1u}^2 & \sum_{u=1}^{N} x_{1u}x_{2u} & \cdots & \sum_{u=1}^{N} x_{1u}x_{iu} & \cdots & \sum_{u=1}^{N} x_{1u}x_{vu} \\ \sum_{u=1}^{N} x_{2u} & \sum_{u=1}^{N} x_{1u}x_{2u} & \sum_{u=1}^{N} x_{2u}^2 & \cdots & \sum_{u=1}^{N} x_{2u}x_{iu} & \cdots & \sum_{u=1}^{N} x_{2u}x_{vu} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{u=1}^{N} x_{iu} & \sum_{u=1}^{N} x_{1u}x_{iu} & \sum_{u=1}^{N} x_{2u}x_{iu} & \cdots & \sum_{u=1}^{N} x_{iu}^2 & \cdots & \sum_{u=1}^{N} x_{iu}x_{vu} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{u=1}^{N} x_{vu} & \sum_{u=1}^{N} x_{1u}x_{vu} & \sum_{u=1}^{N} x_{2u}x_{vu} & \cdots & \sum_{u=1}^{N} x_{iu}x_{vu} & \cdots & \sum_{u=1}^{N} x_{vu}^2 \end{bmatrix}$$

Now to ensure that the terms in the fitted model are uncorrelated with one another *i.e.* to ensure the orthogonality of the parameter estimates, the off-diagonal elements of $\mathbf{X}'\mathbf{X}$ should be zero. Therefore, we have to choose x_{iu} such that $\mathbf{X}'\mathbf{X}$ is diagonal. Hence, x_{iu}'s must satisfy the conditions

(i) $$\sum_{u=1}^{N} x_{iu} = 0; \forall\, i = 1, 2, \ldots, v \text{ and} \tag{3.2.5i}$$

(ii) $$\sum_{u=1}^{N} x_{iu} x_{i'u} = 0; \forall\, i \neq i',\ i, i' = 1, 2, \ldots, v \tag{3.2.5ii}$$

The normal equations (3.2.3) under the conditions (3.2.5) are

$$\begin{bmatrix} N & \mathbf{0}' \\ \mathbf{0} & \mathbf{S} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \boldsymbol{\theta} \end{bmatrix} = \begin{bmatrix} G \\ \mathbf{T} \end{bmatrix} \tag{3.2.6}$$

where

$\mathbf{S} = \text{diag}\,(\sum_{u=1}^{N} x_{1u}^2 \quad \sum_{u=1}^{N} x_{2u}^2 \quad \cdots \quad \sum_{u=1}^{N} x_{iu}^2 \quad \cdots \quad \sum_{u=1}^{N} x_{vu}^2)$; $G = \sum_{u=1}^{N} y_u$ and $\mathbf{T} = (T_1, \cdots, T_i \cdots, T_v)'$;

$T_i = \sum_{u=1}^{N} x_{iu} y_u$; $\forall\, i = 1, 2, \cdots, v$.

The best linear unbiased estimate of the parameter vector $\boldsymbol{\beta}' = (\beta_0, \boldsymbol{\theta}')'$ is

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\boldsymbol{\theta}} \end{bmatrix} = \begin{bmatrix} N^{-1} & \mathbf{0} \\ \mathbf{0}' & \mathbf{S}^{-1} \end{bmatrix} \begin{bmatrix} G \\ \mathbf{T} \end{bmatrix} = \begin{bmatrix} N^{-1}G \\ \mathbf{S}^{-1}\mathbf{T} \end{bmatrix} \tag{3.2.7}$$

where $\mathbf{S}^{-1} = \text{diag}\,(1/\sum_{u=1}^{N} x_{1u}^2 \quad 1/\sum_{u=1}^{N} x_{2u}^2 \quad \cdots \quad 1/\sum_{u=1}^{N} x_{iu}^2 \quad \cdots \quad 1/\sum_{u=1}^{N} x_{vu}^2)$ with

$$D\begin{pmatrix} \hat{\beta}_0 \\ \hat{\boldsymbol{\theta}} \end{pmatrix} = \sigma^2 \begin{bmatrix} N^{-1} & \mathbf{0} \\ \mathbf{0}' & \mathbf{S}^{-1} \end{bmatrix}. \tag{3.2.8}$$

Therefore, $\text{Var}\,(\hat{\beta}_0) = \sigma^2 / N$ and $\text{Var}\,(\hat{\beta}_i) = \sigma^2 / \sum_{u=1}^{N} x_{iu}^2$; $i = 1, 2, \ldots, v$.

The estimated response at a point $\mathbf{x}'_0 = (x_{10}, x_{20}, \ldots, x_{v0})$ is $\hat{y}_0 = (1 \quad \mathbf{x}'_0)\hat{\boldsymbol{\beta}} = \hat{\beta}_0 + \mathbf{x}'_0\hat{\boldsymbol{\theta}}$ with variance as

$$\begin{aligned} \text{Var}\,(\hat{y}_0) &= \sigma^2 (N^{-1} + \mathbf{x}'_0 \mathbf{S}^{-1} \mathbf{x}_0) \\ &= \sigma^2 (N^{-1} + x_{10}^2 / \sum_{u=1}^{N} x_{iu}^2 + x_{20}^2 / \sum_{u=1}^{N} x_{iu}^2 + \cdots + x_{v0}^2 / \sum_{u=1}^{N} x_{iu}^2) \end{aligned} \tag{3.2.9}$$

Now to ensure the constancy of the variances of the parameter estimates in (3.2.5), we take another condition

$$\text{(iii)} \quad \sum_{u=1}^{N} x_{iu}^2 = N\lambda_2 = R, \text{ a constant}; \forall\, i = 1, 2, ..., v \tag{3.2.5iii}$$

As a consequence, $\text{Var}\,(\hat{\beta}_i) = \sigma^2 / R$; $\forall \; i = 1, 2, \ldots, v$. Substituting (3.2.5iii) into (3.2.9), we get,

$$\text{Var}\,(\hat{y}_0) = \sigma^2 (N^{-1} + \sum_{i=1}^{v} x_{i0}^2 / R) \tag{3.2.10}$$

Thus we see that the variance of the estimated response is a function of $\sum_{i=1}^{v} x_{i0}^2$. All such points for which $\sum_{i=1}^{v} x_{i0}^2$ is same the estimated response will have the same variance. The designs satisfying this property are called **first order rotatable designs**. The conditions in (3.2.5i) to (3.2.5iii) can be ensured by coding the real physical level for each factor under investigation.

For construction of the designs, one has to choose N points from s^v in such a way that the conditions in (3.2.5i) to (3.2.5iii) are satisfied. For this we first convert s levels into coded levels. For $s = 2$, the coded levels are -1 and +1; for $s = 3$, the coded levels are -1, 0, +1; for $s = 4$, the coded levels are -3, -1, +1, +3 and so on. The codes can be obtained either through the discussion made in Section 3.2.1 or by taking $\text{Coded value} = \dfrac{\text{Original value} - M}{S}$, where M is the average of the actual physical values for the levels of the factors in the design and S is the half of their difference. It sometimes gives coded levels in fractions, this may be converted into integers by multiplying each by the least common multiple of denominators. From the conditions, it is clear that we have to choose a suitable fraction of s^v in such a way that the main effects are orthogonally estimable. In other words, we choose those fractions of s^v factorial experiment in which no main effect and two-factor interaction is present in the identity group or defining contrasts. Orthogonal main effect plans or orthogonal resolution III plans for s^v factorial experiment also serve as designs for fitting response surfaces. Therefore, all resolution III plans can be used as designs for fitting first order response surfaces. For an exhaustive catalogue of resolution III plans, a reference may be made to Gupta, Dey and Nigam (1984) and Dey (1985). First order response surface designs are more useful for two level factorials. The procedure for obtaining first order response designs for two level factorials that satisfy the conditions (i) to (iii) of (3.2.5) is described in the sequel.

For factors at two levels, Hadamard matrices are useful designs for fitting first order response surfaces. A Hadamard matrix $\mathbf{H}_v$ is a square matrix with entries as +1 and -1 such that $\mathbf{H}_v\mathbf{H}'_v = \mathbf{H}'_v\mathbf{H}_v = v\mathbf{I}_v$. A Hadamard matrix of order v exists if $v = 0\,(\text{mod } 4)$, v = 1, 2 being trivial cases. These matrices were first considered as Hadamard determinants. They were so named because the determinant of a Hadamard matrix satisfies equality in Hadamard's determinant theorem, which states that if $\mathbf{H} = ((h_{ij}))$ is a matrix of order v where $\left|h_{ij}\right| \le 1$ for all i and j, then $\left|\det \mathbf{H}\right| \le v v^{1/2}$. A Hadamard matrix of order v serves as a design for 2^{v-1} factorial experiment. Plackett and Burman (1946) constructed Hadamard matrices for all permissible values of $v \le 100$ with the exception of v=92. The Hadamard matrix of order 92 was discovered by Baumert, Golomb and Hall (1962). The smallest order undecided in Hedayat and Wallis (1978) was 268 and Sewade (1985) obtained the Hadamard matrix of this order. The smallest order for which the existence of a Hadamard matrix is in doubt is currently 428 *(www.research.att.com/~njas/hadamard/).* For those $v \ge 3$, which are not multiple of 4, we can obtain the designs for fitting of first order response surfaces as regular fraction of 2^v-factorials.

3.3 Second Order Response Surface Designs for Response Optimization

Let there be v factors such that s_i denotes the level of factor i; $i = 1, 2, \ldots, v.$ The N-design points are chosen out of $\prod_{i=1}^{v} s_i$ total treatment combinations. Let x_{iu} denotes the level of the i^{th} factor in the u^{th} treatment combination and $\mathbf{X}$, the matrix for a second order response surface. The $\mathbf{X}$ matrix for v = 2 and model (2.2.1) given in Section 2.2 of Chapter II is given by

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{21} & x_{11}^2 & x_{21}^2 & x_{11}x_{21} \\ 1 & x_{12} & x_{22} & x_{12}^2 & x_{22}^2 & x_{12}x_{22} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1u} & x_{2u} & x_{1u}^2 & x_{2u}^2 & x_{1u}x_{2u} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & x_{1N}^2 & x_{2N}^2 & x_{1N}x_{2N} \end{bmatrix}$$

For this,

$$\mathbf{X'X} = \begin{bmatrix} N & \sum_{u=1}^{N} x_{1u} & \sum_{u=1}^{N} x_{2u} & \sum_{u=1}^{N} x_{1u}^2 & \sum_{u=1}^{N} x_{2u}^2 & \sum_{u=1}^{N} x_{1u}x_{2u} \\ \sum_{u=1}^{N} x_{1u} & \sum_{u=1}^{N} x_{1u}^2 & \sum_{u=1}^{N} x_{1u}x_{2u} & \sum_{u=1}^{N} x_{1u}^3 & \sum_{u=1}^{N} x_{1u}x_{2u}^2 & \sum_{u=1}^{N} x_{1u}^2 x_{2u} \\ \sum_{u=1}^{N} x_{2u} & \sum_{u=1}^{N} x_{1u}x_{2u} & \sum_{u=1}^{N} x_{2u}^2 & \sum_{u=1}^{N} x_{1u}^2 x_{2u} & \sum_{u=1}^{N} x_{2u}^3 & \sum_{u=1}^{N} x_{1u}x_{2u}^2 \\ \sum_{u=1}^{N} x_{1u}^2 & \sum_{u=1}^{N} x_{1u}^3 & \sum_{u=1}^{N} x_{1u}^2 x_{2u} & \sum_{u=1}^{N} x_{1u}^4 & \sum_{u=1}^{N} x_{1u}^2 x_{2u}^2 & \sum_{u=1}^{N} x_{1u}^3 x_{2u} \\ \sum_{u=1}^{N} x_{2u}^2 & \sum_{u=1}^{N} x_{1u}x_{2u}^2 & \sum_{u=1}^{N} x_{2u}^3 & \sum_{u=1}^{N} x_{1u}^2 x_{2u}^2 & \sum_{u=1}^{N} x_{2u}^4 & \sum_{u=1}^{N} x_{1u}x_{2u}^3 \\ \sum_{u=1}^{N} x_{1u}x_{2u} & \sum_{u=1}^{N} x_{1u}^2 x_{2u} & \sum_{u=1}^{N} x_{1u}x_{2u}^2 & \sum_{u=1}^{N} x_{1u}^3 x_{2u} & \sum_{u} x_{1u}x_{2u}^3 & \sum_{u=1}^{N} x_{1u}^2 x_{2u}^2 \end{bmatrix}$$

To ensure the orthogonal estimation of parameters, the matrix $\mathbf{X'X}$ should be diagonal. For a second order response surface design, a complete diagonal $\mathbf{X'X}$ is not feasible due to the occurrence of sum of squares terms like $\sum_{u=1}^{N} x_{iu}^2$ and sum of cross products of squares like $\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$ in the off-diagonal positions. We attempt to diagonalize the $\mathbf{X'X}$ to the possible extent. Let us assume that $x_{iu}'s$ satisfy the following conditions on the moments:

(i) $\sum_{u=1}^{N} \left\{ \prod_{u=1}^{v} x_{iu}^{\alpha_i} \right\} = 0$, if any α_i is odd, for $\alpha_i = 0,1,2$ $or\, 3$ and $\sum \alpha_i \le 4.$

(ii) $\sum_{u=1}^{N} x_{iu}^2 =$ constant (for all i) $= N\lambda_2 = R$ (say)

(iii) $\sum_{u=1}^{N} x_{iu}^4 =$ constant (for all i) = $CN\lambda_4 = CL$ (say)

(iv) $\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 =$ constant $= N\lambda_4 = L$ (say), for all $i \ne i'$ (3.3.1)

These conditions are also known as conditions of symmetry. Using the conditions (i), (ii), (iii) and (iv) given in (3.3.1) and using model (2.2.1) given in Section 2.2 of Chapter II, we get

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} N & \mathbf{0}' & R\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & R\mathbf{I}_v & \mathbf{0} & \mathbf{0} \\ & & & \\ R\mathbf{1} & \mathbf{0} & (C-1)L\mathbf{I}_v + L\mathbf{1}\mathbf{1}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & L\mathbf{I}_{v(v-1)/2} \end{bmatrix} \tag{3.3.2}$$

The inverse of the above matrix can be obtained with the help of the following lemmas.

Lemma 3.3.1: If **A** and **D** are symmetric matrices then

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}' & \mathbf{H} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{A}^{-1} + \mathbf{F}\mathbf{E}^{-1}\mathbf{F}' & -\mathbf{F}\mathbf{E}^{-1} \\ -\mathbf{E}^{-1}\mathbf{F}' & \mathbf{E}^{-1} \end{bmatrix} \tag{3.3.3}$$

where $\mathbf{E} = \mathbf{H} - \mathbf{B}'\mathbf{A}^{-1}\mathbf{B}$ and $\mathbf{F} = \mathbf{A}^{-1}\mathbf{B}$.

Lemma 3.3.2: Let $\mathbf{M} = (a-b)\mathbf{I} + b\mathbf{1}\mathbf{1}'$ be a $n \times n$ matrix then

$$\mathbf{M}^{-1} = (x-y)\mathbf{I} + y\mathbf{1}\mathbf{1}'$$

where $x = \dfrac{a+(n-2)b}{(a-b)[a+(n-1)b]} = \dfrac{(a-b)+(n-1)b}{(a-b)[(a-b)+nb]}$

and $y = \dfrac{-b}{(a-b)[a+(n-1)b]} = \dfrac{-b}{(a-b)[(a-b)+nb]}$

Lemma 3.3.3: If $\mathbf{P} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}' & \mathbf{H} \end{bmatrix}$, det ($\mathbf{P}$) = det ($\mathbf{P}$).det ($\mathbf{H} - \mathbf{B}'\mathbf{A}^{-1}\mathbf{B}$). Here det(.) denotes the determinant of a given matrix.

The matrix $\mathbf{X}'\mathbf{X}$ in (3.3.2) can be seen as $\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}' & \mathbf{H} \end{bmatrix}$, where

$$\mathbf{A} = \begin{bmatrix} N & \mathbf{0}' \\ \mathbf{0} & R\mathbf{I}_v \end{bmatrix}_{(v+1)\times(v+1)}; \quad \mathbf{B} = \begin{bmatrix} R\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & \mathbf{0} \end{bmatrix}_{(v+1)\times\frac{v(v+1)}{2}} \text{ and } \mathbf{H} = \begin{bmatrix} (C-1)L\mathbf{I}_v + L\mathbf{1}\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & L\mathbf{I} \end{bmatrix}.$$

Now, we can see that

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{1}{N} & \mathbf{0}' \\ \mathbf{0} & \frac{1}{R}\mathbf{I}_v \end{bmatrix}; \quad \mathbf{F} = \mathbf{A}^{-1}\mathbf{B} = \begin{bmatrix} \frac{R}{N}\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & \mathbf{0} \end{bmatrix}_{(v+1)\times\frac{v(v+1)}{2}};$$

$$\mathbf{B}'\mathbf{A}^{-1}\mathbf{B} = \begin{bmatrix} \frac{R^2}{N}\mathbf{1}\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & \mathbf{0} \end{bmatrix}_{\frac{v(v+1)}{2}\times\frac{v(v+1)}{2}}$$

$$\mathbf{E} = \mathbf{H} - \mathbf{B}'\mathbf{A}^{-1}\mathbf{B} = \begin{bmatrix} (C-1)L\mathbf{I}_v + \left(L - \dfrac{R^2}{N}\right)\mathbf{11}' & \mathbf{0}' \\ \mathbf{0} & L\mathbf{I} \end{bmatrix}.$$

For finding the inverse of the matrix **E** we have to find the inverse of

$(C-1)L\mathbf{I}_v + \left(L - \dfrac{R^2}{N}\right)\mathbf{11}' = \mathbf{G}$ (say) using Lemma 3.3.2.

$$\begin{aligned} \mathbf{G}^{-1} &= \frac{1}{(C-1)L}\mathbf{I} + \frac{-\left(NL - R^2\right)}{(C-1)L\,D}\mathbf{11}' \\ &= \frac{1}{(C-1)L}\left[\mathbf{I} - \frac{\left(NL - R^2\right)}{D}\mathbf{11}'\right] \end{aligned};$$

where $D = (C + v - 1)NL - vR^2$

Therefore,

$$\mathbf{E}^{-1} = \begin{bmatrix} \dfrac{1}{(C-1)L}\left[\mathbf{I} - \dfrac{\left(NL - R^2\right)}{D}\mathbf{11}'\right] & \mathbf{0} \\ \mathbf{0} & \dfrac{1}{L}\mathbf{I} \end{bmatrix}$$

Hence,

$$\mathbf{FE}^{-1} = \begin{bmatrix} \dfrac{R}{D}\left(\dfrac{1}{(C-1)NL}\right)\left(D - v\left(NL - R^2\right)\right)\mathbf{1}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

Simplifying $D - v\left(NL - R^2\right)$, we get

$$D - v\left(NL - R^2\right) = v\left(NL - R^2\right) + (C-1)NL - v\left(NL - R^2\right) = (C-1)NL$$

$$\therefore \quad \mathbf{FE}^{-1} = \begin{bmatrix} \dfrac{R}{D}\mathbf{1}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}; \quad \mathbf{FE}^{-1}\mathbf{F}' = \begin{bmatrix} \dfrac{R^2 v}{ND} & \mathbf{0}' \\ \mathbf{0} & \mathbf{0} \end{bmatrix};$$

$$\therefore \mathbf{A}^{-1} + \mathbf{FE}^{-1}\mathbf{F}' = \begin{bmatrix} \dfrac{1}{N}\left(1 + \dfrac{R^2 v}{D}\right) & \mathbf{0}' \\ \mathbf{0} & \dfrac{1}{R}\mathbf{I}_v \end{bmatrix}$$

where $1+\dfrac{R^2v}{D}=\dfrac{D+R^2v}{D}=\dfrac{v\left(NL-R^2\right)+(C-1)NL+vR^2}{v\left(NL-R^2\right)+(C-1)NL}=\dfrac{(v+C-1)NL}{D}=\dfrac{(v+C-1)NL}{D}$

$$\therefore \mathbf{A}^{-1}+\mathbf{F}\mathbf{E}^{-1}\mathbf{F}'=\begin{bmatrix}\dfrac{(C+v-1)L}{D} & \mathbf{0}' \\ \mathbf{0} & \dfrac{1}{R}\mathbf{I}_v\end{bmatrix}$$

$$\therefore (\mathbf{X}'\mathbf{X})^{-1}=\begin{bmatrix}\dfrac{(C+v-1)L}{D} & \mathbf{0}' & \dfrac{-R}{D}\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & \dfrac{1}{R}\mathbf{I}_v & \mathbf{0} & \mathbf{0} \\ \dfrac{-R}{D}\mathbf{1} & \mathbf{0} & \dfrac{1}{(C-1)L}\left[\mathbf{I}+\dfrac{\left(R^2-NL\right)}{D}\mathbf{1}\mathbf{1}'\right] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dfrac{1}{L}\mathbf{I}_{v(v-1)/2}\end{bmatrix} \tag{3.3.4}$$

Now D is appearing in the denominator and also a factor of det($\mathbf{X}'\mathbf{X}$)= $R^v L^{v(v-1)/2}[(C-1)L]^{v-1}D$, therefore D>0, we get one more condition on $x_{iu}'s$ other than those given in (3.2.1) for choosing N design points

$$\frac{NL}{R^2}>\frac{v}{v+C-1} \tag{3.3.5}$$

Here, det (.) denotes the determinant of a given matrix. Now, if we write $(v+1)(v+2)/2$-component vector $\boldsymbol{\beta}$ of unknown parameters in (2.2.2) as $\boldsymbol{\beta}'=(\beta_0 \quad \boldsymbol{\theta}' \quad \boldsymbol{\gamma}' \quad \boldsymbol{\varphi}')$ with $\boldsymbol{\theta}'=(\beta_1,\beta_2,\cdots,\beta_v)$; $\boldsymbol{\gamma}'=(\beta_{11},\beta_{22},\cdots,\beta_{vv})$ and $\boldsymbol{\varphi}'=(\beta_{12},\beta_{13},\cdots,\beta_{v-1,v})$. Then using the method of ordinary least squares, the normal equations $\mathbf{X}'\mathbf{X}\boldsymbol{\beta}=\mathbf{X}'\mathbf{y}$ as given in (2.2.3) can be written as

$$\begin{bmatrix} N & \mathbf{0}' & R\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & R\mathbf{I}_v & \mathbf{0} & \mathbf{0} \\ R\mathbf{1} & \mathbf{0} & (C-1)L\mathbf{I}_v+L\mathbf{1}\mathbf{1}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & L\mathbf{I}_{v(v-1)/2}\end{bmatrix}\begin{bmatrix}\beta_0 \\ \boldsymbol{\theta} \\ \boldsymbol{\gamma} \\ \boldsymbol{\varphi}\end{bmatrix}=\begin{bmatrix}G \\ \mathbf{T} \\ \mathbf{P} \\ \mathbf{B}\end{bmatrix} \tag{3.3.6}$$

where $G=\sum_{u=1}^{N} y_u=\mathbf{1}'\mathbf{y}$; y_u is the observation pertaining to u^{th} design point; $u=1,2,\ldots,N$;

$\mathbf{T}' = (T_1, T_2, \cdots, T_v)$ and $T_i = \sum_{u=1}^{N} x_{iu} y_u$; $i = 1, 2, \ldots, v$;

$\mathbf{P}' = (P_1, P_2, \cdots, P_v)$ and $P_i = \sum_{u=1}^{N} x_{iu}^2 y_u$; $i = 1, 2, \ldots, v$ and

$\mathbf{B}' = (B_{12}, B_{13}, \cdots, B_{v-1,v})$ and $B_{ii'} = \sum_{u=1}^{N} x_{iu} x_{i'u} y_u$; $i < i' = 1, 2, \ldots, v$.

$\hat{\boldsymbol{\beta}}$ and variance-covariance matrix of $\hat{\boldsymbol{\beta}}$ can easily be obtained by using (2.2.4), (2.2.5) and (3.3.4). As a consequence, we have

$$\hat{\beta}_0 = b_0 = \left[L(C+v-1)G - R\sum_{i=1}^{v}\sum_{u=1}^{N} x_{iu}^2 y_u \right] \Big/ D \ ;$$

$$\hat{\beta}_i = b_i = \sum_{u=1}^{N} x_{iu} y_u / R; \quad \forall\ i = 1,2,\ldots,v$$

$$\hat{\beta}_{ii} = b_{ii} = \frac{1}{L(C-1)} \sum_{u=1}^{N} x_{iu}^2 y_u + \frac{R^2 - NL}{DL(C-1)} \sum_{i=1}^{v}\sum_{u=1}^{N} x_{iu}^2 y_u - \frac{R}{D} \sum_{u=1}^{N} y_u \quad \forall\ i = 1,2,\ldots,v \text{ and}$$

$$\hat{\beta}_{ii} b_{ii'} = \sum_{u=1}^{N} x_{iu} x_{i'u} y_u / L; \qquad \forall\ i < i' = 1,2,\ldots,v \tag{3.3.7}$$

Using these solutions variances and co- variances of these estimates are obtained as below:

$$\begin{aligned}
&\operatorname{var}(b_0) = \{L(C+v-1)/D\}\sigma^2 && \\
&\operatorname{var}(b_i) = \sigma^2 / R; && \forall\, i = 1, 2, \ldots, v \\
&\operatorname{var}(b_{ii}) = \left\{1 + \left(R^2 - NL\right)/D\right\} / \{L(C-1)\}\sigma^2 && \forall\, i = 1, 2, \ldots, v \\
&\operatorname{var}(b_{ii'}) = \sigma^2 / L && \forall\, i < i' = 1, 2, \ldots, v \\
&\operatorname{covar}(b_0, b_{ii}) = (-R/D)\sigma^2 && \forall\, i = 1, 2, \ldots, v \\
&\operatorname{covar}(b_{ii}, b_{i'i'}) = \left(R^2 - NL\right)\sigma^2 / \{DL(C-1)\} && \forall\, i \neq i' = 1, 2, \ldots, v
\end{aligned} \tag{3.3.8}$$

Other covariances are zero. The estimated response at a point $\mathbf{x}_0' = (x_{10}, x_{20}, \ldots, x_{v0})$ is

$$\hat{y}_0 = b_0 + \sum_{i=1}^{v} b_i x_{i0} + \sum_{i=1}^{v} b_{ii} x_{i0}^2 + \sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} b_{ii'} x_{i0} x_{i'0}$$

with variance as

$$\begin{aligned}
\operatorname{Var}(\hat{y}_0) = {} & \operatorname{Var}(b_0) + \operatorname{Var}(b_i)\sum_{i=1}^{v} x_{i0}^2 + \operatorname{Var}(b_{ii})\sum_{i=1}^{v} x_{i0}^4 + \operatorname{Var}(b_{ii'})\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2 x_{i'0}^2 \\
& + 2\operatorname{Covar}(b_0, b_{ii})\sum_{i=1}^{v} x_{i0}^2 + 2\operatorname{Covar}(b_{ii}, b_{i'i'})\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2 x_{i'0}^2
\end{aligned} \tag{3.3.9}$$

Let $\sum_{i=1}^{v} x_{i0}^2 = d^2$ so that $\sum_{i=1}^{v} x_{i0}^4 = d^4 - 2\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2 x_{i'0}^2$. Substituting these values in (3.3.9) results

$$\begin{aligned}\text{Var}(\hat{y}_0) &= \text{Var}(b_0) + d^2\{\text{Var}(b_i) + 2\,\text{Covar}(b_0, b_{ii})\} + d^4\ \text{Var}(b_{ii}) \\ &\quad + \sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2 x_{i'0}^2 \{Var(b_{ii'}) - 2\,\text{Var}(b_{ii}) + 2\,\text{Covar}(b_{ii}, b_{i'i'})\}\end{aligned} \tag{3.3.10}$$

Using (3.3.8), we get

$$\begin{aligned}\text{Var}(\hat{y}_0) &= \left[L(C+v-1)/D + d^2\left(D-2R^2\right)/RD + d^4\left\{1+\left(R^2-NL\right)/D\right\}/\left(L(C-1)\right)\right]\sigma^2 \\ &\quad + \sigma^2\{(C-3)/(C-1)L\}\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2 x_{i'0}^2\end{aligned} \tag{3.3.11}$$

Consider the coefficient of $\sum_{i=1}^{v-1}\sum_{i'=i+1}^{v} x_{i0}^2 x_{i'0}^2$ in (3.3.11) given by $(C-3)\sigma^2/(C-1)L$. If $C=3$, then this term vanishes and the expression in (3.3.11) becomes

$$\text{Var}(\hat{y}_0) = \left[L(C+v-1)/D + d^2\left(D-2R^2\right)/RD + d^4\left\{1+\left(R^2-NL\right)/D\right\}/\left(L(C-1)\right)\right]\sigma^2 \tag{3.3.12}$$

This expression of variance of the estimated response is a function of $\sum_{i=1}^{v} x_{i0}^2 = d^2$. It, therefore, follows that for all such points $\mathbf{x}$ for which $\sum_{i=1}^{v} x_i^2$ is same constant, the variance of the estimated response at all these points $\mathbf{x}$ will be same. Such property of the designs is known as rotatability and the designs satisfying this property are known as **rotatable designs**. The designs for fitting second order response surfaces satisfying this property alongwith conditions of symmetry (i) to (iv) in (3.3.1) and (3.3.5) are called **Second Order Rotatable Response Surface Designs** (SORD). If (3.3.5) is not satisfied, then it is known as **Second Order Rotatable Arrangement** (SORA).

Thus, the rotatability property of second order response surface designs requires that $\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$ *i.e.*, $C=3$ in the conditions of symmetry (3.3.1) and (3.3.5). This condition actually gives a relationship between fourth order moments (pure and joint). Some other restrictions are also possible, like the relationship between square of the second order moments and fourth order moments, though it seems that these have not been exploited yet. Therefore, in the present investigation, we put another condition

$$\left(\sum_{u=1}^{N} x_{iu}^2\right)^2 = N \sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 \;\; i.e.,\; R^2 = NL \qquad (3.3.13)$$

to get another series of symmetrical response surface designs which provide more precise estimates of response at specific points of interest than what is available from the corresponding existing designs. A design for fitting second order response surfaces satisfying conditions in (3.3.1), (3.3.5) and (3.3.13) will be called a **modified second order response surface design**. If the designs satisfies these conditions along with $C = 3$, then it is called as **modified second order rotatable response surface design**. It is seen that if $R^2 = NL$, then $\mathrm{Co\,var}(b_{ii}, b_{jj}) = 0$. Further, $\mathrm{Var}(b_{ii})$ becomes $\sigma^2 / \{L(C-1)\}$ and D becomes $NL(C-1)$.

Remark 3.3.1: Besides rotatability, D-optimality criterion has been widely advocated in the literature for selection of a response surface design. D-optimal design is one which maximizes determinant of $\mathbf{X}'\mathbf{X}$ in a specified experimental region, where $\mathbf{X}$ is the design matrix for the response surface design. Another criterion for selection of a design is the minimization of variance of predicted response at a given point. It may be seen easily that $R^2 = NL$ maximizes the determinant and minimizes the variance of the predicted response to a reasonable extent, if not the absolute maximization and minimization. For a rotatable design, *i.e.*, $C = 3$ and also if $R^2 = NL$ is satisfied, then $D = 2\,NL$ and

$$\mathrm{Var}(\hat{y}_0) = \left[\frac{v+2}{2N} + \frac{d^4}{2L}\right]\sigma^2. \qquad (3.3.14)$$

Therefore, the application of the condition $R^2 = NL$ in obtaining D-optimal designs needs further attention.

3.3.1 Methods of Construction of Modified and /or rotatable designs for Symmetrical Factorial Experiments

In this section, we give the methods of construction of designs for fitting second order response surfaces for response optimization when various factors are with equispaced levels and/or have unequal dose ranges for both symmetrical as well as asymmetrical factorials. In general, a second order response surface design is at least resolution V plan. Several methods of construction of designs for fitting response surfaces are available in literature. Our main emphasis is on designs obtainable from Central Composite designs of Box and Wilson (1951) and Symmetrical Block Designs with Unequal Block Sizes (SUBA arrangement) of Kishen (1940), balanced incomplete block designs and cyclic designs. The catalogues of the designs obtainable from these methods of construction with $3 \le v \le 10$ and $N \le 500$ are also prepared and included here for a ready reference.

Method 3.3.1: The method is similar to that of Central Composite Designs given by Box and Wilson (1951) on slightly different symbolism. Some modifications have been made for obtaining designs with equispaced doses as well. A central composite design for v-factors is obtained as follows:

1. Take a 2^v factorial arrangement with factorial levels coded as +1or –1 or a 2^p factorial combinations out of 2^v factorial combinations such that no interaction with less than 5 factors is confounded . (In the absence of this condition, the symmetry condition (3.3.1i) are not satisfied). Associate these points to $(\alpha,\alpha,...,\alpha)$. Association is carried out by multiplying the factorial combinations with the set $(\alpha,\alpha,...,\alpha)$. These points are the vertices of a cube and are called as factorial points.

2. 2- axial points on the axis of each design variable at a distance of β from the design centre. As there are v-axis, therefore, this process yield 2v-axial points $(\pm\beta,0,...,0)$, $(0,\pm\beta,0,...,0),\ldots,(0,0,...0,\pm\beta)$. These points are also known as star points and help in the estimation of curvature of the surface. The values of α and β depends on certain properties desired for the design and on the number of factors involved.

3. Add $(n_0 \geq 1)$ center points. The number of center points to be added also depends upon the design properties.

The designs obtained from this method are for 5-level factorial experiments. The level codes are represented by $-\beta,-\alpha,0,\alpha,\beta$. To make the presentation covering a broad class, we take s copies, that is, repetition of the factorial points, and t copies of axial points such that the total number of design points is $N = s.2^v + 2tv + n_0$ or $N = s.2^p + 2tv + n_0$. Here 2^v or 2^p denote the number of factorial combination and let these be denoted by w.

For these designs, $\sum_{u=1}^{N} x_{iu}^2 = R = sw\alpha^2 + 2t\beta^2$; $\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = L = sw\alpha^4$ and $\sum_{u=1}^{N} x_{iu}^4 = CL$. $= sw\alpha^4 + 2t\beta^4$.

To make the design rotatable, we take $C = 3$ and get the following equation,

$$sw\alpha^4 + 2t\beta^4 = 3sw\alpha^4$$

$$\Rightarrow \frac{t\beta^4}{s\alpha^4} = w \tag{3.3.15}$$

For obtaining a modified design, we take $R^2 = NL$ and get the following equation

$$\left(sw\alpha^2 + 2t\beta^2\right)^2 = (sw + 2tv + n_0)sw\alpha^4$$

$$\Rightarrow 4t^2\beta^4 + 4stw\alpha^2\beta^2 = 2stvw\alpha^4 + n_0 sw\alpha^4$$

$$\Rightarrow n_0 = \frac{4t^2\beta^4 + 4stw\alpha^2\beta^2 - 2stvw\alpha^4}{sw\alpha^4} \tag{3.3.16}$$

For obtaining modified second order response surface designs alone, we have to fix n_0 and obtain the values for α, β, s and t satisfying (3.3.16). Since, there is only one equation, we can estimate only one parameter. Hence, we fix three of them, α, s and t (say) and obtain the value of β. For $s=1$, $t=1$ and $\alpha=1$, the value of β is generally different from that of rotatable designs. Also the values of α and β change with the change in the value of n_0 and hence, N in modified design whereas the values of α and β remains unchanged with the change in the value of n_0 and hence, N in a rotatable design. This is explained with the help of following example.

Let a design with $v=3$ and $N=14$ is obtained by using the sets $(1)\alpha\alpha\alpha$, $(2)\beta 0 0$ $(3) 0 \beta 0$ and $(4) 0 0 \beta$, where α and β are unknowns. Associating the factorial 2^3 with these sets the distinct combinations give the design. Some more points of the type $(0\,0\,0)$ can be added to the design, which are known as center points. This in general is the design obtained using central composite designs. The design points (without center points) are the following

α	α	α
α	α	-α
α	-α	α
α	-α	-α
-α	α	α
-α	α	-α
-α	-α	α
-α	-α	-α
β	0	0
-β	0	0
0	β	0
0	-β	0
0	0	β
0	0	-β

$R=8\alpha^2+2\beta^2$, $L=8\alpha^4$ $CL=8\alpha^4+2\beta^4$

For obtaining a modified design, we use the relation $R^2=NL$ and get

$$\left(8\alpha^2+2\beta^2\right)^2=14\times 8\alpha^4$$

or $8\alpha^2+2\beta^2=4\times 2.645751311\alpha^2$

or $\beta^2=1.291503\alpha^2$

Now fixing α, conveniently, β is known. Thus the design as combination of level codes is obtained along with R, L and CL. For $\alpha=1$, $\beta=1.136443$. It may be seen easily that as N changes for a modified response surface design, the ratio β/α also changes, *e.g.*, with the addition of one central point in the above design. Taking $n_0=1$ and N = 15 in the relation $R^2=NL$ we get $\beta^2=1.477226\alpha^2$. For $\alpha=1$, $\beta=1.215412$.

For a rotatable design *i.e.*, for $C = 3,\ \beta^4 = 8\alpha^4$. For $\alpha = 1,\ \beta = 1.682$. For a rotatable design this ratio remains the same if the change in N is due to addition of center points only. Taking $\alpha = 1$ the variances of estimated responses at the center, axial and factorial points of interest for modified and rotatable designs are presented in the following table.

Number of Design Points	Nature of the Point	Variance of the estimated response $\left[\operatorname{var}(\hat{y}_0)/\sigma^2\right]$	
		Modified	Rotatable
14	Center	0.58531	*85.65518
	Axial	0.62203	0.70716
	Factorial	0.78347	0.71996
15	Center	0.43327	0.98846
	Axial	0.50113	0.60831
	Factorial	0.76553	0.67021

** This variance is exceptionally high due to the fact that in case of a rotatable design for 3 factors with 14 runs, the* $\mathbf{X}'\mathbf{X}$ *matrix is almost singular.*

It can easily be seen that for this design both the conditions *viz.* $C = 3$ and $R^2 = NL$ cannot be satisfied simultaneously for fixed $N = 14$ or $N = 14 + n_0$, where n_0 is the number of center points. However, we can see that both these conditions $C = 3$ and $R^2 = NL$ can be satisfied simultaneously, if we obtain n_0 through (3.16) by substituting the ratio of β/α obtained for a rotatable design. This is given in the sequel.

If we want to get a modified and rotatable design, then substituting $\dfrac{\beta^4}{\alpha^4} = \dfrac{sw}{t}$ in (3.3.16), gives

$$n_0 = 2t\left[2 + 2\sqrt{\frac{sw}{t}} - v\right] \tag{3.3.17}$$

The number of center points is a whole number only when (sw/t) is a perfect square. As a consequence, construction of a modified and rotatable design is possible only when (sw/t) is a perfect square.

For obtaining most commonly used central composite designs {Box and Wilson, 1951}, $s = 1,\ t = 1$. Therefore, we substitute $s = 1,\ t = 1$ in (3.3.15) and get $\dfrac{\beta}{\alpha} = w^{1/4}$. Now taking $\alpha = 1,\ \beta$ can be obtained as fourth root of the number of factorial runs. Some typical values of β for a second order response surface design with $2 \le v \le 10$ and $N \le 500$ are given in Table 3.3.1. In this table n_0 denotes the number of center points, it can be chosen as per requirement and availability of the resources. For $s = 1,\ t = 1$, the number of central points in modified and rotatable design using (3.3.17) are

$$n_0 = 2\left[2 + 2\sqrt{w} - v\right] \qquad (3.3.18)$$

As a consequence, the construction of a modified and rotatable design from the above method with $s = 1,\ t = 1$ is possible only for those situations, in which *w*, the number of factorial runs is a perfect square. For a design to be modified and rotatable n_0 for the feasible cases are also given in Table 3.3.1.

Table 3.3.1: The value of β and N for a second order response surface design with $2 \le v \le 10$.

v	p	β	N (for a rotatable design)	N (for a modified rotatable design)
2	2	1.4142	8+ n_0	8+8=16
3	3	1.6818	14+ n_0	
4	4	2.0000	24+ n_0	24+12=36
5	4	2.0000	26+ n_0	26+10=36
5	5	2.3784	42+ n_0	
6	5	2.3784	44+ n_0	
6	6	2.8284	76+ n_0	76+24=100
7	6	2.8284	78+ n_0	78+22=100
7	7	3.3636	142+ n_0	
8	6	2.8284	80+ n_0	80+20=100
8	7	3.3636	144+ n_0	
8	8	4.0000	272+ n_0	272+52=324
9	7	3.3636	146+ n_0	
9	8	4.0000	274+ n_0	274+50=324
10	8	4.0000	276+ n_0	276+48=324

Designs for Response Optimization when the Factors have Equispaced Levels

In agricultural experiments, the factors considered may have equispaced doses (levels) as discussed above. The response surface designs with *v* factors each having equispaced doses may be obtained through a central composite design by using the following procedure of Method 3.3.1. Let the dose codes be $-2,-1,0,1,2$, then the design can be obtained by taking $\alpha = 1, \beta = 2$. For this situation

$$R = s.2^p + 8t, \quad L = s.2^p, \quad CL = s.2^p + 32t.$$

To make the design rotatable, we take $C = 3$ and get the following equation,

$$sw + 32t = 3.s.w$$

$$\Rightarrow 16t = sw$$

$$\Rightarrow (s/t) = 16/w \qquad (3.3.19)$$

Therefore, a central composite type rotatable design with equispaced doses can now be obtained by taking s and t in the ratio $16:w$. Some center points can also be added when required. We know that for a modified and rotatable design $R^2 = NL$ and $C = 3$. These two conditions are satisfied simultaneously by adding n_0 central points where $n_0 = 2t(10 - v)$. This is so because of the following

$$s^2w^2 + 64t^2 + 16tsw = (sw + 2tv + n_0).sw \tag{3.3.20}$$

If $C = 3$, then $sw = 16t$. Substituting for sw above, we get

$$256t^2 + 64t^2 + 256t^2 = (16t + 2tv + n_0) \times 16t$$
$$\Rightarrow n_0 = 2t(10 - v). \tag{3.3.21}$$

Thus choosing s, t and n_0 as above, we get modified and rotatable designs when each of the factors is at 5 equispaced levels. The values of s, t, n_0 and N for modified and rotatable designs for factorials with equispaced doses with $3 \le v \le 10$ and $N \le 500$ are given in Table 3.3.2 . The design for $v = 2$ is not included in this table as the number of design points required are more than the total factorial combinations. Table 3.3.2 also does not contain any design with $v = 10$, as $N \ge 500$.

Table 3.3.2: The values of v, p, s, t, n_0 **and** N **for modified and rotatable second order response surface designs for equispaced doses with** $3 \le v \le 10$ **and** $N \le 500$**.**

v	p	s	t	n_0	N
3	3	2	1	14	36
4	4	1	1	12	36
5	4	1	1	10	36
5	5	1	2	20	72
6	5	1	2	16	72
6	6	1	4	32	144
7	6	1	4	24	144
7	7	1	8	48	288
8	6	1	4	16	144
8	7	1	8	32	288
9	7	1	8	16	288

It may be noted here that with the same number of copies of s and t the design remains rotatable with some copies of n_0, so as to make $D > 0$. Here n_0 may be smaller or greater than the value indicated in the above table.

To obtain a modified design only, the condition to be satisfied is $R^2 = NL$, *i.e.*,

$$s^2w^2 + 64t^2 + 16tsw = (sw + 2tv + n_0).sw$$

By fixing $s=1$ and $t=1$ we get

$$n_0 = \frac{64+(16-2v)w}{w} \tag{3.3.22}$$

The value of n_0 in (3.3.22) may be a fraction or negative integers. We present only those designs with $3 \le v \le 10$ and $N \le 500$ for which n_0 is a positive integer in Table 3.3.3. The design for $v=2$ is not included in this table as the number of design points required are more than the total factorial combinations.

Table 3.3.3: The values of v, p, n_0 **and** N **for modified second order response surface designs for equispaced doses with** $3 \le v \le 10$ **and** $N \le 500$**.**

v	p	n_0	N
3	3	18	32
4	4	12	36
5	4	10	36
5	5	8	50
6	5	6	50
6	6	5	81
7	6	3	81
8	6	1	81

Method 3.3.2: This method is based on BIB designs and uses the methods of construction given by Box and Behnken (1960) and Das and Narsimham (1962) with slight modifications so as to get modified and/or rotatable designs with equispaced doses.

A balanced incomplete block design is an arrangement of *v* treatments in *b* blocks each of size *k* *(v<k)* such that a treatment is applied atmost once in a block, each treatment occurs exactly in *r* blocks and each pair of treatment occur together in λ blocks.

Let $\mathbf{M} = (m_{ji})$ be the incidence matrix of a BIB design with parameters *v, b, r, k,* λ where **M** is defined as follows:

$$m_{ji} = \begin{cases} 1, & \text{if the } i^{th} \text{ treatment occurs in the } j^{th} \text{ block} \\ 0, & \text{otherwise} \end{cases} \qquad (i=1,\ldots,v; \quad j=1,\ldots,b)$$

The element 1 in the incidence matrix is replaced by an unknown α.. From the rows of this matrix involving 0 and the unknown α, we shall get *b* combinations. Each of these combinations is then associated with a 2^k factorial or a suitable Resolution V fraction, say 2^p, of it, the levels being coded as ± 1. Let these 2^k or 2^p be denoted by *w*. For these bw points, we have

$$R=\sum_{u=1}^{N}x_{iu}^{2}=rw\alpha^{2};\; CL=\sum_{u=1}^{N}x_{iu}^{4}=rw\alpha^{4} \quad \text{and} \quad L=\sum_{u=1}^{N}x_{iu}^{2}x_{i'u}^{2}=\lambda w\alpha^{4}$$

For obtaining a rotatable design, we take $C=3$, *i.e.*, $\sum_{u=1}^{N}x_{iu}^{4}=3\sum_{u=1}^{N}x_{iu}^{2}x_{i'u}^{2}$ and get the following equation

$$rw\alpha^{4}=3\lambda w\alpha^{4} \quad \Rightarrow \quad r=3\lambda. \tag{3.3.23}$$

If a BIB design with $r=3\lambda$ exists for given v, then no further combinations need to be taken excepting center points. By taking $\alpha=1$, we can get designs with v factors each at three levels coded as -1, 0, +1. The number of design points is $N=bw+n_0$.

For getting a rotatable design, we take $R^2=NL$ and get the following equation

$$r^2w^2\alpha^4=(bw+n_0)\lambda w\alpha^4$$
$$\Rightarrow r^2w^2=b\lambda w^2+n_0\lambda w$$
$$\Rightarrow n_0=\frac{w(r^2-b\lambda)}{\lambda} \tag{3.3.24}$$

For obtaining the number of center points for a modified and rotatable design, we substitute (3.3.23) in (3.3.24) and get

$$n_0=w(9\lambda-b) \tag{3.3.25}$$

The values of v, p, n_0, N for modified and rotatable designs obtainable from BIB designs with $r=3\lambda$ for $3\le v\le 10$ and $N\le 500$ are given in Table 3.3.4. For a rotatable design alone n_0 may be smaller or greater than the value indicated in the above table. For this value of n_0, the non-singularity condition is satisfied.

Table 3.3.4: The values of $v, p,\ n_0$ and N for modified and rotatable second order response surface designs for three equispaced doses with $3\le v\le 10$ and $N\le 500$ obtainable from Method 3.3.2.

v	p	n_0	N	Source BIB design
4	2	12	36	(4,6,3,2,1)
7	3	16	72	(7,7,3,3,1)
10	4	48	288	(10,15,6,4,2)

From (3.3.24), it is clear that the condition $r=3\lambda$ is not required for obtaining a modified second order response surface design alone. The values of v, p, n_0, N for modified designs obtainable from BIB designs with $r\ne 3\lambda$ for $3\le v\le 10$ and $N\le 500$ are given in Table 3.3.5. In this Table the design for 3 factors with 16 design points is same as studied by De Baun (1959). De Baun (1959) reported that for 3^3 factorial with less than 20 design points, this design provides orthogonality, 3 degrees of freedom for pure error and provides almost rotatable information surface.

Table 3.3.5: The values of v, p, n_0 and N for modified second order response surface designs for three equispaced doses with $3 \le v \le 10$ and $N \le 500$ obtainable from Method 3.3.2.

v	p	n_0	N	Source BIB design
3	2	4	16	(3,3,2,2,1)
5	2	24	64	(5,10,4,2,1)
6	2	40	100	(6,15,5,2,1)
6	3	20	100	(6,10,5,3,2)
6	4	4	100	(6,6,5,5,4)
6	5	8	200	(6,6,5,5,4)
7	2	60	144	(7,21,6,2,1)
8	2	84	196	(8,28,7,2,1)
9	2	112	256	(9,36,8,2,1)
9	3	32	128	(9,12,4,3,1)
9	4	32	320	(9,18,10,5,5)
10	2	144	324	(10,45,9,2,1)
10	3	84	324	(10,30,9,3,2)
10	4	36	324	(10,18,9,5,4)

If however, the relation $r = 3\lambda$ does not hold in a BIB design, we have to take further combinations of another unknown β as indicated below.

If $r < 3\lambda$, we take the combinations $(\pm\beta, 0,...,0)$, $(0,\pm\beta, 0,...,0)$,... $(0,...,0,\pm\beta)$. The values of the unknowns have to be fixed in this case by using the relation

$$\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 \text{ and /or } \left(\sum_{u=1}^{N} x_{iu}^2\right)^2 = N\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 .$$

If again, $r > 3\lambda$, the combinations $(\pm\beta, \pm\beta,...,\pm\beta)$ have to be taken along with the combinations obtained from the incidence matrix of the BIB design. Here, again the restriction $\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$ and /or $\left(\sum_{u=1}^{N} x_{iu}^2\right)^2 = N\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$ has to be used for determining one of the unknown levels.

For obtaining modified and/or rotatable designs when each of the factors at 5 equispaced levels (-2,-1,0,1,2) using BIB designs, we take s copies of the points obtained from the incidence matrix and t copies of the added points (other than the center points). We get the following.

When $r < 3\lambda$

$\sum_{u=1}^{N} x_{iu}^2 = R = s\,r\,w + 8t$, $\quad \sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = L = s\,\lambda\,w$ and $\quad \sum_{u=1}^{N} x_{iu}^4 = CL = s\,r\,w + 32t$

$$N = bsw + 2vt + n_0 .$$

For a second order rotatable design, $C = 3,$ *i.e.*,

$$\sum_{u=1}^{N} x_{iu}^4 = 3 \sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$$

$$\Rightarrow srw + 32t = 3s\lambda w$$

$$\Rightarrow \frac{s}{t} = \frac{32}{(3\lambda - r)w} \tag{3.3.26}$$

We know that for a modified and rotatable second order response surface design both the conditions $R^2 = NL$ and $C = 3$ are satisfied simultaneously. Therefore, to obtain a modified and rotatable second order response surface design, we have to choose n_0 center points so that the condition $R^2 = NL$ is satisfied, *i.e.*.

$$(s\,r\,w + 8t)^2 = (bsw + 2vt + n_0)s\lambda w$$

$$\Rightarrow n_0 = t\left[\frac{r^2 - b\lambda}{\lambda}\frac{sw}{t} + \frac{16r - 2v\lambda}{\lambda} + \frac{64}{\lambda}\frac{t}{sw}\right] \tag{3.3.27}$$

Now substituting (3.3.26) in (3.3.27), we get the number of center points to be added as:

$$n_0 = 2t\left[\frac{16(r^2 - b\lambda)}{\lambda(3\lambda - r)} + \frac{7r - \lambda(v-3)}{\lambda}\right] \tag{3.3.28}$$

In some cases, the above formula, may give the value of n_0 in fraction. Therefore, we have to be careful and construct the designs only for those situations, where n_0 is a positive integer.

The values of v, p, s, t, n_0, N for modified and rotatable designs obtainable from BIB designs with $r < 3\lambda$ for $3 \le v \le 10$ and $N \le 500$ are given in Table 3.3.6. For a rotatable design alone n_0 may be smaller or greater than the value indicated in the above table. For this value of n_0, $D > 0$.

Table 3.3.6: The values of v, p, s, t, n_0 and N for modified and rotatable second order response surface designs for five equispaced doses with $3 \le v \le 10$ and $N \le 500$ obtainable from BIB designs with $r < 3\lambda$.

v	p	s	t	n_0	N	BIBD
4	3	4	3	136	288	(4, 4, 3, 3, 2)
*5	3	4	3	304	654	(5,10,6,3,3)
6	3	4	1	144	476	(6, 10, 5, 3, 2)
6	4	2	7	456	732	(6, 6, 5, 5, 4)
*6	5	1	7	456	732	(6, 6, 5, 5, 4)
7	4	1	1	64	190	(7, 7, 4, 4, 2)

*These designs have been included here because the rotatable design can be obtained in number of design points $N \le 500$ by taking smaller number of center points.

To obtain a modified design only, the condition to be satisfied is (3.3.27). By fixing $s = 1$ and $t = 1$, we get

$$\frac{1}{\lambda w}\left[\left(r^2 - b\lambda\right)w^2 + \left(16r - 2v\lambda\right)w + 64\right] = n_0 \tag{3.3.29}$$

Using the above, one can construct a modified second order response surface design with the parameters $v = 10, p = 4, s = 2, t = 15, n_0 = 128, N = 748.$ This design can be obtained by using a BIB design (10,10,9,9,8).

For $r > 3\lambda$, we have

$$\sum_{u=1}^{N} x_{iu}^2 = R = s\,r\,w_1 + 4tw_2 \quad \text{where } 2^p = w_1 \text{ and } 2^v \text{ or a fraction of it} = w_2$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = L = s\,\lambda w_1 + 16tw_2 \quad \text{and} \quad \sum_{u=1}^{N} x_{iu}^4 = CL = s\,rw_1 + 16tw_2\,; \quad N = bsw_1 + tw_2 + n_0$$

For rotatability, we have $C = 3$, *i.e.*

$$\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$$

$$\Rightarrow \left(srw_1 + 16tw_2\right) = 3\left(s\lambda w_1 + 16tw_2\right)$$

$$\Rightarrow \frac{s}{t} = \frac{32}{r - 3\lambda}\frac{w_2}{w_1} \tag{3.3.30}$$

We know that for a modified and rotatable second order response surface design both the conditions $R^2 = NL$ and $C = 3$ are satisfied simultaneously. Therefore, to obtain a modified and rotatable second order response surface design, we have to choose n_0 central points so that the condition $R^2 = NL$ is satisfied, *i.e.*.

$$\Rightarrow \left(s\, r\, w_1 + 4tw_2\right)^2 = \left(bsw_1 + tw_2 + n_0\right)\left(s\lambda w_1 + 16tw_2\right)$$

$$\Rightarrow n_0 = \frac{s^2 w_1^2\left(r^2 - b\lambda\right) + stw_1 w_2\left(8r - \lambda - 16b\right)}{s\lambda w_1 + 16tw_2} \qquad (3.3.31)$$

Now substituting (3.3.30) in (3.3.31), we can get the number of center points to be added as

$$\Rightarrow n_0 = \frac{32sw_1\left(r^2 - b\lambda\right) + 32w_2\left(8r - \lambda - 16b\right)}{16r - 47\lambda} \qquad (3.3.32)$$

In some cases, the above formula may give the value of n_0 in fraction. Therefore, we have to careful and construct the designs only for those situations, where n_0 is a positive integer. Using conditions (3.3.30) and (3.3.32), modified and rotatable second order response surface designs obtainable from BIB desings with $r > 3\lambda$ can easily be obtained.

To obtain a modified design only, the condition to be satisfied is (3.3.31). By fixing $s = 1$ and $t = 1$, we get

$$n_0 = \frac{w_1^2\left(r^2 - b\lambda\right) + w_1 w_2\left(8r - \lambda - 16b\right)}{\lambda w_1 + 16w_2} \qquad (3.3.33)$$

Remark 3.3.2: A generalization of Method 3.3.2 was given by Raghavarao (1963) by using symmetrical unequal block arrangement with two distinct block sizes (SUBA) instead of BIB designs. SUBA was introduced by Kishen (1940) and is defined as: An arrangement of v treatments in b blocks, where b_1 blocks are of size k_1 and b_2 blocks are of size k_2 such that $b_1 + b_2 = b$ is said to be a SUBA if

(i) every treatment occurs in $\left(b_i k_i / v\right) = r_i$ blocks of size k_i; $(i = 1,2)$ and

(ii) every pair of first block associates occur together in u blocks of size k_1 and in $\lambda - u$ blocks of size k_2 and every pair of second block associates occur together in λ blocks of size k_2.

These arrangements can easily be obtained by $D_1 \cup D_2$, where D_1 and D_2 are two associate partially balanced incomplete block (PBIB) designs based on same association scheme and with parameters

$D_1 : v, b_1, r_1, k_1, n_1, n_2, \lambda_1 = u, \lambda_2 = 0$ and $D_2 : v, b_2, r_2, k_2, n_1, n_2, \lambda_1 = \lambda - u, \lambda_2 = \lambda$.

The method of construction is as follows: Let $v, b, r = r_1 + r_2, k_1, k_2, b_1, b_2$ and λ be the parameters of a SUBA. Obtain the incidence matrix $\mathbf{M}$ as in Method 3.3.2. Let $k_1 < k_2$ and $\frac{1}{2^{k_2 - k_1}}$ th replicate of 2^{k_2} factorial exists without including any interaction of less than five factors in the identity relation, then by multiplying the unknown combinations of α arising from the blocks of size k_1 with 2^{k_1} factorial with levels being coded as ± 1 and the unknown combinations arising from blocks of size k_2 with a $\frac{1}{2^{k_2-k_1}}$ th replicate of 2^{k_2} combinations.

For this design $R=\sum_{u=1}^{N} x_{iu}^2 = rw\alpha^2$; $CL=\sum_{u=1}^{N} x_{iu}^4 = rw\alpha^4$; $L=\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = \lambda w\alpha^4$ and $N = bw + n_0$; where $r = r_1 + r_2$ and $w = 2^{k_1}$. We get a second order rotatable design, if $r = 3\lambda$. If $r \neq 3\lambda$ then the modifications as given in Method 3.3.2 gives second order rotatable designs with 5 equispaced factors. Further, proceeding on the similar lines of Method 3.3.2, the modified and/or rotatable designs with 5 equispaced doses can be obtained.

Remark 3.3.3: Following the method of construction given in Remark 3.3.2, we can get a modified and/or rotatable design by using any equireplicated pairwise balanced block design with two distinct block sizes if the design is equireplicated separately for the two sets of blocks of different sizes.

Designs with Four Levels

The Method 3.3.1 gives the modified and/or rotatable designs for the situation where each of the factor has five levels and Method 3.3.2 yield designs for 3 and 5 level factorial experiments. In agricultural and allied sciences, many experiments are conducted with 4 level factors. Here, we present a method for obtaining designs with 4 level factorial experiments. The method was originally given by Das (1961) and modified by Nigam and Dey (1970). A further refinement is suggested in the present investigation.

Method 3.3.3: Let there be *v*-factors at 4 levels each. Let the level codes be denoted by $-\beta, -\alpha, \alpha, \beta$. Now consider a set of *v*-combinations obtained by cyclic permutations of $(\alpha\, \beta\, \beta \cdots \beta)$. Call these combinations as Type I. Consider another set of combinations as the design points of a 2^v factorial (or a suitable fraction of 2^v, at least of Resolution V) and call these combinations as Type II. Now associate each of the combinations of Type I with each of the combinations of Type II. This can be achieved by multiplying Type I combinations with Type II combinations. This process yields an arrangement of $v.\ 2^{v-p}$ points in *v* factors, where 2^{v-p} denotes the smallest Resolution V fraction of 2^v. Denote 2^v or 2^{v-p} by *w*.

From the above vw design points, it can easily be verified that these points satisfy the conditions of symmetry given in (3.3.1) and

$$R=\sum_{u=1}^{N} x_{iu}^2 = w(\alpha^2 + (v-1)\beta^2)\,;\ CL=\sum_{u=1}^{N} x_{iu}^4 = w(\alpha^4 + (v-1)\beta^4)\,;$$

$$L=\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = w(2\alpha^2\beta^2 + (v-2)\beta^4) \text{ and } N = vw.$$

For a rotatable design, $C = 3$, therefore, we obtain the values of α and β satisfying

$$w\{\alpha^4 + (v-1)\beta^4\} = w\{6\alpha^2\beta^2 + 3(v-2)\beta^4\}$$
$$\Rightarrow \frac{\alpha^2}{\beta^2} = 3 \pm (4+2v)^{1/2} \quad (3.3.34)$$

Now taking $\beta = 1$, we get $\alpha = \pm\{3 \pm (4+2v)^{1/2}\}^{1/2}$

Both Das (1961) and Nigam and Dey (1970) have given these values for α and β. However, for square root to be real number, all these values must be positive, i.e.

$$3-(4+2v)^{1/2} \geq 0; \quad \Rightarrow v \leq 5/2$$

In other words, it holds only for $v = 2$. Hence, for $v \geq 3$ and $\beta = 1$, this value of α will not give any result. *Therefore, only* $\alpha = \pm\{3+(4+2v)\}^{1/2}$ *should be taken*.

Further, it can easily be verified that $vR^2 = (v+2)NL$. As a consequence, the condition (3.3.5) is not satisfied and above procedure results into a second order rotatable arrangement rather than a second order rotatable design. This was also pointed out by Nigam and Dey (1970). They modified this second order rotatable arrangement in *v* factors and *N* design points by deleting any $x \geq 1$ columns from $N \times v$ arrangement. Now the $N \times v - x$ matrix is a SORD with $v - x$ factors. For $x = 1$, the values of α when $\beta = 1$ are given in Table 3.3.7 for $3 \leq v \leq 10$.

Table 3.3.7: The values of α, p and $N \leq 500$ for a SORA in *v* factors and SORD in $v - x$ factors obtainable from Method 3.3.3.

v	$v-x$	p	alpha	N
3	2	3	2.482394	24
4	3	4	2.54246	64
5	4	4	2.59647	80
5	4	5	2.59647	160
6	5	5	2.645751	192
6	5	6	2.645751	384
7	6	6	2.691215	448

This result can further be improved upon and is stated in the following result:

Result 3.3.1: {Nigam and Dey (1970)}. Let There exist a SORD in *v* factors, then the design obtained by omitting any *x* columns of the design is also a SORD in *(v – x)* factors.

Remark 3.3.4: In this particular case, the designs developed are with factors at 4 levels each. Therefore, we cannot add center points to get a modified and rotatable second order response surface design. Therefore, we make an attempt to obtain modified second order response surface design alone. For a modified design $R^2 = NL$ which implies that $\alpha = \beta$ in this case. Therefore, it is not possible to obtain a modified second order response surface design using Method 3.3.3.

Remark 3.3.5: We can see that the SORD for $v - x$ factors at 4 levels each obtained from the Method 3.3.3 are not for the situations with equispaced doses. If we take, $\beta = 1, \alpha = 3$, the levels will be -3, -1, 1, 3 and are equispaced. If we take these values of α and β in the above method, then the construction of a SORD is not possible. Then $R = w(8+v)$; $CL = w(80+v)$; $L = w(16+v)$. For this case $C = \dfrac{80+v}{16+v}$. Now if we take $\beta = 3, \alpha = 1$, then $R = w(9v-8)$; $CL = \sum_{u=1}^{N} x_{iu}^4 = w(81v-80)$; $L = w(81v-144)$. For this case $C = \dfrac{81v-80}{81v-144}$.

Remark 3.3.5 provides only one solution for obtaining the designs for fitting second order response surface designs. To obtain the methods of construction of modified second order rotatable response surface designs needs further attention.

3.3.2 Asymmetric Response Surface Designs

In Section 3.3.1, we have discussed the methods of construction of modified and/ or rotatable second order response surface designs for symmetric factorial experiments *i.e.* when all the factors have same number of levels. In practice, however, there do occur experimental situations in which it is not possible to maintain same number of levels for all the factors. Ramchander (1963) initiated the work on obtaining response surface designs for asymmetrical factorials and gave two series of response surface designs for asymmetrical factorials of the type 3×5^m, but no systematic method of construction was developed. Mehta and Das (1968) gave a general method of construction of rotatable response surface designs for asymmetrical factorials by applying orthogonal transformations on the design points of a suitably chosen symmetric rotatable design. The method is described in the sequel.

Method 3.3.4: Consider a symmetric rotatable design in *v*-factors each at *s* levels. Let $\mathbf{x}'_u = (x_{1u}\ x_{2u} \cdots x_{iu} \cdots x_{vu})$ denote the u^{th} design point of the symmetric rotatable design, $\mathbf{B}$ is an $v \times v$ orthonormal transformation matrix, then the new design point $\mathbf{z}'_u = (z_{1u}\ z_{2u} \cdots z_{iu} \cdots z_{vu})$ can be obtained through the relationship

$$\mathbf{z}'_u = \mathbf{x}'_u \mathbf{B} \qquad u = 1, 2, \cdots, N \qquad (3.3.35)$$

A proper choice of $\mathbf{B}$, helps in obtaining an Asymmetric Rotatable Design from a second order rotatable design. To illustrate, we consider the following example.

Let us consider a second order rotatable central composite design in 4 factors $(\pm\alpha, \pm\alpha, \pm\alpha, \pm\alpha)$, $(\pm 2\alpha,\ 0,\ 0,\ 0)$, $(0,\ \pm 2\alpha,\ 0,\ 0)$, $(0,\ 0,\ \pm 2\alpha,\ 0)$, $(0,\ 0,\ 0,\ \pm 2\alpha)$, (0, 0, 0, 0), where α is a non-zero constant. The notation $(\pm\alpha, \pm\alpha, \pm\alpha, \pm\alpha)$ is used to denote the 16 points generated by all possible combinations of signs. $(\pm 2\alpha,\ 0,\ 0,\ 0)$ will also the similar meaning. If we choose the matrix $\mathbf{B}$ as follows

$$\mathbf{B} = \begin{bmatrix} e & -f & -c & -d \\ f & e & d & -c \\ c & -d & e & f \\ d & c & -f & e \end{bmatrix} \qquad (3.3.36)$$

where $c^2+d^2+e^2+f^2=1$, and transform the design points of the central composite design using (3.3.36), then the transformed design has the levels $(\pm c, \pm d, \pm e, \pm f)\alpha$, $\pm c\beta$, $\pm d\beta$, $\pm e\beta$ and $\pm f\beta$, for all the factors. The maximum number of levels for each factor is obviously 24.

Next, the elements of $\mathbf{B}$ are chosen in such a manner that desired asymmetry is induced in the transformed design. For example, if $\mathbf{B}$ is chosen as

$$\mathbf{B}=\begin{bmatrix} e & -f & 0 & 0 \\ f & e & 0 & 0 \\ 0 & 0 & c & d \\ 0 & 0 & -d & c \end{bmatrix} \qquad (3.3.37)$$

then the first two factors of the transformed design will have the levels as $(\pm e, \pm f)\alpha$, $\pm e\beta$, $\pm f\beta$, and 0 and the last two factors will have the levels $(\pm c, \pm d)\alpha$, $\pm cb$, $\pm db$, and 0. Through a proper choice of c, d, e, f one can make the number of levels of the two pairs of two factors unequal. Therefore, $e=f=1/\sqrt{2}$ and $c=1/\sqrt{5}$, $d=2/\sqrt{5}$ will give a transformed design which is an incomplete factorial $3^2\times 7^2$ having three levels $0, \pm\sqrt{2}a$ for the first two factors and the seven levels $0, \pm a/\sqrt{5}$, $\pm 2a/\sqrt{5}$ and $\pm 3a/\sqrt{5}$ for the remaining two factors.

This transformation permits the factors to have different numbers of levels while preserving rotatability. The numbers of levels of the factors depend upon the orthogonal transformation matrix. As a consequence, *it is not always possible to achieve the specified number of levels of each factor*.

Draper and Stoneman (1968) have also studied the response surface designs for asymmetric factorials when some factors are at two levels and other factors are at 3 or 4 levels each. For these designs, the response surface cannot include quadratic terms in factors that are at two levels each but all second order terms for variables to be examined at 3 or 4 levels can be permitted. Dey (1969) gave methods of construction of both rotatable and non-rotatable asymmetric response surface designs. The non-rotatable type of designs have a special feature that a part of the design retains the property of rotatability and as such these designs have been called as partially rotatable designs. A direct and straightforward method of construction of asymmetric rotatable designs is also given. This method yields response surface designs for the $5^{v-2}\times 3^2$ factorial experiments i.e. when two factors are at three levels and others are at five levels. The method of construction with some modifications is described in the sequel.

Method 3.3.5: Let the levels of factors that are at five levels each are denoted by $\pm\alpha$, 0, $\pm\beta$ and for those, which are at three levels by $\pm\alpha'$ and 0. α, α' and β can be obtained satisfying the conditions of rotatability and will be described later. A set $(\alpha, \alpha, ..., \alpha)$ is considered for $v-2$ factors which are 5 levels. This set is associated with 2^{v-2} factorial (or a fraction thereof without confounding any interaction with less than five factors for obtaining the fraction), the levels of the factorial being -1 and $+1$. Let the number of points thus obtained be denoted by *w*. A further half fraction of these points are taken. Against one of the fractions containing $\frac{w}{2}$ points, write $(\alpha' \ 0)$ and then again $(-\alpha' \ 0)$ for the two factors at three levels each. Thus, we get in all $\frac{w}{2}+\frac{w}{2}=w$ design points. Against the remaining half fraction of $\frac{w}{2}$ points, write $(0 \ \alpha')$ and then again $(0 \ -\alpha')$. In this way we get another *w* points.

Further consider the following set of combinations

1	2	...	...	...	$v-2$	$v-1$	v
β	0	...	...	...	0	0	0
0	β	...	...	...	0	0	0
:							
:							
:							
0	0	...	...	...	β	0	0

and associate each of them with $+1$ and -1 in all possible ways. This process yields $2(v-2)$ points. Further, take s_1 copies of $2w$ points obtained earlier and t copies of $2(v-2)$ points obtained above so as to make $\beta = 2\alpha$ under the condition of rotatability. This ensures that the doses of the factors at 5 levels each are equispaced.

Finally the set $(0, \ 0, \ ... \ ...; \alpha', \alpha')$ is taken and associated with the combinations of a 2^2 factorial with levels $+1$ and -1. Repeat these points s_2. Thus we have $N = 2ws_1 + 2t(v-2) + 4s_2$ and

$$\sum_{u=1}^{N} x_{iu}^2 = 2ws_1\alpha^2 + 2t\beta^2 \tag{3.3.38i}$$

$$\sum_{u=1}^{N} x_{iu}^4 = 2ws_1\alpha^4 + 2t\beta^4 \tag{3.3.38ii}$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = 2ws_1\alpha^4 \qquad i \neq i', \ i, i' = 1, 2, ..., \ v-2 \tag{3.3.38iii}$$

For satisfying the rotatability condition, $\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$

$$2ws_1\alpha^4 + 2t\beta^4 = 6ws_1\alpha^4 \tag{3.3.38iv}$$

If $\beta = 2\alpha$, we get

$$4ws_1\alpha^4 = 32t\alpha^4$$

$$\Rightarrow \frac{s_1}{t} = \frac{8}{w} \qquad (3.3.38v)$$

Next, for the two factors (which are at three levels each)

$$\sum_{u=1}^{N} x_{iu}^2 = ws_1\alpha'^2 + 4s_2\alpha'^2 \qquad (3.3.38vi)$$

$$\sum_{u=1}^{N} x_{iu}^4 = ws_1\alpha'^4 + 4s_2\alpha'^4 \qquad (3.3.38vii)$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = 4s_2\alpha'^4 \qquad i \neq i',\ i, i' = v-1, v-2 \qquad (3.3.38viii)$$

Applying the condition of rotatability, we get

$$\frac{s_2}{s_1} = \frac{w}{8} \qquad (3.3.38ix)$$

Also $\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = ws_1\alpha^2\alpha'^2 \qquad i \neq i',\ i = 1,...,v-2;\ i' = v-1, v \qquad (3.3.38x)$

From (3.3.38i), (3.3.38ii), (3.3.38vi), (3.3.38vii) and (3.3.38x) we get $\alpha'^2 = 2\alpha^2$. Hence the unknown levels are completely determined. For $\alpha = 1$, the level codes of the factors at 5 levels each are -2, -1, 0, 1, 2 and for factors at 3 levels each are $-\sqrt{2}, 0, \sqrt{2}$. Therefore, we may consider that levels are equispaced. Further, for these values of α', α and β, $L = \sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = 2ws_1$ and $R = \sum_{u=1}^{N} x_{iu}^2 = 2ws_1 + 8t$ and using (3.3.38v) and (3.3.38ix), $ws_1 = 8t$ and $s_2 = t$. Using these it can easily be seen that the condition (3.3.5) *i.e.* $\frac{NL}{R^2} > \frac{v}{v+C-1}$ $\Rightarrow (v-4)^2 > 0$. As a consequence, for $v > 4$, there is no need of adding any center points as far as estimation of parameters are concerned. However, for estimating the pure error for testing the lack of fit, a few center points may be added. For $v = 4$, the number of center points $n_0 \geq 5$ so as to satisfy (3.3.5). The procedure is explained with the help of following example:

For obtaining a asymmetric rotatable design for $5^3 \times 3^2$. In this case, following method 3.3.5, we get $w = 8$ and for $\alpha = 1$ and $\beta = 2$, using (3.3.8v) we get $s_1 = t = 1$ and further using (3.3.8ix) we get $s_2 = 1$. The design obtained is

-1	-1	-1	$\sqrt{2}$	0
1	1	-1	$\sqrt{2}$	0
1	-1	1	$\sqrt{2}$	0
-1	1	1	$\sqrt{2}$	0
1	-1	-1	$-\sqrt{2}$	0
-1	1	-1	$-\sqrt{2}$	0
-1	-1	1	$-\sqrt{2}$	0
1	1	1	$-\sqrt{2}$	0
-1	-1	-1	0	$\sqrt{2}$
1	1	-1	0	$\sqrt{2}$
1	-1	1	0	$\sqrt{2}$
-1	1	1	0	$\sqrt{2}$
1	-1	-1	0	$-\sqrt{2}$
-1	1	-1	0	$-\sqrt{2}$
-1	-1	1	0	$-\sqrt{2}$
1	1	1	0	$-\sqrt{2}$
2	0	0	0	0
-2	0	0	0	0
0	2	0	0	0
0	-2	0	0	0
0	0	2	0	0
0	0	-2	0	0
0	0	0	$-\sqrt{2}$	$-\sqrt{2}$
0	0	0	$-\sqrt{2}$	$\sqrt{2}$
0	0	0	$\sqrt{2}$	$-\sqrt{2}$
0	0	0	$\sqrt{2}$	$\sqrt{2}$

Here N = 26, $R = 24$; $L = 16$ and $CL = 48$. One can see that the condition (3.3.5) *i.e.* $\frac{NL}{R^2} > \frac{v}{v+C-1}$ is satisfied. The values of $v-2$, p, s_1, s_2, t and N for asymmetric rotatable designs with $v-2$ factors at 5 levels each and 2 factors at 3 levels with $2 \le v \le 10$ and $N \le 500$ are given in Table 3.3.8.

Table 3.3.8: The values of $v-2$, p, s_1, s_2, t and N for asymmetric rotatable designs with $v-2$ factors at 5 levels each and 2 factors at 3 levels each with $2 \le v \le 10$ and $N \le 500$ obtainable from Method 3.3.5.

v-2	p	s_1	t	s_2	N
2	2	2	1	1	$24+n_0$; $n_0 \ge 5$
3	3	1	1	1	26
4	4	1	2	2	56
5	4	1	2	2	60
5	5	1	4	4	120
6	5	1	4	4	128
6	6	1	8	8	256
7	6	1	8	8	272
8	6	1	8	8	288

As pointed out by Das, Parsad and Manocha (1999), the main problem in obtaining asymmetric rotatable designs is how best to place the unknowns among the level codes of each factor and how many of them. This problem is discussed in Method 3.3.6 and then the problems of forming the equations and their solutions are taken.

Method 3.3.6: {Das, Parsad and Manocha, 1999}. The technique used for construction of asymmetrical response surface designs is first to take v factors with number of levels, $s_1, s_2, ..., s_v$ where all s_i's are not equal. For each factor equidistant level codes like $k\alpha$ and $-k\alpha$ are taken in pairs where some of the k's may be unknown. Using such codes the complete factorial with $N = \prod_{i=1}^{v} s_i$ level combinations is written. Some of the level codes in these combinations are unknown. Denoting the level codes in the design by x_{iu} for the level codes of the i^{th} factor in the u^{th} combination of the design as used for the symmetrical designs and taking the same quadratic polynomial, the expression for $S_2, S_{22,} S_4$ are obtained for each factor.

In such designs the condition (3.3.1i) , $S(pqrt) = \sum_{u=1}^{N} x_{iu}^{p} x_{i'u}^{q} x_{i''u}^{r} x_{i'''u}^{t} = 0$, when at least one of the p, q, r, t is odd holds and the dose codes for each factor are equidistant and the factorial is complete. The condition $S_2 = R = \sum_{u=1}^{N} x_{iu}^2 =$ constant for different factors and similar others do not hold as such in these designs. We shall denote for these expressions like $\sum_{u=1}^{N} x_{iu}^2$ by R_i,

$\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$ by $L_{ii'}$ and $\sum_{u=1}^{N} x_{iu}^4$ by CL_i. The unknowns in the level codes will be obtained by solving equations like $R_i = R_{i'}$, $L_{ii'} = L_{ii''}$ and $CL_i = CL_{i'}$ for different values of i, i', i'' etc.

Choice of level codes: Scheme A

For factors with 3 levels the codes are taken as $-\alpha\ 0\ \alpha$ where α is an unknown constant and same for all factors with 3 levels. For factors with 4 levels the codes are $-k_2\alpha\ \ -k_1\alpha\ \ k_1\alpha\ \ k_2\alpha$ where k_1 and k_2 are unknowns. For factors with 5 levels the codes are similar as for 4 levels and one code is taken as 0. The unknown constants are, however, different from those for 4 levels. For factors with 6 levels there are likewise 3 unknowns. Actually, the scaling constant is the same for all factors in this scheme and for factors with same number of levels the codes are the same.

The response surface design is now obtained from the complete factorial obtained by using such level codes. For example, let there be 3 factors A, B and C with number of levels as 3, 4 and 5 respectively. The following level codes are used.

Factor A	$-\alpha$	0	α		
Factor B	$-k_2\alpha$	$-k_2\alpha$	$-k_2\alpha$	$-k_2\alpha$	
Factor C	$-k_2\alpha$	$-k_2\alpha$	0	$-k_2\alpha$	$-k_2\alpha$

Number of combinations in the design is $N = 60$.

Using this design and method of obtaining sum of squares and products as discussed in section 3.3, the following are obtained:

$$R_1 = N\,2\alpha^2/3,\ R_2 = N\,2\alpha^2\,(k_1^2 + k_2^2)/4,\ R_3 = N\,2\alpha^2\,(p_1^2 + p_2^2)/5,$$

$$L_{12} = N\,2\alpha^2\,2(k_1^2 + k_2^2)\alpha^2/(3\times 4) = 4N\alpha^4\,(k_1^2 + k_2^2)/12,\ L_{13} = 4N\alpha^4\,(p_1^2 + p_2^2)/15,$$

$$L_{23} = N\alpha^4\,(k_1^2 + k_2^2)(p_1^2 + p_2^2)/20,$$

$$CL_1 = N\,2\alpha^4/3,\ CL_2 = N\,2\alpha^4\,(k_1^4 + k_2^4)/4,\ CL_3 = N\,2\alpha^4\,(p_1^4 + p_2^4)/5.$$

Restriction $R_1 = R_2$ gives the equation

$$N\,2\alpha^2/3 = N\,2\alpha^2\,(k_1^2 + k_2^2)/4$$

or $\quad k_1^2 + k_2^2 = 4/3 \qquad (3.3.39)$

Restriction $R_1 = R_3$ gives the equation

$$N\,2\alpha^2/3 = N\,2\alpha^2\,(p_1^2 + p_2^2)/5$$

or $\quad p_1^2 + p_2^2 = 5/3 \qquad (3.3.40)$

It will be noticed that R_1, that is, the expression for the factor A without any unknown constant in its codes beside the scaling constant has been necessarily used in each such restriction.

Restriction $L_{12} = L_{13}$ gives the equation

$$4N\alpha^4(k_1^2 + k_2^2)/12 = 4N\alpha^4(p_1^2 + p_2^2)/15$$
$$or\ (k_1^2 + k_2^2)\big/(p_1^2 + p_2^2) = 4/5 \qquad (3.3.41)$$

Restriction $L_{12} = L_{23}$ gives the equation

$$4N\alpha^4(k_1^2 + k_2^2)/12 = N\alpha^4(k_1^2 + k_2^2)(p_1^2 + p_2^2)/20$$
$$or\ \ p_1^2 + p_2^2 = 5/3 \qquad (3.3.42)$$

It will be seen that when conditions (3.3.39) and (3.3.40) hold then conditions (3.3.41) and (3.3.42) automatically hold. This fact is true in general for all designs constructed as discussed above.

Restriction $CL_1 = CL_2$ gives the equation

$$N\,2a^4/3 = N\,2a^4(k_1^4 + k_2^4)/4$$
$$or\ k_1^4 + k_2^4 = 4/3 \qquad (3.3.43)$$

Restriction $CL_1 = CL_3$ gives the equation

$$N\,2a^4/3 = N\,2a^4(p_1^4 + p_2^4)/5$$
$$or\ p_1^4 + p_2^4 = 5/3 \qquad (3.3.44)$$

Solving the biquadratic equations (3.3.39) and (3.3.43) k_1 and k_2 are obtained. Again solving similar equations (3.3.40) and (3.3.44) p_1 and p_2 are obtained. Putting $x = k_1^2$ and $x = k_2^2$ the equations (3.3.39) and (3.3.43) become

$x + y = 4/3;\ x^2 + y^2 = 4/3$

The equations (3.3.40) and (3.3.44) become

$x + y = 5/3;\quad x^2 + y^2 = 5/3$

where $x = p_1^2$ and $x = p_2^2$

The solutions are given below.

$k_1 = 0.4419;\ k_2 = 1.0668;\ p_1 = 0.6787;\ p_2 = 1.0982.$

These solutions for each of factors at 4 and 5 levels remain the same whatever may be the design.

For factors with 6 levels, 3 unknowns are involved in the codes. But there will be only two equations to solve them out *viz.*

$x+y+z=6/3;\ x^2+y^2+z^2=6/3$

To get unique solutions one of x, y or z has to be fixed conveniently.

Now in the level codes only the scaling constant α remains and this has to be fixed conveniently. At this stage the design is asymmetrical response surface design but without any added property like the modified designs or rotatable designs although conditions of symmetry are satisfied. But these designs can be converted to them by taking some more initial sets of level combinations and the unknowns in them appear in the equations to satisfy $C=3$ or $R^2=NL$ or both. We shall discuss an example in this regard subsequently.

It will be seen that the level codes of one of the factors in the above design *viz.* factor A do not involve any unknown beside the scaling constant and the expression R for this factor has been used in each restriction for forming equation.

It is necessary to have a factor with known constant like the factor A in the above example and in all the restrictions R and CL corresponding expressions of this factor have to be used.

Choice of level codes: Scheme B

In this scheme also a factor with conveniently chosen known codes have to be taken along with a scaling constant. If there is a factor with 3 levels then this is the factor with known constant *viz.* 1 along with a scaling constant.

For other factors only one pair of equidistant codes need involve an unknown along with its own scaling constant and the rest can be fixed suitably in equidistant pairs. The codes for some number of levels of factors are shown below:

A	$-\alpha$	0				
B	$-k_1\beta_1$	$-s_1\beta_1$	$s_1\beta_1$	$k_1\beta_1$		
C	$-k_2\beta_2$	$-s_2\beta_2$	0	$s_2\beta_2$	$k_2\beta_2$	
D	$-k_3\beta_3$	$-s_{32}\beta_3$	$-s_{31}b_3$	$s_{31}\beta_3$	$s_{32}\beta_3$	$k_3\beta_3$

In all these factors except A the scheme codes involve one unknown for each factor and the rest codes are known except the scaling constants, that is, all $k's$ are unknowns and $s's$ are known. For these factors

$$R_1=(N/3)\,2\alpha^2;\ R_2=(N/4)\,2\left(k_1^2+s_1^2\right)\beta_1^2;$$
$$R_3=(N/5)\,2\left(k_2^2+s_2^2\right)\beta_2^2;R_4=(N/6)\,2\left(k_3^2+s_{32}^2+s_{31}^2\right)\beta_3^2.$$

Different restrictions involving $R's$ give the following equations

$$\left(k_1^2 + s_1^2\right) = (4/3)\left(\beta_1^2 / \alpha^2\right) \tag{3.3.45}$$
$$\left(k_2^2 + s_2^2\right) = (5/3)\left(\beta_2^2 / \alpha^2\right) \tag{3.3.46}$$
$$\left(k_3^2 + s_{31}^2 + s_{32}^2\right) = (5/3)\left(\beta_3^2 / \alpha^2\right) \tag{3.3.47}$$

The equations to make L expressions equal come out to be the same as above. The equations to make CL expressions equal come out to be the above equations except that wherever there is power 2 it should be made 4, *i.e.*,

$$\left(k_1^4 + s_1^4\right) = (4/3)\left(\beta_1^4 / \alpha^4\right) \tag{3.3.48}$$
$$\left(k_2^4 + s_2^4\right) = (5/3)\left(\beta_2^4 / \alpha^4\right) \tag{3.3.49}$$
$$\left(k_3^4 + s_{31}^4 + s_{32}^4\right) = (5/3)\left(\beta_3^4 / \alpha^4\right) \tag{3.3.50}$$

These equations are biquadratic equations in pairs (3.3.45 and 3.3.48) form one pair. (3.3.46 and 3.3.49) another and the remaining two the third pair. The unknowns in each pair are k_i^2 and the ratio β_i^2 / α^2 $(i = 1,2,3)$. All $s's$ are constants as given while writing the codes. After the codes are known through positive solutions of the equations these can be used in any design provided one of the factors has 3 levels. One of the scaling constants can be fixed conveniently and the other is worked from the solution of their ratio.

The design is now an asymmetrical response surface design where R, L and CL are constants and as such can be treated just like symmetrical response surface designs regarding parameter estimates, variances and co-variances. Taking further sets of combinations with fresh unknowns these designs can be converted into rotatable or modified designs.

Fractional asymmetrical response surface designs

The designs obtained previously in Choice A and Choice B are based on complete factorial. When there are more than 4 factors, suitable fractions of the complete asymmetrical factorial where no interaction with less than 5 factors is confounded can be used without any change in procedure and solutions except for change of N.

Another procedure of getting fractional designs is first to take some initial sets with unknowns and generate design points as is done for obtaining symmetrical designs with s as number of levels of each factor. Let this design be denoted by D. Next each unknown level code of an additional factor X with m levels, m not equal to s is associated (pre-fixed) with each combination of the symmetrical design D. The resulting design will have mN combinations where N is the number of combinations in the symmetrical design D. If factor X which we shall call 1, has 3 levels with unknown scaling constant there will be only two unknowns. The constancy restrictions are three *viz.* $R_1 = R_2, L_{12} = L_{23}$ and $CL_1 = CL_2$ and each one gives a separate equation unlike what happened in design based on complete factorial. Thus a 3-level factor cannot be used as the additional factor X. As there are 3 equations there should be at least three unknowns in the sets of D and in the additional factor together. The following illustration clarifies different issues. The design D is obtained as below:

We take the factor X at 4 levels involving two unknowns. Design D is obtained from the sets *(1)*$(\alpha \quad \alpha \quad \alpha \quad \alpha)$, *(2)*$(\beta \quad 0 \quad 0 \quad 0)$, *(3)*$(0 \quad \beta \quad 0 \quad 0)$, *(4)*$(0 \quad 0 \quad \beta \quad 0)$ and *(5)*$(0 \quad 0 \quad 0 \quad \beta)$. The factor X has the 4 levels *viz.* $-p \quad -q \quad q \quad p$. The codes are each associated with the 16 points from set (1) only. Against the points generated from sets (2) to (5) the factor X will have levels 1 and -1 as shown below. The design will thus have 72 points in 5 factors with X at 6 levels including $+1$ and -1 and rest at 5 levels each. The design is shown below:

Design Points

Factors					Factors					Points				
X	**A**	**B**	**C**	**D**	**X**	**A**	**B**	**C**	**D**	**X**	**A**	**B**	**C**	**D**
$-p$	$-\alpha$	$-\alpha$	$-\alpha$	$-\alpha$	$-q$	$-\alpha$	$-\alpha$	$-\alpha$	$-\alpha$	1	β	0	0	0
$-p$	$-\alpha$	$-\alpha$	$-\alpha$	α	$-q$	$-\alpha$	$-\alpha$	$-\alpha$	α	1	$-\beta$	0	0	0
$-p$	$-\alpha$	$-\alpha$	α	$-\alpha$	$-q$	$-\alpha$	$-\alpha$	α	$-\alpha$	-1	0	β	0	0
$-p$	$-\alpha$	α	$-\alpha$	$-\alpha$	$-q$	$-\alpha$	α	$-\alpha$	$-\alpha$	-1	0	$-\beta$	0	0
$-p$	α	$-\alpha$	$-\alpha$	$-\alpha$	$-q$	α	$-\alpha$	$-\alpha$	$-\alpha$	1	0	0	β	0
$-p$	$-\alpha$	$-\alpha$	α	α	$-q$	$-\alpha$	$-\alpha$	α	α	1	0	0	$-\beta$	0
$-p$	$-\alpha$	α	$-\alpha$	α	$-q$	$-\alpha$	α	$-\alpha$	α	-1	0	0	0	β
$-p$	$-\alpha$	α	α	$-\alpha$	$-q$	$-\alpha$	α	α	$-\alpha$	-1	0	0	0	$-\beta$
$-p$	α	$-\alpha$	$-\alpha$	α	$-q$	α	$-\alpha$	$-\alpha$	α					
$-p$	α	$-\alpha$	α	$-\alpha$	$-q$	α	$-\alpha$	α	$-\alpha$					
$-p$	α	α	$-\alpha$	$-\alpha$	$-q$	α	α	$-\alpha$	$-\alpha$					
$-p$	α	α	α	$-\alpha$	$-q$	α	α	α	$-\alpha$					
$-p$	α	α	$-\alpha$	α	$-q$	α	α	$-\alpha$	α					
$-p$	α	$-\alpha$	α	α	$-q$	α	$-\alpha$	α	α					
$-p$	$-\alpha$	α	α	α	$-q$	$-\alpha$	α	α	α					
$-p$	α	α	α	α	$-q$	α	α	α	α					

There are 4 sets of 16 points each set having a different level of X. Two of the sets with levels $-p$ and $-q$ are shown along with the 8 points from the initial sets from (2) to (5). There are two more groups of 16 points which are identical to the above two groups except that $-p$ has to be replaced by p and $-q$ by q. This way all the 72 points in the design are obtained.

Different R, L etc. expressions are shown below:

$$R_1 = 32\left(p^2 + q^2\right) + 8;\; R_2 = 64\alpha^2 + 2\beta^2 = R_3$$
$$L_{12} = 32\alpha^2\left(p^2 + q^2\right) + 2\beta^2;\; L_{23} = 64\alpha^4$$
$$CL_1 = 32\left(p^4 + q^4\right) + 8;\; CL_2 = 64\alpha^4 + 2\beta^4$$

The following 3 equations follow from the constancy restrictions:

$$32\left(p^2+q^2\right)+8=64\alpha^2+2\beta^2 \tag{3.3.51}$$

$$32\alpha^2\left(p^2+q^2\right)+2\beta^2=64\alpha^4 \tag{3.3.52}$$

$$32\left(p^4+q^4\right)+8=64\alpha^4+2\beta^4 \tag{3.3.53}$$

Dividing the second by α^2 and then subtracting from the first equation

$$2\beta^2+2\beta^2/\alpha^2=8$$

Taking $\alpha=1$ we get $\beta^2=2$. With these values of α and β the first two equations are satisfied. Substituting these values in equations (3.3.51) and (3.3.53) above

$$p^2+q^2=15/8; \quad p^4+q^4=2$$

Solving these equations

$$p^2=(15+5.568)/16=1.285; q^2=(15-5.568)/16=0.5895$$
$$\Rightarrow p=1.13 \text{ and } q=0.76$$

All the unknowns are now known and the design is complete except for its conversion to actual levels, which can be obtained by following the method given earlier after the level ranges for the factors are known.

Conversion to rotatable or modified designs

By taking the initial set $(d \quad d \quad d \quad d \quad d)$ we obtain 16 design points from it using half fraction of 2^5. The sets $(d \quad 0 \quad 0 \quad 0 \quad 0)$ that give 10 additional points can also be taken. Taking these points along with 72 points of the design obtained above each value of expressions R, L and CL will increase by a constant separately for each category of expressions. Thus the asymmetrical design obtained earlier is not disturbed due to addition of these points except for change of number of levels by increase of 2 or 3 for each factor. Now by using restrictions either $C=3$ or $R^2=NL$, d can be obtained and the design will be rotatable or modified.

Another method for converting the design to rotatable or modified response surface design is to generate another equation in addition to the three at (3.3.51), (3.3.52), (3.3.53) by using the restriction $C=3$ or $R^2=NL$. This is possible as there are 4 unknowns in the equations. When $C=3$ no positive solution of p^2 is possible.

Using $R^2=NL$ we get the equation

$$\left(32\left(p^2+q^2\right)+8\right)^2 = 72\times 64\alpha^4$$
$$or\ 32\left(p^2+q^2\right)+8 = 8\times 8.48828\alpha^2, \tag{3.3.54}$$

Solving these 4 equations, we get $\alpha^2 = 1.0607; \beta^2 = 2.05888; p = 1.1679; q = 0.7975.$ With these values of the unknowns the design becomes modified response surface design with 72 points and with 82 points the design becomes both modified and rotatable as discussed earlier.

3.3.3 Group Divisible Rotatable Designs

The above discussion relates to the situations where it is possible to obtain designs that ensure that the variance of the predicted response remains constant at all points that are equidistant from the design center. However, it may not always be achievable for all the factors or if achievable may require a large number of runs. To take care of this problem Herzberg (1966) introduced another class of designs called **cylindrically rotatable designs**. These designs are rotatable with respect to all factors except one. To be specific, a $v-$dimensional design is cylindrically rotatable if the variance of the predicted response is constant at points on the same $(v-1)$-dimensional hypersphere that is centered on a specified axis. Das and Dey (1967) attempted a modification of rotatable designs. They divided the *v*-dimensional space corresponding to *v* factors into two mutually orthogonal spaces, one of v_1-dimension and the other of $v_2\left(=v-v_1\right)$-dimension. The projection of any treatment combination in the v-dimensional space can be thought upon on each of the above two spaces. Without loss of generality the v_1-dimensional space can be defined by the first v_1 factors and the other space by the remaining factors. Therefore the projection of the point $\mathbf{x}_0' = \left(x_{10}, x_{20}, ..., x_{v0}\right)$ on the first space gives $\left(x_{10}, x_{20}, ..., x_{v_1 0}, 0, ..., 0\right)$ and on the second space gives $\left(0, ..., 0, x_{v_1+1,0}, ..., x_{v,0}\right)$. If the distances of these projections from a suitable origin are d_1^2 and d_2^2 respectively, then.

$$\sum_{i=1}^{v_1} x_{i0}^2 = d_1^2, \qquad \sum_{q=v_1+1}^{v} x_{j0}^2 = d_2^2.$$

Knowing that in rotatable designs the variance of the estimated response at a point is a function of the distance of that point from the origin, Das and Dey (1967) introduced a new class of response surface designs, such that the variance of a response estimated through such designs at the point $\left(x_{10}, x_{20}, ..., x_{v0}\right)$ is a function of the distances d_1^2 and d_2^2. These designs will not be rotatable in the *v*-dimensional space, but they will be certainly rotatable in v_1-dimensional space for all those points whose projection in the v_2-dimensional space are at a constant distance from the origin and vice-versa. These designs have been termed as **group divisible rotatable designs** as the factors get divided into groups such that for the factors within each group the design is rotatable. We may now formally define a group divisible second order response surface designs (GDSORD).

Let there be v-factors each at s levels. The *v*-factors in the experiment are divided into two groups of factors, one group consisting of v_1-factors and the other, the rest $v_2\left(=v-v_1\right)$ factors.

Without loss of generality, the factors in the first group may be denoted as $1, 2, \ldots, v_1$ and the factors in the second group are denoted by $v_1+1, v_1+2, \ldots, v_1+v_2(=v)$. Then the set of points $\{x_{iu}\}$, $i = 1, 2, ..., v$, $u = 1, 2, ..., N$ will be a GDSORD if and only if

(i) $\sum_{u=1}^{N}\left\{\prod_{u=1}^{k} x_{iu}^{\alpha_i}\right\} = 0$, if any α_i is odd, for $\alpha_i = 0,1,2$ *or* 3 and $\sum \alpha_i \le 4$.

(v) $\sum_{u=1}^{N} x_{iu}^2 = \text{constant} = R_1$ (say) for all $i = 1, 2, \ldots, v_1$

(vi) $\sum_{u=1}^{N} x_{iu}^4 = \text{constant} = 3L_1$ (say) for all $i = 1, 2, \ldots, v_1$

(vii) $\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = \text{constant} = L_1$ (say), for all $i \ne i'$, $i, i' = 1, 2, \ldots, v_1$

(viii) $\sum_{u=1}^{N} x_{qu}^2 = \text{constant} = R_2$ (say) for all $q = v_1+1, v_1+2, \ldots, v$

(ix) $\sum_{u=1}^{N} x_{qu}^4 = \text{constant} = 3L_2$ (say) for all $q = v_1+1, v_1+2, \ldots, v$

(x) $\sum_{u=1}^{N} x_{qu}^2 x_{q'u}^2 = \text{constant} = L_2$ (say), for all $q \ne q'$, $q, q' = v_1+1, v_1+2, \ldots, v$

(xi) $\sum_{u=1}^{N} x_{iu}^2 x_{qu}^2 = \text{constant} = \theta$ (say), for all $i = 1, 2, \ldots, v_1$; $q = v_1+1, v_1+2, \ldots, v$

(3.3.55)

Das and Dey (1967) also gave some methods of construction of GDSORD using central composite type designs, BIB designs and Group divisible designs. All their methods of construction give designs for experiments where each of the factors is at 5 levels. The level codes for the factors in the first group are denoted by $-\beta, -\alpha, 0, \alpha, \beta$ and for the factors within second group are denoted by $-\gamma, -\alpha, 0, \alpha, \gamma$. The designs obtained are not suitable for the situations where doses are equispaced. Dey (1969) has obtained some designs where the factors in one group are at 3 levels each and factors in the second group are at 5 levels each. Dey (1969) has also given a very simple method of construction of GDSORD.

Method 3.3.7: {Dey (1969)}. Let there exist a SORD in v_t factors and N_t design points; $t = 1,2$. Let the set of points $\{x_{tiu}\}$ be denoted by $\mathbf{A}_t$. Then a GDSORD can always be obtained in $v = v_1 + v_2$ factors with $N = N_1 + N_2$ points by considering the rows of the design matrix as

$$\mathbf{X} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 \end{bmatrix} \qquad (3.3.56)$$

This method in general enables us to get GDSORD for symmetrical as well as asymmetrical factorials with smaller number of points. Using this method, the GDSORD's with equispaced doses can be obtained using the SORD's obtained through the methods of construction given in

Section 3.3.1. However, since $\sum_{u=1}^{N} x_{iu}^2 x_{qu}^2 = \theta = 0$, therefore, the parameters b_{iq}; $i = 1, 2, \ldots, v_1$; $q = v_1 + 1, v_1 + 2, \ldots, v$ are non-estimable in the second order response surface.

In the present investigation, a simplification in the GDSORD has been introduced. For these designs $R_1 = R_2$ and $L_1 = L_2$ and $\theta > 0$. A method of construction based on a group divisible designs. A group divisible design is defined as follows:

Let $v = mn$ treatments that can be arranged in *m* groups of size *n* each. The two treatments are first associates if they occur in the same group and second associates otherwise. Then a group divisible design is an arrangement of $v = mn$ treatments in b blocks each of size $k < v$ such that a treatment is applied at most once in a block, each treatment occurs exactly in *r* blocks and each pair of first associates occur together in λ_1 blocks and each pair of second associates occur together in λ_2 blocks. The method is described in the sequel.

Method 3.3.8: Consider a group divisible (GD) design with parameters $v = 2n, b, r, k, \lambda_1, \lambda_2 > 0, m = 2, n$. Then following the procedure of Method 3.3.2, Let $\mathbf{M} = (m_{ji})$ be the incidence matrix of the group divisible design where:

$$m_{ji} = \begin{cases} 1, & \text{if the } i^{th} \text{ treatment occurs in the } j^{th} \text{ block} \\ 0, & \text{otherwise} \end{cases} \qquad (j = 1, \ldots, v; \quad i = 1, \ldots, b)$$

The element 1 in the incidence matrix is replaced by an unknown α.. From the rows of this matrix involving *0* and the unknown α, we shall get *b* combinations. Each of these combinations is then associated with a 2^k factorial or a suitable Resolution V fraction, say 2^p, of it, the levels being coded as ± 1. Let the number of 2^k or 2^p points be denoted by *w*. For these bw points, we have

$$R_1 = R_2 = rw\alpha^2; \; CL_1 = CL_2 = rw\alpha^4 \; ; \; L_1 = L_2 = \lambda_1 w\alpha^4 \text{ and } \theta = \lambda_2 w\alpha^4$$

For obtaining a rotatable design within groups, we take $C = 3$ *i.e.*

$$rw\alpha^4 = 3\lambda_1 w\alpha^4 \qquad \Rightarrow \qquad r = 3\lambda_1. \tag{3.3.57}$$

If a GD design with $r = 3\lambda_1$ exists for given $v = 2n$, then no further combinations need to be taken excepting center points. By taking $\alpha = 1$, we can get designs with v factors each at three levels coded as -1, 0, +1. The number of design points is $N = bw + n_0$.

The values of v, p, N for group divisible rotatable designs obtainable from GD designs with $r = 3\lambda_1$ for $3 \le v \le 10$ and $N \le 500$ are given in Table 3.3.9. In this Table X# denotes the design of Type X given at serial number # in Clatworthy (1973). The parameters of the GD design are given in the order $v, b, r, k, \lambda_1, \lambda_2, m, n$.

Table 3.3.9: The values of v, p, and N for group divisible second order response surface designs for three equispaced doses with $3 \le v \le 10$ and $N \le 500$ obtainable from Method 3.3.8.

v	p	N	Source GD design
6	2	$108+n_0$	R25:(6,27,9,2,3,1,2,3)
6	3	$144+n_0$	R52: (6,18,9,3,3,4,2,3)
8	4	$192+n_0$	SR38: (8,12,6,4,2,3,2,4)

If however, the relation $r = 3\lambda_1$ does not hold in a GD design, we have to take further combinations of another unknown β as indicated below.

If $r < 3\lambda_1$, then we take the combinations $(\pm\beta, 0,...,0), (0,\pm\beta, 0,...,0),... (0,...,0,\pm\beta)$. If again, $r > 3\lambda_1$, the combinations $(\pm\beta, \pm\beta,...,\pm\beta)$ have to be taken along with the combinations obtained from the incidence matrix of the GD design. The values of the unknowns have to be fixed in this case by using the relations $C = 3$, *i.e.*, $\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2$ and $\sum_{u=1}^{N} x_{qu}^4 = 3\sum_{u=1}^{N} x_{qu}^2 x_{q'u}^2$.

For obtaining group divisible rotatable designs when each of the factors at 5 equispaced levels (-2,-1,0,1,2) using GD designs, we take s copies of the points obtained from the incidence matrix and t copies of the added points (other than the central points). We get the following.

When $r < 3\lambda_1$
$R_1 = R_2 = s\,r\,w + 8t$; $L_1 = L_2 = s\,\lambda_1 w$; and $\theta = s\lambda_2 w$;
$N = bsw + 2vt + n_0$.

For a group divisible rotatable design, $C = 3$, *i.e.*,

$$srw + 32t = 3s\lambda_1 w$$

$$\Rightarrow \frac{s}{t} = \frac{32}{(3\lambda_1 - r)w} \tag{3.3.58}$$

The values of v, p, s, t, N for group divisible rotatable designs obtainable from GD designs with $r < 3\lambda_1$ for $3 \le v \le 10$ and $N \le 500$ are given in Table 3.3.10.

Table 3.3.10: The values of v, p,s,t and N for group divisible second order response surface designs for five equispaced doses with $3 \le v \le 10$ and $N \le 500$ obtainable from Method 3.3.8.

v	p	s	t	N	*Source GD design*
4	2	4	1	$136+n_0$	R1: (4,8,4,2,2,1,2,2)
4	2	2	1	$88+n_0$	R2: (4,10,5,2,3,1,2,2)
4	2	4	3	$216+n_0$	R4: (4,12,6,2,4,1,2,2)
4	2	1	1	$64+n_0$	R5: (4,14,7,2,5,1,2,2)
4	2	4	1	$232+n_0$	R6: (4,14,7,2,3,2,2,2)
4	2	4	5	$296+n_0$	R8: (4,16,8,2,6,1,2,2)
4	2	2	1	$136+n_0$	R9: (4,16,8,2,4,2,2,2)
4	2	2	3	$168+n_0$	R11: (4,18,9,2,7,1,2,2)
4	2	4	3	$312+n_0$	R12: (4,18,9,2,5,2,2,2)
4	2	4	7	$376+n_0$	R14: (4,20,10,2,8,1,2,2)
4	2	1	1	$88+n_0$	R15: (4,20,10,2,6,2,2,2)
4	2	4	1	$328+n_0$	R16: (4,20,10,2,4,3,2,2)
6	4	2	3	$324+n_0$	SR35: (6,9,6,4,3,4,2,3)
6	3	4	3	$420+n_0$	R43: (6,12,6,3,3,2,2,3)
6	4	2	5	$252+n_0$	R94: (6,6,4,4,3,2,2,3)
8	4	1	2	$288+n_0$	R98: (8,16,8,4,4,3,2,4)
8	4	1	3	$336+n_0$	R100: (8,18,9,4,5,3,2,4)
8	4	1	4	$384+n_0$	R102: (8,20,10,4,6,3,2,4)
8	4	2	7	$368+n_0$	R133: (8,8,5,5,4,2,2,4)
8	4	1	7	$368+n_0$	R135: (8,16,10,5,8,4,2,4)

X# denotes the design of Type X given at serial number # in Clatworthy (1973).

For $r > 3\lambda_1$, we have $R_1 = R_2 = s\,r\,w_1 + 4tw_2$ where $2^p = w_1$ and 2^v or a fraction of it $= w_2$
$L_1 = L_2 = s\,\lambda_1 w_1 + 16tw_2$ and $CL_1 = CL_2 = s\,rw_1 + 16tw_2$; $\theta = s\lambda_2 w + 16tw_2$;
$N = bsw_1 + tw_2 + n_0$. For group divisible rotatability, we have $C = 3$, *i.e.*
$(srw_1 + 16tw_2) = 3(s\lambda_1 w_1 + 16tw_2)$

$$\Rightarrow \frac{s}{t} = \frac{32}{r - 3\lambda_1}\frac{w_2}{w_1} \qquad (3.3.59)$$

Using conditions (3.3.59), group divisible second order response surface designs obtainable from GD designs with $r > 3\lambda_1$ can easily be obtained.

Adhikary and Panda (1983) extended the concept of group divisible second order rotatable response surface designs when the factor space is divisible into $m > 2$ groups. These designs can be obtained using Method 3.3.8 by taking the GD design with $m > 2$.

3.4 Designs for Slope Estimation

The response surface designs given in Section 3.3 are suitable for the experimental situations where the experimenter is interested in determining the level combination of the factors that optimize the response. In many practical situations, however, the experimenter is interested in estimation of the rate of change of response for given value of independent variable(s) rather than optimization of response. This problem is frequently encountered *e.g.*, in estimating rates of reaction in chemical experiments; rates of growth of biological populations; rates of changes in response of a human being or an animal to a drug dosage, rate of change of yield per unit of fertilizer dose, etc. The work on the problem of obtaining designs for slope estimation was initiated by Ott and Mendenhall (1972) and Murty and Studden (1972). Since, then lot of efforts have been made in the literature for obtaining efficient designs for the estimation of differences in responses *i.e.*, for estimating the slope of a response surface. Hader and Park (1978) introduced the concept of slope rotatability over axial directions. According to them, the designs possessing the property that the estimate of derivative is equal for all points equidistant from the origin are known as **slope rotatable designs**. For a second order response surface as defined in (2.1.3) and (2.2.6) of Chapter II, the rate of change of response due to i^{th} independent variable is given by

$$\frac{\partial \hat{y}(\mathbf{x})}{\partial x_i} = b_i + 2b_{ii}x_i + \sum_{i' \neq i = 1}^{v} b_{ii'}x_{i'} \tag{3.4.1}$$

For second order response design obtained in Section 3.3satisfying the conditions of symmetry given in (3.3.1) and condition of non-singularity given in (3.3.5), we have

$$\mathrm{Cov}(b_i, b_{ii}) = \mathrm{Cov}(b_i, b_{ii'}) = \mathrm{Cov}(b_{ii}, b_{ii'}) = 0$$

Using (3.3.8) and (3.3.60), the variance of $\frac{\partial \hat{y}(\mathbf{x})}{\partial x_i}$ at point $(x_{1u}, x_{2u}, \cdots, x_{iu}, \cdots, x_{vu})$ is given by

$$\mathrm{Var}\left(\frac{\partial \hat{y}(\mathbf{x})}{\partial x_i}\right) = \mathrm{Var}(b_i) + d^2\,\mathrm{Var}(b_{ii}) + \sum_{i' \neq i = 1}^{v} x_{i'}^2\left[4\,\mathrm{Var}(b_{ii}) - \mathrm{Var}(b_{ii'})\right]; \text{ where } d^2 = \sum_{i=1}^{v} x_{iu}^2$$

It can easily be seen that the above expression will be a function of d^2 only if

$$4\,\mathrm{Var}(b_{ii}) = \mathrm{Var}(b_{ii'}) \tag{3.4.2}$$

The designs possessing the property (3.4.2) provide the estimate of derivative (slope) with same variance at all points equidistant from the origin and are known as **slope rotatable designs over axial directions**.

Further, it can easily be seen that no rotatable design can be a slope rotatable. This can be proved by using the fact that for a rotatable design

$$\mathrm{V}ar(b_{ii}) = \left\{1 + \left(R^2 - NL\right)/D\right\}/(2L)\,\sigma^2 \qquad \forall\, i = 1, 2, \ldots, v$$

$$\mathrm{V}ar(b_{ii'}) = \sigma^2/L \qquad \forall\, i < i' = 1, 2, \ldots, v$$

Now, (3.3.61) implies that $\dfrac{NL}{R^2} = \dfrac{v-2}{v}$ and for rotatability $\dfrac{NL}{R^2} > \dfrac{v}{v+2}$.

Now if we take $R^2 = NL$ design, then condition (3.4.2) and (3.3.8), we get $C = 5$. We call such designs as modified slope rotatable designs. In nutshell for a modified second order slope rotatable design following conditions have to be satisfied

- Conditions of symmetry (3.3.1)
- $R^2 = NL$ (3.3.13) and $C = 5$. (3.4.3)

Hader and Park (1978) and Gupta (1989) obtained slope rotatable designs over axial directions through Central Composite designs and BIB designs respectively. The designs obtained by these authors are not with equispaced levels. Hence, in this section, we obtain modified second order slope rotatable designs over axial directions for equispaced doses.

Using the method of construction of designs for fitting response surfaces with factor levels as equispaced doses given in Section 3.3.1, one can get a modified second order slope rotatable design with equispaced doses.

For the modified slope rotatable designs obtainable from central composite designs following the procedure of Method 3.3.1, $C = 5$ implies that

$$sw + 32t = 5\,sw$$
$$\Rightarrow 32\,t = 4\,sw \qquad (3.4.4)$$
$$\Rightarrow \frac{s}{t} = \frac{8}{w}$$

and $R^2 = NL$

$$s^2w^2 + 64t^2 + 16tsw = (sw + 2tv + n_0)sw$$

If $C = 5$, then $sw = 8t$. Substituting for sw in above, we get

$$64t^2 + 64t^2 + 128t^2 = (8t + 2tv + n_0)8t$$
$$\Rightarrow n_0 = 2t(12 - v) \qquad (3.4.5)$$

Now choosing the values of s, t, n_0 using equations (3.4.4) and (3.4.5), we get a modified second order slope rotatable design with each of the factors at 5 equispaced levels. The values of p, s, t, n_0 and N for modified slope rotatable designs for factorial experiments with 5 equispaced doses with $3 \le v \le 10$ and $N \le 500$ are given in Table 3.4.1.

Table 3.4.1: The values of v, p, s, t, n_0 **for modified slope rotatable designs for 5 equispaced doses with** $3 \le v \le 10$ **and** $N \le 500$ **obtainable from Central Composite Designs.**

v	p	s	t	n_0	N
3	3	1	1	18	32
4	4	1	2	32	64
5	4	1	2	28	64
5	5	1	4	56	128
6	5	1	4	48	128
6	6	1	8	96	256
7	6	1	8	80	256
8	6	1	8	64	256

Now, using Method 3.3.2 and the conditions in (3.4.3), a modified slope rotatable design with v factors each with three levels can be obtained using the above method, provided there exists a BIB design with $r = 5\lambda$. There is only one BIB design for $v \le 10$ that satisfies the condition $r = 5\lambda$. The parameters of this design are $v = 6, b = 15, r = 5, k = 2, \lambda = 1$. Following Method 3.3.2, for the design obtainable from this BIB design, we have $w = 2^2 = 4$ and get $R = 20, CL = 20$ and $L = 4$. The number of design points is $N = 60 + n_0$. The condition $C = 5$ is satisfied. To obtain a modified slope rotatable design, the condition $R^2 = NL$ must also be satisfied. To meet this requirement, we get $n_0 = 40$. Therefore, we get a modified slope rotatable design with 100 design points for a 3^6-factorial experiment.

For the case of $r < 5\lambda$, we can proceed on the steps of Method 3.3.2. The condition $C = 5$ requires that

$$\sum_{u=1}^{N} x_{iu}^2 = 5 \sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 .$$

Following Method 3.3.2 with equispaced doses, the above condition implies that

$$\frac{s}{t} = \frac{32}{(5\lambda - r)w} \tag{3.4.6}$$

Using $R^2 = NL$, we have

$$\frac{(r^2 - b\lambda)s^2 w^2 + (16r - 2v\lambda)swt + 64t^2}{s\lambda w} = n_0$$

$$\Rightarrow 2t\left[\frac{16(r^2 - b\lambda)}{\lambda(5\lambda - r)} + \frac{7r + \lambda(5 - v)}{\lambda}\right] = n_0 \tag{3.4.7}$$

Table 3.4.2 gives the list of the modified slope rotatable second order response surface designs obtainable from BIB dressings with $r < 5\lambda$.

Table 3.4.2: The values of v, p, s, t, n_0 **for modified slope rotatable designs for 5 equispaced doses with** $3 \le v \le 10$ **and** $N \le 500$ **obtainable from BIB designs with** $r < 5\lambda$ **.**

v	k	p	s	t	n_0	N	Source BIB Design
4	2	2	4	1	92	196	(4,6,3,2,1)
4	3	3	4	7	177	361	(4, 4, 3,3,2)
5	2	2	8	1	248	578	(5,10,4,2,1)
5	3	3	4	9	316	726	(5,10,6,3,3)
5	4	4	2	11	216	486	(5,5,4,4,3)
6	3	3	4	5	245	625	(6,10,5,3,2)
6	4	4	1	10	240	600	(6,15,10,4,6)
7	3	3	2	1	70	196	(7,7,3,3,1)
7	4	4	1	3	88	242	(7,7,4,4,2)
8	4	4	1	4	144	432	(8,14,7,4,3)
8	7	4	2	23	243	867	(8,8,7,7,6)
8	7	5	1	23	243	867	(8,8,7,7,6)
9	3	3	4	1	176	578	(9,12,4,3,1)

In case of $r > 5\lambda$, for a modified slope rotatable response surface design, we get

$$\frac{s}{t} = \frac{64}{r-5\lambda}\frac{w_2}{w_1} \tag{3.4.8}$$

Substituting (3.4.8) in (3.3.31) we will get a modified slope rotatable design when $C = 5$. The number of design points obtainable from this are quite large and are not presented here.

One may observe that the number of center points added in the designs obtained in this section is quite large. For obtaining slope rotatable designs for equispaced doses, this is difficult to avoid. Further, efforts need to be made to obtain slope rotatable designs over axial directions with equispaced doses.

The concept of slope rotatability over axial directions requires that the variance of the estimated slope in every axial direction be constant at points equidistant from the design origin. Park (1987) and Jang and Park (1993) extended the concept of slope rotatability over axial directions to the class of slope rotatable designs over all directions. This requires that average variance slope is constant for all the points equidistant from the origin. To be clearer, consider the following:

Let the estimated slope vector be

$$\hat{g}(\mathbf{x}) = \begin{bmatrix} \dfrac{\partial \hat{y}}{\partial x_1} \\ \dfrac{\partial \hat{y}}{\partial x_2} \\ \vdots \\ \dfrac{\partial \hat{y}}{\partial x_v} \end{bmatrix} = \mathbf{Db} \tag{3.4.9}$$

where $\mathbf{D} = \begin{bmatrix} \mathbf{0} & \mathbf{I}_v & 2diag(x_1, x_2, \cdots, x_v) & \mathbf{D}^* \end{bmatrix}$ is the matrix arising from the differentiation of (2.2.6) in Chapter II with respect to each of the v variables and $\mathbf{b}$ is the vector of estimated parameters of a second order response surface and given in (2.2.4) of Chapter II. Here the matrix $\mathbf{D}^*$ is

$$\mathbf{D}^* = \begin{bmatrix} x_2 & x_3 & \cdots & x_v & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ x_1 & 0 & \cdots & 0 & x_3 & x_4 & \cdots & x_v & \cdots & 0 & 0 & 0 \\ 0 & x_1 & \cdots & 0 & x_2 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & x_2 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & x_{v-1} & x_v & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & x_{v-2} & 0 & x_k \\ 0 & 0 & \cdots & x_1 & 0 & 0 & \cdots & x_2 & \cdots & 0 & x_{v-2} & x_{v-1} \end{bmatrix}$$

The estimated derivative at any point $\mathbf{x}$ in the direction specified by the $v \times 1$ vector of direction cosines, $\mathbf{v} = (v_1,\ v_2,\ ...,\ v_v)$, is $\mathbf{v}'\hat{g}(\mathbf{x})$, where $\sum_{i=1}^{v} v_i^2 = 1$. The variance of this slope is

$$\begin{aligned} \text{Var}_v(\mathbf{x}) &= \text{var}[\mathbf{v}'\hat{g}(\mathbf{x})] \\ &= \mathbf{v}'\mathbf{D}\,\text{var}(\hat{\boldsymbol{\beta}})\mathbf{D}'\mathbf{v} \\ &= \sigma^2 \mathbf{v}'\mathbf{D}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{D}'\mathbf{v}. \end{aligned} \tag{3.4.10}$$

If we are interested in all possible directions of $\mathbf{v}$, we want to consider the average of $\text{Var}_v(\mathbf{x})$ over all possible directions, which is referred to as the **average slope variance**. Park (1987) showed that the average slope variance is

$$\bar{V}(\mathbf{x}) = \frac{\sigma^2}{v}\,\text{trace}\left[\mathbf{D}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{D}'\right] \tag{3.4.11}$$

Note that $\bar{V}(\mathbf{x})$ is a function of $\mathbf{x}$, the point at which the derivative is being estimated, and also a function of the design. By choice of design it is possible to make this variance $\bar{V}(\mathbf{x})$ constant for all points equidistant from the design origin. This is the property of **slope rotatability over all directions**. In other words, we can say that the property of slope rotatability over all directions requires that the sum of the variances of the estimates of slopes in all directions at any point is a function of the distance of the point from the origin. This covers a very wide class of designs. If we call a second order response surface design satisfying the conditions of symmetry in (3.3.1) as symmetric second order response design, then we have the following result:

Result 3.4.1: {Park (1987) and Anjaneyulu, Varma and Narasimham (1997)}. Any symmetric second order response surface design is a second order slope rotatable design over all directions.

Proof: For any general v-factor symmetric second order response surface design, we have

$$\operatorname{Var}\left(\frac{\partial\hat{y}(\mathbf{x})}{\partial x_i}\right)=\operatorname{Var}(b_i)+4x_i^2\operatorname{Var}(b_{ii})+\sum_{i'\neq i=1}^{v}x_{i'}^2\operatorname{Var}(b_{ii'})\text{ (from (3.4.1)}$$

Now the sum of the variances of the estimates of slopes in all directions at any point is

$$\sum_{i=1}^{v}\operatorname{Var}\left(\frac{\partial\hat{y}(\mathbf{x})}{\partial x_i}\right)=\sum_{i=1}^{v}\operatorname{Var}(b_i)+4\sum_{i=1}^{v}x_i^2\operatorname{Var}(b_{ii})+\sum_{i=1}^{v}\sum_{i'\neq i=1}^{v}x_{i'}^2\operatorname{Var}(b_{ii'})$$

Now using (3.3.8) and taking $d^2=\sum_{i=1}^{v}x_i^2$, we get

$$\sum_{i=1}^{v}\operatorname{Var}\left(\frac{\partial\hat{y}(\mathbf{x})}{\partial x_i}\right)=v\operatorname{Var}(b_i)+4d^2\operatorname{Var}(b_{ii})+(v-1)d^2\operatorname{Var}(b_{ii'})$$
$$=f(d^2)\qquad(3.4.11)$$

Hence proved.

As a consequence of the Result 3.4.1, we have the following designs that are Second Order Slope Rotatable designs over all directions:

- *All the second order rotatable designs for response optimization obtained in Section (3.3.1) and modified second order slope rotatable designs over axial directions obtained in this Section.*
- *All second order rotatable designs for response optimization and modified second order slope rotatable designs over axial directions obtained in Sections 3.3.1 and Section 3.4.1 even when* $s=t=1$ *and* n_0*, the number of center points may be different from those given in the catalogues.*
- *The designs obtained in Method 3.3.3 with factors at 4 equispaced doses {although do not satisfy the property of rotatability for response optimization}.*
- *All asymmetric rotatable designs obtainable from Method 3.3.4 and Method 3.3.5.*
- *All designs for factors at three equispaced levels obtainable from incidence matrix of a BIB design either with* $r=3\lambda$ *or* $r\neq 3\lambda$.

Park and Kwon (1998) introduced yet another concept viz. **Slope-rotatable design with equal maximum directional variance** in obtaining designs for slope estimation. Such designs are defined as

Let

$$\operatorname{Var}_{\max}(\mathbf{x})=\max_{v:v'v=1}\operatorname{Var}_v(\mathbf{x})$$
$$=\max_{v:v'v=1}\mathbf{v}'\mathbf{D}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{D}'\mathbf{v}$$

If $\text{Var}_{\max}(\mathbf{x})$ is constant on the circles ($v=2$), spheres ($v=3$) or hyperspheres ($v \geq 4$) centered at the design origin, the estimates of the slope would be equally reliable for all points equidistant from the design origin.

The design, which gives this property, is called **slope-rotatable design with equal maximum directional variance**. Park and Kwon (1998) have shown that a rotatable designs for response optimization is a slope-rotatable design with equal maximum directional variance. As a consequence, all rotatable designs obtained in Section 3.3.1 are also slope-rotatable designs with equal maximum directional variance.

Minimax Designs for Estimating the Slope of a Response Surface

The study of optimal designs for estimating the slope of a response surface was initiated by Mukerjee and Huda (1985) using the criterion of minimizing the variance of the estimated slope maximized over all points in the factor space. They have termed such designs as **Minimax designs**. The concept of Minimax is described in the sequel:

Consider v quantitative factors $x_1, x_2, ..., x_v$ taking values in a v- ball having unit radius and suppose that the response at a point $\mathbf{x}$ is given by the second order polynomial given in (2.1.3) and (2.2.2). The *N*-observations in this model have been assumed to be uncorrelated w ith a common variance σ^2. Without loss of generality, let $\sigma^2 = 1$. A second order design ¶ is a probability measure on $\mathbf{X} = \left[(x_1, x_2, ..., x_v); \sum_{i=1}^{v} x_{iu}^2 \leq 1 \right]$ which allows the estimation of all parameters in (2.2.2) and let $M(¶) = \int f(\mathbf{x})\ f'(\mathbf{x})\ ¶(d\,\mathbf{x})$ be the information matrix of ¶. Then

$$N\,D(\mathbf{b}) = \mathbf{M}^{-1}(¶)$$

where $\mathbf{b}$ is the least squares estimator of $\boldsymbol{\beta}$ given in (2.2.2) and $D(.)$ stands for the dispersion matrix.

It can be shown that for polynomial regression in spherical regions, optimal designs under the present type of criterion are symmetric (Kiefer (1960)). Hence, restricting to symmetric designs, we observe that for a second order design ¶ the conditions for symmetry are

$$\begin{aligned} &\int x_i^2\ ¶(d\,\mathbf{x}) = R/N, \\ &\int x_i^4\ ¶(d\,\mathbf{x}) = CL/N, \\ &\int x_i^2 x_{i'}^2\ ¶(d\,\mathbf{x}) = L/N \quad (i \neq i') \\ &R > 0, \quad C > 1, L > 0, \quad (C+v-1)N^2 L > vR^2 \end{aligned} \tag{3.4.12}$$

and all other moments upto order four are zero.

The vector of estimated slopes along the factor axes at a point $\mathbf{x}$ is $\hat{g}(\mathbf{x})$ as given in (3.4.9). One can obtain the covariance matrix of $\hat{g}(\mathbf{x})$ and consider the variance of the estimated slope averaged over all directions as in (3.4.11). Following Atkinson (1970), this is equivalent to considering the trace of the covariance matrix and the minimax design will be that which minimizes this trace maximized over all points in $\mathbf{X}$.

After substituting the variance of the estimated parameters from (3.3.8) in (3.4.11), the trace of the covariance matrix can be shown to be

$$vNR^{-1} + \left[4N\{(C-1)L\}^{-1}\left(1 + D_1^{-1}(R^2 - N^2L)\right) + NL^{-1}(v-1)\right]d^2 \qquad (3.4.13)$$

where $d^2 = \sum_{i=1}^{v} x_i^2$ and $D_1 = \left[(C+v-1)N^2L - vR^2\right]$

Note that (3.4.13) is a function of d^2 even though the design has been assumed to be only symmetric and not necessarily rotatable. This has also been shown in Result 3.4.1.

Since the radius of the spherical design region is taken as unity, then noting that the coefficient of d^2 in (3.4.13) is non-negative, it follows that (3.4.13) is maximum over the factor space when $d^2=1$ and this maximum, after some rearrangement of terms, can be expressed as

$$\mathrm{V} = vNR^{-1} + (v-1)NL^{-1} + 4v^{-1}N(v-1)\{L(C-1)\}^{-1} + 4v^{-1}D_1^{-1} \qquad (3.4.14)$$

where $0 < R < v^{-1}$, $C > 1, L > 0$, $vR^2 < (C+v-1)N^2L \le R$

For fixed R and L, clearly (3.4.14) is decreasing in CL and is a minimum when $CL = R - (v-1)L$ in which case (3.4.14) becomes

$$\mathrm{V} = vNR^{-1} + (v-1)NL^{-1} + 4Nv^{-1}(v-1)(R - vL)^{-1} + 4v^{-1}(N^2R - vR^2) \qquad (3.4.15)$$

with $0 < R/N < v^{-1}$, $0 < L/N \le RN^{-1}(v+2)^{-1}$

Differentiation with respect to L shows that for fixed R expression (3.4.15) is a minimum when $L = (v+2)^{-1}R$ and if this is substituted in (3.4.15), the resulting expression, as a function of R, is a minimum when $R = \left[v + 2(v+4)^{-1/2}\right]^{-1} = \alpha_{20}$, say. Thus for the minimax design $R = \alpha_{20}$, as stated above and

$$N^{-1}L = (v+2)^{-1}\alpha_{20}, \quad N^{-1}CL = 3\,(v+2)^{-1}\alpha_{20} \qquad (3.4.16)$$

Since $C = 3$, the minimax design is rotatable (Box and Hunter (1957)). Since in practice, we are only concerned with discrete (exact) designs for which the weights are integer multiples of N^{-1}, the optimal design moments specified in (3.4.16) may not be achieved by implementable designs. Thus, it is important to study the performance of an implementable design in comparison with the optimal design. A measure of efficiency may be taken as the ratio of the value of (3.4.15) for the optimal design (denoted by V) to that for the design under consideration (denoted by Var). Mukerjee and Huda (1985) studied the efficiencies of rotatable designs obtainable from central composite designs. Gupta (1989) studied the minimax property of the response surface designs obtained through BIB designs. In the presented investigation, the minimax property of second order rotatable designs for various factors with equispaced doses are investigated. All the rotatable designs obtained in Section 3.3.1 are found to have reasonably high efficiencies.

As discussed above second order rotatable designs for various factors with equispaced doses also possess the property of slope rotatability over all directions, slope-rotatability with equal maximum directional variance and have reasonably good efficiencies as per minimax criterion. Therefore, the second order rotatable designs for response optimization obtained in Sections 3.3.1 and 3.3.2 can usefully be employed in agricultural experiments for both response optimization and slope estimation.

3.5 Blocking in Second Order Response Surface Designs

In many experimental situations, it may not be possible to have as many homogeneous experimental units as are the design points of a second order response surface design *i.e.* the conditions under which a trial for fitting second order response surface cannot be run under homogenous conditions. To deal with such situations, it is required that the design points be grouped into blocks such that experimental conditions for design points within a block are homogeneous. For a thorough discussion on orthogonal blocking of second order response surface designs one may refer to Box and Hunter (1957), Dey (1968), Dey and Das (1970), Gill and Das (1974) and Khuri and Cornell (1996), Chapter 8. For completeness, we give a brief description of the designs with orthogonal blocking. Let the N design points of a v-factor response surface design be divided into b blocks. The second order response surface with block effect can be represented as

$$y_u = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} + \sum_{i=1}^{v} \beta_{ii} x_{iu}^2 + \sum_{i=1}^{v-1} \sum_{j=i+1}^{v} \beta_{ij} x_{iu} + \sum_{j=1}^{b} \alpha_j z_{ju} + e_u ; \ \forall u = 1, \ldots, N \qquad (3.5.1)$$

where α_j is the effect of j^{th} block and z_{ju} is a dummy variable which takes the value '1' if the u^{th} observation pertains to j^{th} block and '0' otherwise. The other symbols have the same meaning as in Chapter II.

In general the linear and quadratic effects (polynomial effects) in (3.5.1) are not independent of the block effects. However, the experimenter would generally be interested in assessing the polynomial effects independent of block effects. Therefore, the design points of the second order response surface design should be so chosen that the least square estimators of the values of polynomial effects $\boldsymbol{\beta}$ are independent of block effects. A design, which allows the estimation of polynomial effects independent of block effects, is known as orthogonally blocked second order response surface design. Further blocks are assumed to have no impact on the nature and shape of the response surface. To obtain the conditions, we rewrite the model (3.5.1) by adding and subtracting $\sum_{j=1}^{b}\alpha_j \bar{z}_j$ as

$$y_u = \beta_0' + \sum_{i=1}^{v}\beta_i x_{iu} + \sum_{i=1}^{v}\beta_{ii} x_{iu}^2 + \sum_{i=1}^{v-1}\sum_{i'=i+1}^{v}\beta_{ii'} x_{iu} x_{i'u} + \sum_{j=1}^{b}\alpha_j\left(z_{ju} - \bar{z}_j\right) + e_u \qquad (3.5.2)$$

where $\bar{z}_j = \frac{1}{N}\sum_{u=1}^{N} z_{ju}$ and $\beta_0' = \beta_0 + \sum_{s=1}^{b}\alpha_j \bar{z}_j$.

The model (3.5.2) can be re-written in matrix notations as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha} + \mathbf{e} \qquad (3.5.3)$$

where $\mathbf{X}, \boldsymbol{\beta}$ and $\mathbf{e}$ are same as defined in (2.2.2) and $\mathbf{Z} = ((z_{ju}))$ and $\alpha = (\alpha_1, \ldots, \alpha_b)'$.

One can easily see that for the orthogonal estimation of $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$, $\mathbf{X}'\mathbf{Z} = \mathbf{0}$, *i.e.* the conditions for orthogonal blocking are

(i) $\sum_{u=1}^{N} x_{iu}\left(z_{ju} - \bar{z}_j\right) = 0 \qquad \forall\, i = 1,\ldots,v;\quad j = 1,\ldots,b$

(ii) $\sum_{u=1}^{N} x_{iu} x_{i'u}\left(z_{ju} - \bar{z}_j\right) = 0 \qquad \forall\, i \neq i',\ i, i' = 1,\ldots,v;\quad j = 1,\ldots,b$

(iii) $\sum_{u=1}^{N} x_{iu}^2\left(z_{ju} - \bar{z}_j\right) = 0 \qquad \forall\, i = 1,\ldots,v;\quad j = 1,\ldots,b$ (3.5.4)

Since it is desirable for an orthogonally blocked design to be rotatable also, therefore, the symmetry conditions of the second order response surface designs given in section (3.3) should also be satisfied. Here let us take that

(iv) $\sum_{u=1}^{N} x_{iu} = 0 \qquad \forall\, i = 1,\ldots,v$

(v) $\sum_{u=1}^{N} x_{iu} x_{i'u} = 0 \qquad \forall\, i \neq i',\ i, i' = 1,\ldots,v$ (3.5.5)

As z_{su} is a 0-1 variable, therefore, using (3.5.4) and (3.5.5), the following conditions are obtained for orthogonal blocking [(see e.g. Box and Hunter (1957)]

(a) $\sum_{u(j)} x_{iu} = 0 \qquad \forall\, i = 1,\ldots,v;\quad j = 1,\ldots,b$

(b) $\quad \sum_{u(j)} x_{iu} x_{i'u} = 0 \qquad \forall\, i \neq i',\ i, i' = 1,\ldots,v; \quad j = 1,\ldots,b$

(c) $$\frac{\sum_{u(j)} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_j}{N} \qquad \forall\, i = 1,\ldots,v; \quad j = 1,\ldots,b \tag{3.5.6}$$

where $\sum_{u(j)}$ denotes the summation extended only over those values of u in the j^{th} block and n_j is the number of design points in the j^{th} block. To be specific, conditions (3.5.6a) and (3.5.6b) imply that the sum of $x_{iu}'s$ within each block should be zero. It implies that the each block is a first order orthogonal design. According to the condition (3.5.6c), the fraction of the total of sum of squares of $x_{iu}'s$ $(i = 1,\ldots,v)$ in each block must be equal to the fraction of the total number of design points allotted in that block. We now discuss the methods of construction of second order response surface designs with orthogonal blocking.

The methods of blocking in response surface designs obtainable from central composite designs and BIB designs have been studied in literature. Dey (1968) has studied the blocking in response surface designs with equispaced doses. These methods of blocking with some modifications are given as below:

3.5.1 Blocking in Central Composite Designs

1. Take a central composite design for v factors having 5 equispaced levels each denoted by –2, -1, 0, 1,2. Now divide $w = 2^p$, $p \leq v$ in blocks of size 2^{3+m}, where m is a positive integer such that interaction of third order or less is not confounded with blocks. This results into 2^{p-3-m} blocks.
2. Now take the $2v$ axial points 2^m times in one block. We get a block of size $v.2^{m+1}$.
3. If $v.2^{m+1} > 2^{3+m}$, then add $v.2^{m+1} - 2^{3+m}$ center points in each of the blocks of size 2^{3+m}. If, however, $v.2^{m+1} < 2^{3+m}$, then add $2^{3+m} - v.2^{m+1}$ center points in the block of size $v.2^{m+1}$.
4. To satisfy the desired property of rotatability or slope rotatability over axial directions copies of these blocks may be adjusted so that the design without blocks satisfy the conditions of the desired property.

3.5.2 Blocking in Designs obtainable from BIB designs

The blocking procedure for the designs obtainable from BIB designs can be classified intro two categories viz. (i) resolvable BIB designs (ii) non-resolvable BIB designs. These are described in the sequel.

Designs obtainable from resolvable BIB designs

Consider a $\alpha-$resolvable BIB design with parameters $v, b = h\beta, r = h\alpha, k, \lambda$. In this design, the blocks can be grouped into h sets such that each set contains β-blocks and in every set every treatment is replicated $\alpha-$times. Obtain bw, $w = 2^p$, $p \le k$ points as per procedure of Method 3.3.2. Call these points as points obtained from incidence matrix.

Now take the βwpoints obtained from one set of blocks of $\alpha-$resolvable BIB design into one block. This gives h blocks each of size βw. Add n_{0b} center points to each of the blocks. If $r = 3\lambda$, then this procedure yields a second order rotatable design with orthogonal blocking for v factors each at 3 levels. If the number of center points n_0 for a modified and rotatable design are a multiple of h, then taking $n_{0b} = n_0 / h$ gives a modified and rotatable design with orthogonal blocking. The βwpoints can further be divided into blocks of size $\beta.2^r$ each, such that no three factor or less interaction is confounded with the block effects. This will give $hw/2^r$ blocks each of size $\beta.2^r$.

If, however, $r < 3\lambda$, then the $2v$-axial points of the type $(\pm 2, 0, \cdots, 0)$; $\cdots, (0, 0, \ldots, \pm 2)$, 2^m times in one block. This requires that $\alpha.2^r = 2^{3+m}$. The center points are added as per procedure of Step 3 of blocking in Central composite designs. Now the copies of the blocks can be taken as per procedure of Method 3.3.2 so as to satisfy the condition of rotatability for response optimization or slope rotatability over axial directions.

Designs obtainable from non-resolvable BIB designs

Consider a BIB design with parameters *v, b, r, k,* λ. Now take its complementary which is also a BIB design with parameters *v, b, b - r, v - k, b - 2r +* λ. Form the groups of 2*b* blocks so obtained such that each group consists of two blocks, one block from the original BIB design and other is its corresponding block from the complementary design. This process always yields a 1-resolvable variance balanced block design. It can easily be seen that this design is essentially a symmetrical unequal block arrangement with two distinct block sizes as introduced by Kishen (1940) with parameters $v, b_1 = b, b_2 = b, r = b, k_1 = k, k_2 = v - k, \lambda^* = b - 2r + 2\lambda$. Following the procedure described in Remark 3.3.2, one can get a second order rotatable design by associating the rows of the incidence matrix with 2^{k_2} factorial or 2^p fraction of 2^{k_2} factorial, $k_1 \le p \le k_2$. In this case, it may be noted that the fraction of 2^{k_2} factorial need no necessarily be a Resolution 5 plan as the design is second order response surface design with non-singularity condition with original BIB design itself. Now for blocking, follow the same procedure as described for resolvable block designs.

The procedures of blocking described above are quite general in nature. In the sequel we give the block contents of second order rotatable designs with orthogonal blocking for $3 \le v \le 8$ factors each at 3 or 5 equispaced doses. In some cases, if the number of center points in blocks are more than one, then they can be used for estimation for pure error and hence appropriately identified blocks can be used for fitting of first order response surface and testing the lack of fit and rest of the blocks can be used for sequential build up of second order response surface design.

3-factors each at 3 levels; Block Size: 9 (obtained using BIB design 3,3,2,2,1 and its complementary 3,3,1,1,0)

Block-I			Block-II			Block-III		
A	B	C	A	B	C	A	B	C
-1	-1	0	-1	0	-1	0	-1	-1
-1	1	0	-1	0	1	0	-1	1
1	-1	0	1	0	-1	0	1	-1
1	1	0	1	0	1	0	1	1
0	0	1	0	1	0	1	0	0
0	0	1	0	1	0	1	0	0
0	0	-1	0	-1	0	-1	0	0
0	0	-1	0	-1	0	-1	0	0
0	0	0	0	0	0	0	0	0

*to make it modified and rotatable add three more points to each of the blocks.

4-factors each at 3 levels; Block Size: 9 (Obtained using BIB design 4,6,3,2,1)

Block-I				Block-II				Block-III			
A	B	C	D	A	B	C	D	A	B	C	D
-1	-1	0	0	-1	0	-1	0	0	-1	-1	0
-1	1	0	0	-1	0	1	0	0	-1	1	0
1	-1	0	0	1	0	-1	0	0	1	-1	0
1	1	0	0	1	0	1	0	0	1	1	0
0	0	-1	-1	0	-1	0	-1	-1	0	0	-1
0	0	-1	1	0	-1	0	1	-1	0	0	1
0	0	1	-1	0	1	0	-1	1	0	0	-1
0	0	1	1	0	1	0	1	1	0	0	1
0	0	0	0	0	0	0	0	0	0	0	0

*to make it modified and rotatable add three more points to each of the blocks.

4-factors each at 5 equispaced levels; Block Size 9 (Obtained through Central Composite Designs)

Block-I				Block-II				Block-III			
A	B	C	D	A	B	C	D	A	B	C	D
-1	-1	-1	-1	-1	-1	-1	1	2	0	0	0
-1	-1	1	1	-1	-1	1	-1	-2	0	0	0
-1	1	-1	1	-1	1	-1	-1	0	2	0	0
1	-1	-1	1	1	-1	-1	-1	0	-2	0	0
1	-1	1	-1	-1	1	1	1	0	0	2	0
1	1	-1	-1	1	-1	1	1	0	0	-2	0
-1	1	1	-1	1	1	-1	1	0	0	0	2
1	1	1	1	1	1	1	-1	0	0	0	-2
0	0	0	0	0	0	0	0	0	0	0	0

*if we take 3 more center points in each block then it is a modified second order rotatable design.

5-factors each at 5 equispaced levels (ABC, CDE, ABDE are confounded); Block Size: 10 (Obtained through Central Composite Designs)

Block-I					Block-II					Block-III				
A	B	C	D	E	A	B	C	D	E	A	B	C	D	E
-1	-1	-1	-1	-1	-1	-1	-1	-1	1	2	0	0	0	0
-1	-1	-1	1	1	-1	-1	-1	1	-1	-2	0	0	0	0
-1	1	1	-1	1	-1	1	1	-1	-1	0	2	0	0	0
-1	1	1	1	-1	-1	1	1	1	1	0	-2	0	0	0
1	-1	1	-1	1	1	-1	1	-1	-1	0	0	2	0	0
1	-1	1	1	-1	1	-1	1	1	1	0	0	-2	0	0
1	1	-1	-1	-1	1	1	-1	-1	1	0	0	0	2	0
1	1	-1	1	1	1	1	-1	1	-1	0	0	0	-2	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2

Block-IV					Block-V					Block-VI				
A	B	C	D	E	A	B	C	D	E	A	B	C	D	E
-1	-1	1	-1	1	-1	-1	1	-1	-1	2	0	0	0	0
-1	-1	1	1	-1	-1	-1	1	1	1	-2	0	0	0	0
-1	1	-1	-1	-1	-1	1	-1	-1	1	0	2	0	0	0
-1	1	-1	1	1	-1	1	-1	1	-1	0	-2	0	0	0
1	-1	-1	-1	-1	1	-1	-1	-1	1	0	0	2	0	0
1	-1	-1	1	1	1	-1	-1	1	-1	0	0	-2	0	0
1	1	1	-1	1	1	1	1	-1	-1	0	0	0	2	0
1	1	1	1	-1	1	1	1	1	1	0	0	0	-2	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2

*to make this design modified and rotatable add two more center points to each of the blocks.

5-factors each at 5 equispaced levels (ABCDE is confounded): Block size 20 (Obtained through Central Composite Designs)

Block-I						Block-II						Block-III				
A	B	C	D	E		A	B	C	D	E		A	B	C	D	E
-1	-1	-1	-1	-1		1	-1	-1	-1	-1		2	0	0	0	0
1	1	-1	-1	-1		-1	1	-1	-1	-1		-2	0	0	0	0
1	-1	1	-1	-1		-1	-1	1	-1	-1		0	2	0	0	0
1	-1	-1	1	-1		-1	-1	-1	1	-1		0	-2	0	0	0
1	-1	-1	-1	1		-1	-1	-1	-1	1		0	0	2	0	0
-1	1	1	-1	-1		1	1	1	-1	-1		0	0	-2	0	0
-1	1	-1	1	-1		1	1	-1	1	-1		0	0	0	2	0
-1	1	-1	-1	1		1	1	-1	-1	1		0	0	0	-2	0
-1	-1	1	1	-1		1	-1	1	1	-1		0	0	0	0	2
-1	-1	1	-1	1		1	-1	1	-1	1		0	0	0	0	-2
-1	-1	-1	1	1		1	-1	-1	1	1		2	0	0	0	0
1	1	1	1	-1		-1	1	1	1	-1		-2	0	0	0	0
1	1	1	-1	1		-1	1	1	-1	1		0	2	0	0	0
1	1	-1	1	1		-1	1	-1	1	1		0	-2	0	0	0
1	-1	1	1	1		-1	-1	1	1	1		0	0	2	0	0
-1	1	1	1	1		1	1	1	1	1		0	0	-2	0	0
0	0	0	0	0		0	0	0	0	0		0	0	0	2	0
0	0	0	0	0		0	0	0	0	0		0	0	0	-2	0
0	0	0	0	0		0	0	0	0	0		0	0	0	0	2
0	0	0	0	0		0	0	0	0	0		0	0	0	0	-2

*to make the design modified and rotatable add four more points to each of the blocks.

5-factors each at 5 equispaced levels (ABCDE is confounded): Block size 16 (Obtained through BIB design 5,10,4,2,1 and its complementary 5,10,6,3,3)

Block-I						Block-II						Block-III				
A	B	C	D	E		A	B	C	D	E		A	B	C	D	E
-1	-1	-1	0	0		0	-1	-1	-1	0		0	0	-1	-1	-1
-1	-1	1	0	0		0	-1	-1	1	0		0	0	-1	-1	1
-1	1	-1	0	0		0	-1	1	-1	0		0	0	-1	1	-1
1	-1	-1	0	0		0	1	-1	-1	0		0	0	1	-1	-1
-1	1	1	0	0		0	-1	1	1	0		0	0	-1	1	1
1	-1	1	0	0		0	1	-1	1	0		0	0	1	-1	1
1	1	-1	0	0		0	1	1	-1	0		0	0	1	1	-1
1	1	1	0	0		0	1	1	1	0		0	0	1	1	1
0	0	0	-1	-1		-1	0	0	0	-1		-1	-1	0	0	0
0	0	0	-1	1		1	0	0	0	-1		-1	1	0	0	0
0	0	0	1	-1		-1	0	0	0	1		1	-1	0	0	0
0	0	0	1	1		1	0	0	0	1		1	1	0	0	0
0	0	0	-1	-1		-1	0	0	0	-1		-1	-1	0	0	0
0	0	0	-1	1		1	0	0	0	-1		-1	1	0	0	0
0	0	0	1	-1		-1	0	0	0	1		1	-1	0	0	0
0	0	0	1	1		1	0	0	0	1		1	1	0	0	0

Block-IV

A	B	C	D	E
-1	0	0	-1	-1
1	0	0	-1	-1
-1	0	0	-1	1
-1	0	0	1	-1
1	0	0	-1	1
1	0	0	1	-1
-1	0	0	1	1
1	0	0	1	1
0	-1	-1	0	0
0	-1	1	0	0
0	1	-1	0	0
0	1	1	0	0
0	-1	-1	0	0
0	-1	1	0	0
0	1	-1	0	0
0	1	1	0	0

Block-V

A	B	C	D	E
-1	-1	0	0	-1
-1	1	0	0	-1
1	-1	0	0	-1
-1	-1	0	0	1
1	1	0	0	-1
-1	1	0	0	1
1	-1	0	0	1
1	1	0	0	1
0	0	-1	-1	0
0	0	-1	1	0
0	0	1	-1	0
0	0	1	1	0
0	0	-1	-1	0
0	0	-1	1	0
0	0	1	-1	0
0	0	1	1	0

Block-VI

A	B	C	D	E
-1	-1	0	-1	0
-1	-1	0	1	0
-1	1	0	-1	0
1	-1	0	-1	0
-1	1	0	1	0
1	-1	0	1	0
1	1	0	-1	0
1	1	0	1	0
0	0	-1	0	-1
0	0	-1	0	1
0	0	1	0	-1
0	0	1	0	1
0	0	-1	0	-1
0	0	-1	0	1
0	0	1	0	-1
0	0	1	0	1

Block-VII

A	B	C	D	E
0	-1	-1	0	-1
0	-1	-1	0	1
0	-1	1	0	-1
0	1	-1	0	-1
0	-1	1	0	1
0	1	-1	0	1
0	1	1	0	-1
0	1	1	0	1
-1	0	0	-1	0
-1	0	0	1	0
1	0	0	-1	0
1	0	0	1	0
-1	0	0	-1	0
-1	0	0	1	0
1	0	0	-1	0
1	0	0	1	0

Block-VIII

A	B	C	D	E
-1	0	-1	-1	0
1	0	-1	-1	0
-1	0	-1	1	0
-1	0	1	-1	0
1	0	-1	1	0
1	0	1	-1	0
-1	0	1	1	0
1	0	1	1	0
0	-1	0	0	-1
0	-1	0	0	1
0	1	0	0	-1
0	1	0	0	1
0	-1	0	0	-1
0	-1	0	0	1
0	1	0	0	-1
0	1	0	0	1

Block-IX

A	B	C	D	E
0	-1	0	-1	-1
0	1	0	-1	-1
0	-1	0	-1	1
0	-1	0	1	-1
0	1	0	-1	1
0	1	0	1	-1
0	-1	0	1	1
0	1	0	1	1
-1	0	-1	0	0
1	0	-1	0	0
-1	0	1	0	0
1	0	1	0	0
-1	0	-1	0	0
1	0	-1	0	0
-1	0	1	0	0
1	0	1	0	0

Block-X

A	B	C	D	E
-1	0	-1	0	-1
-1	0	1	0	1
1	0	-1	0	-1
-1	0	-1	0	-1
1	0	1	0	1
-1	0	1	0	1
1	0	-1	0	-1
1	0	1	0	1
0	-1	0	-1	0
0	-1	0	1	0
0	1	0	-1	0
0	1	0	1	0
0	-1	0	-1	0
0	-1	0	1	0
0	1	0	-1	0
0	1	0	1	0

10 more blocks are obtained by repeating Blocks I to X once

Block-XXI

A	B	C	D	E
2	0	0	0	0
-2	0	0	0	0
0	2	0	0	0
0	-2	0	0	0
0	0	2	0	0
0	0	-2	0	0
0	0	0	2	0
0	0	0	-2	0
0	0	0	0	2
0	0	0	0	-2
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

6 factors each at 5 equispaced levels; (Defining Contrast : ABCDEF and ABC and DEF are confounded); Block Size :24 (Obtained through Central Composite Designs)

Block-I

A	B	C	D	E	F
-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	1	1
-1	-1	-1	1	-1	1
-1	-1	-1	1	1	-1
-1	1	1	-1	-1	-1
-1	1	1	-1	1	1
-1	1	1	1	-1	1
-1	1	1	1	1	-1
1	-1	1	-1	-1	-1
1	-1	1	-1	1	1
1	-1	1	1	-1	1
1	-1	1	1	1	-1
1	1	-1	-1	-1	-1
1	1	-1	-1	1	1
1	1	-1	1	-1	1
1	1	-1	1	1	-1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-II

A	B	C	D	E	F
-1	-1	1	-1	-1	1
-1	-1	1	-1	1	-1
-1	-1	1	1	-1	-1
-1	-1	1	1	1	1
-1	1	-1	-1	-1	1
-1	1	-1	-1	1	-1
-1	1	-1	1	-1	-1
-1	1	-1	1	1	1
1	-1	-1	-1	-1	1
1	-1	-1	-1	1	-1
1	-1	-1	1	-1	-1
1	-1	-1	1	1	1
1	1	1	-1	-1	1
1	1	1	-1	1	-1
1	1	1	1	-1	-1
1	1	1	1	1	1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-III

A	B	C	D	E	F
2	0	0	0	0	0
-2	0	0	0	0	0
0	2	0	0	0	0
0	-2	0	0	0	0
0	0	2	0	0	0
0	0	-2	0	0	0
0	0	0	2	0	0
0	0	0	-2	0	0
0	0	0	0	2	0
0	0	0	0	-2	0
0	0	0	0	0	2
0	0	0	0	0	-2
2	0	0	0	0	0
-2	0	0	0	0	0
0	2	0	0	0	0
0	-2	0	0	0	0
0	0	2	0	0	0
0	0	-2	0	0	0
0	0	0	2	0	0
0	0	0	-2	0	0
0	0	0	0	2	0
0	0	0	0	-2	0
0	0	0	0	0	2
0	0	0	0	0	-2

6 factors each at 5 equispaced levels; (ABC, CDE, ADF, ABDE, ACEF, BCDF, BDEF confounded); Block Size :12 (Obtained through Central Composite Designs)

Block-I

A	B	C	D	E	F
-1	-1	-1	-1	-1	-1
-1	-1	-1	1	1	1
-1	1	1	-1	1	-1
-1	1	1	1	-1	1
1	-1	1	-1	1	1
1	-1	1	1	-1	-1
1	1	-1	-1	-1	1
1	1	-1	1	1	-1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-II

A	B	C	D	E	F
-1	-1	-1	-1	-1	1
-1	-1	-1	1	1	-1
-1	1	1	-1	1	1
-1	1	1	1	-1	-1
1	-1	1	-1	1	-1
1	-1	1	1	-1	1
1	1	-1	-1	-1	-1
1	1	-1	1	1	1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-III

A	B	C	D	E	F
2	0	0	0	0	0
-2	0	0	0	0	0
0	2	0	0	0	0
0	-2	0	0	0	0
0	0	2	0	0	0
0	0	-2	0	0	0
0	0	0	2	0	0
0	0	0	-2	0	0
0	0	0	0	2	0
0	0	0	0	-2	0
0	0	0	0	0	2
0	0	0	0	0	-2

Block-IV

A	B	C	D	E	F
-1	-1	-1	-1	1	-1
-1	-1	-1	1	-1	1
-1	1	1	-1	-1	-1
-1	1	1	1	1	1
1	-1	1	-1	-1	1
1	-1	1	1	1	-1
1	1	-1	-1	1	1
1	1	-1	1	-1	-1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-V

A	B	C	D	E	F
-1	-1	-1	-1	1	1
-1	-1	-1	1	-1	-1
-1	1	1	-1	-1	1
-1	1	1	1	1	-1
1	-1	1	-1	-1	-1
1	-1	1	1	1	1
1	1	-1	-1	1	-1
1	1	-1	1	-1	1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-VI

A	B	C	D	E	F
2	0	0	0	0	0
-2	0	0	0	0	0
0	2	0	0	0	0
0	-2	0	0	0	0
0	0	2	0	0	0
0	0	-2	0	0	0
0	0	0	2	0	0
0	0	0	-2	0	0
0	0	0	0	2	0
0	0	0	0	-2	0
0	0	0	0	0	2
0	0	0	0	0	-2

Block-VII

A	B	C	D	E	F
-1	-1	1	-1	1	-1
-1	-1	1	1	-1	1
-1	1	-1	-1	-1	-1
-1	1	-1	1	1	1
1	-1	-1	-1	-1	1
1	-1	-1	1	1	-1
1	1	1	-1	1	1
1	1	1	1	-1	-1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-VIII

A	B	C	D	E	F
-1	-1	1	-1	1	1
-1	-1	1	1	-1	-1
-1	1	-1	-1	-1	1
-1	1	-1	1	1	-1
1	-1	-1	-1	-1	-1
1	-1	-1	1	1	1
1	1	1	-1	1	-1
1	1	1	1	-1	1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-IX

A	B	C	D	E	F
2	0	0	0	0	0
-2	0	0	0	0	0
0	2	0	0	0	0
0	-2	0	0	0	0
0	0	2	0	0	0
0	0	-2	0	0	0
0	0	0	2	0	0
0	0	0	-2	0	0
0	0	0	0	2	0
0	0	0	0	-2	0
0	0	0	0	0	2
0	0	0	0	0	-2

Block-X

A	B	C	D	E	F
-1	-1	1	-1	-1	-1
-1	-1	1	1	1	1
-1	1	-1	-1	1	-1
-1	1	-1	1	-1	1
1	-1	-1	-1	1	1
1	-1	-1	1	-1	-1
1	1	1	-1	-1	1
1	1	1	1	1	-1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-XI

A	B	C	D	E	F
-1	-1	1	-1	-1	1
-1	-1	1	1	1	-1
-1	1	-1	-1	1	1
-1	1	-1	1	-1	-1
1	-1	-1	-1	1	-1
1	-1	-1	1	-1	1
1	1	1	-1	-1	-1
1	1	1	1	1	1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

Block-XII

A	B	C	D	E	F
2	0	0	0	0	0
-2	0	0	0	0	0
0	2	0	0	0	0
0	-2	0	0	0	0
0	0	2	0	0	0
0	0	-2	0	0	0
0	0	0	2	0	0
0	0	0	-2	0	0
0	0	0	0	2	0
0	0	0	0	-2	0
0	0	0	0	0	2
0	0	0	0	0	-2

7 factors each at 5 equispaced levels; (Block Size :16 (Obtained through BIB design 7,7,3,3,1 and its complementary 7,7,4,4,2)

Block - I

A	B	C	D	E	F	G
-1	-1	0	-1	0	0	0
-1	-1	0	1	0	0	0
-1	1	0	-1	0	0	0
1	-1	0	-1	0	0	0
-1	1	0	1	0	0	0
1	-1	0	1	0	0	0
1	1	0	-1	0	0	0
1	1	0	1	0	0	0
0	0	-1	0	-1	-1	-1
0	0	-1	0	-1	1	1
0	0	-1	0	1	-1	1
0	0	-1	0	1	1	-1
0	0	1	0	-1	-1	1
0	0	1	0	-1	1	-1
0	0	1	0	1	-1	-1
0	0	1	0	1	1	1

Block-II

A	B	C	D	E	F	G
-1	-1	0	-1	0	0	0
-1	-1	0	1	0	0	0
-1	1	0	-1	0	0	0
1	-1	0	-1	0	0	0
-1	1	0	1	0	0	0
1	-1	0	1	0	0	0
1	1	0	-1	0	0	0
1	1	0	1	0	0	0
0	0	-1	0	-1	-1	1
0	0	-1	0	-1	1	-1
0	0	-1	0	1	-1	-1
0	0	-1	0	1	1	1
0	0	1	0	-1	-1	-1
0	0	1	0	-1	1	1
0	0	1	0	1	-1	1
0	0	1	0	1	1	-1

Block - III

A	B	C	D	E	F	G
0	-1	-1	0	-1	0	0
0	-1	-1	0	1	0	0
0	-1	1	0	-1	0	0
0	1	-1	0	-1	0	0
0	-1	1	0	1	0	0
0	1	-1	0	1	0	0
0	1	1	0	-1	0	0
0	1	1	0	1	0	0
-1	0	0	-1	0	-1	-1
1	0	0	-1	0	-1	1
1	0	0	-1	0	1	-1
-1	0	0	-1	0	1	1
1	0	0	1	0	-1	-1
-1	0	0	1	0	-1	1
-1	0	0	1	0	1	-1
1	0	0	1	0	1	1

Block-IV

A	B	C	D	E	F	G
0	-1	-1	0	-1	0	0
0	-1	-1	0	1	0	0
0	-1	1	0	-1	0	0
0	1	-1	0	-1	0	0
0	-1	1	0	1	0	0
0	1	-1	0	1	0	0
0	1	1	0	-1	0	0
0	1	1	0	1	0	0
1	0	0	-1	0	-1	-1
-1	0	0	-1	0	-1	1
-1	0	0	-1	0	1	-1
1	0	0	-1	0	1	1
-1	0	0	1	0	-1	-1
1	0	0	1	0	-1	1
1	0	0	1	0	1	-1
-1	0	0	1	0	1	1

Block - V

A	B	C	D	E	F	G
0	0	-1	-1	0	-1	0
0	0	-1	-1	0	1	0
0	0	-1	1	0	-1	0
0	0	1	-1	0	-1	0
0	0	-1	1	0	1	0
0	0	1	-1	0	1	0
0	0	1	1	0	-1	0
0	0	1	1	0	1	0
-1	-1	0	0	-1	0	-1
1	1	0	0	-1	0	-1
-1	1	0	0	-1	0	1
1	-1	0	0	-1	0	1
-1	1	0	0	1	0	-1
1	-1	0	0	1	0	-1
-1	-1	0	0	1	0	1
1	1	0	0	1	0	1

Block-VI

A	B	C	D	E	F	G
0	0	-1	-1	0	-1	0
0	0	-1	-1	0	1	0
0	0	-1	1	0	-1	0
0	0	1	-1	0	-1	0
0	0	-1	1	0	1	0
0	0	1	-1	0	1	0
0	0	1	1	0	-1	0
0	0	1	1	0	1	0
-1	1	0	0	-1	0	-1
1	-1	0	0	-1	0	-1
-1	-1	0	0	-1	0	1
1	1	0	0	-1	0	1
-1	-1	0	0	1	0	-1
1	1	0	0	1	0	-1
-1	1	0	0	1	0	1
1	-1	0	0	1	0	1

Block - VII

A	B	C	D	E	F	G
0	0	0	-1	-1	0	-1
0	0	0	-1	-1	0	1
0	0	0	-1	1	0	-1
0	0	0	1	-1	0	-1
0	0	0	-1	1	0	1
0	0	0	1	-1	0	1
0	0	0	1	1	0	-1
0	0	0	1	1	0	1
-1	-1	-1	0	0	-1	0
-1	1	1	0	0	-1	0
1	-1	1	0	0	-1	0
1	1	-1	0	0	-1	0
-1	-1	1	0	0	1	0
-1	1	-1	0	0	1	0
1	-1	-1	0	0	1	0
1	1	1	0	0	1	0

Block-VIII

A	B	C	D	E	F	G
0	0	0	-1	-1	0	-1
0	0	0	-1	-1	0	1
0	0	0	-1	1	0	-1
0	0	0	1	-1	0	-1
0	0	0	-1	1	0	1
0	0	0	1	-1	0	1
0	0	0	1	1	0	-1
0	0	0	1	1	0	1
-1	-1	1	0	0	-1	0
-1	1	-1	0	0	-1	0
1	-1	-1	0	0	-1	0
1	1	1	0	0	-1	0
-1	-1	-1	0	0	1	0
-1	1	1	0	0	1	0
1	-1	1	0	0	1	0
1	1	-1	0	0	1	0

Block - IX

A	B	C	D	E	F	G
-1	0	0	0	-1	-1	0
1	0	0	0	-1	-1	0
-1	0	0	0	-1	1	0
-1	0	0	0	1	-1	0
1	0	0	0	-1	1	0
1	0	0	0	1	-1	0
-1	0	0	0	1	1	0
1	0	0	0	1	1	0
0	-1	-1	-1	0	0	-1
0	-1	1	1	0	0	-1
0	1	-1	1	0	0	-1
0	1	1	-1	0	0	-1
0	-1	-1	1	0	0	1
0	-1	1	-1	0	0	1
0	1	-1	-1	0	0	1
0	1	1	1	0	0	1

Block-X

A	B	C	D	E	F	G
-1	0	0	0	-1	-1	0
1	0	0	0	-1	-1	0
-1	0	0	0	-1	1	0
-1	0	0	0	1	-1	0
1	0	0	0	-1	1	0
1	0	0	0	1	-1	0
-1	0	0	0	1	1	0
1	0	0	0	1	1	0
0	-1	-1	1	0	0	-1
0	-1	1	-1	0	0	-1
0	1	-1	-1	0	0	-1
0	1	1	1	0	0	-1
0	-1	-1	-1	0	0	1
0	-1	1	1	0	0	1
0	1	-1	1	0	0	1
0	1	1	-1	0	0	1

Block - XI

A	B	C	D	E	F	G
0	-1	0	0	0	-1	-1
0	1	0	0	0	-1	-1
0	-1	0	0	0	-1	1
0	-1	0	0	0	1	-1
0	1	0	0	0	-1	1
0	1	0	0	0	1	-1
0	-1	0	0	0	1	1
0	1	0	0	0	1	1
-1	0	-1	-1	-1	0	0
-1	0	-1	1	1	0	0
-1	0	1	-1	1	0	0
-1	0	1	1	-1	0	0
1	0	-1	-1	1	0	0
1	0	-1	1	-1	0	0
1	0	1	-1	-1	0	0
1	0	1	1	1	0	0

Block-XII

A	B	C	D	E	F	G
0	-1	0	0	0	-1	-1
0	1	0	0	0	-1	-1
0	-1	0	0	0	-1	1
0	-1	0	0	0	1	-1
0	1	0	0	0	-1	1
0	1	0	0	0	1	-1
0	-1	0	0	0	1	1
0	1	0	0	0	1	1
-1	0	-1	-1	1	0	0
-1	0	-1	1	-1	0	0
-1	0	1	-1	-1	0	0
-1	0	1	1	1	0	0
1	0	-1	-1	-1	0	0
1	0	-1	1	1	0	0
1	0	1	-1	1	0	0
1	0	1	1	-1	0	0

Block - XIII

A	B	C	D	E	F	G
-1	0	-1	0	0	0	-1
-1	0	1	0	0	0	-1
1	0	-1	0	0	0	-1
-1	0	-1	0	0	0	1
1	0	1	0	0	0	-1
-1	0	1	0	0	0	1
1	0	-1	0	0	0	1
1	0	1	0	0	0	1
0	-1	0	-1	-1	-1	0
0	-1	0	-1	1	1	0
0	-1	0	1	-1	1	0
0	-1	0	1	1	-1	0
0	1	0	-1	-1	1	0
0	1	0	-1	1	-1	0
0	1	0	1	-1	-1	0
0	1	0	1	1	1	0

Block-XIV

A	B	C	D	E	F	G
-1	0	-1	0	0	0	-1
-1	0	1	0	0	0	-1
1	0	-1	0	0	0	-1
-1	0	-1	0	0	0	1
1	0	1	0	0	0	-1
-1	0	1	0	0	0	1
1	0	-1	0	0	0	1
1	0	1	0	0	0	1
0	-1	0	-1	-1	1	0
0	-1	0	-1	1	-1	0
0	-1	0	1	-1	-1	0
0	-1	0	1	1	1	0
0	1	0	-1	-1	-1	0
0	1	0	-1	1	1	0
0	1	0	1	-1	1	0
0	1	0	1	1	-1	0

Block - XV

A	B	C	D	E	F	G
2	0	0	0	0	0	0
-2	0	0	0	0	0	0
0	2	0	0	0	0	0
0	-2	0	0	0	0	0
0	0	2	0	0	0	0
0	0	-2	0	0	0	0
0	0	0	2	0	0	0
0	0	0	-2	0	0	0
0	0	0	0	2	0	0
0	0	0	0	-2	0	0
0	0	0	0	0	2	0
0	0	0	0	0	-2	0
0	0	0	0	0	0	2
0	0	0	0	0	0	-2
0	0	0	0	0	0	0
0	0	0	0	0	0	0

8 factors each at 5 equispaced levels; (Block Size :17 (Obtained through BIB design 8,14,7,4,3)

Block - I

A	B	C	D	E	F	G	H
-1	-1	0	-1	0	0	0	-1
-1	-1	0	1	0	0	0	1
-1	1	0	-1	0	0	0	1
-1	1	0	1	0	0	0	-1
1	-1	0	-1	0	0	0	1
1	-1	0	1	0	0	0	-1
1	1	0	-1	0	0	0	-1
1	1	0	1	0	0	0	1
0	0	-1	0	-1	-1	-1	0
0	0	-1	0	-1	1	1	0
0	0	-1	0	1	-1	1	0
0	0	-1	0	1	1	-1	0
0	0	1	0	-1	-1	1	0
0	0	1	0	-1	1	-1	0
0	0	1	0	1	-1	-1	0
0	0	1	0	1	1	1	0
0	0	0	0	0	0	0	0

Block-II

A	B	C	D	E	F	G	H
-1	-1	0	-1	0	0	0	1
-1	-1	0	1	0	0	0	-1
-1	1	0	-1	0	0	0	-1
-1	1	0	1	0	0	0	1
1	-1	0	-1	0	0	0	-1
1	-1	0	1	0	0	0	1
1	1	0	-1	0	0	0	1
1	1	0	1	0	0	0	-1
0	0	-1	0	-1	-1	1	0
0	0	-1	0	-1	1	-1	0
0	0	-1	0	1	-1	-1	0
0	0	-1	0	1	1	1	0
0	0	1	0	-1	-1	-1	0
0	0	1	0	-1	1	1	0
0	0	1	0	1	-1	1	0
0	0	1	0	1	1	-1	0
0	0	0	0	0	0	0	0

Block - III

A	B	C	D	E	F	G	H
0	-1	-1	0	-1	0	0	-1
0	-1	-1	0	1	0	0	1
0	-1	1	0	-1	0	0	1
0	-1	1	0	1	0	0	-1
0	1	-1	0	-1	0	0	1
0	1	-1	0	1	0	0	-1
0	1	1	0	-1	0	0	-1
0	1	1	0	1	0	0	1
-1	0	0	-1	0	-1	-1	0
1	0	0	-1	0	-1	1	0
1	0	0	-1	0	1	-1	0
-1	0	0	-1	0	1	1	0
1	0	0	1	0	-1	-1	0
-1	0	0	1	0	-1	1	0
-1	0	0	1	0	1	-1	0
1	0	0	1	0	1	1	0
0	0	0	0	0	0	0	0

Block-IV

A	B	C	D	E	F	G	H
0	-1	-1	0	-1	0	0	1
0	-1	-1	0	1	0	0	-1
0	-1	1	0	-1	0	0	-1
0	-1	1	0	1	0	0	1
0	1	-1	0	-1	0	0	-1
0	1	-1	0	1	0	0	1
0	1	1	0	-1	0	0	1
0	1	1	0	1	0	0	-1
1	0	0	-1	0	-1	-1	0
-1	0	0	-1	0	-1	1	0
-1	0	0	-1	0	1	-1	0
1	0	0	-1	0	1	1	0
-1	0	0	1	0	-1	-1	0
1	0	0	1	0	-1	1	0
1	0	0	1	0	1	-1	0
-1	0	0	1	0	1	1	0
0	0	0	0	0	0	0	0

Block - V

A	B	C	D	E	F	G	H
0	0	-1	-1	0	-1	0	-1
0	0	-1	-1	0	1	0	1
0	0	-1	1	0	-1	0	1
0	0	-1	1	0	1	0	-1
0	0	1	-1	0	-1	0	1
0	0	1	-1	0	1	0	-1
0	0	1	1	0	-1	0	-1
0	0	1	1	0	1	0	1
-1	-1	0	0	-1	0	-1	0
1	1	0	0	-1	0	-1	0
-1	1	0	0	-1	0	1	0
1	-1	0	0	-1	0	1	0
-1	1	0	0	1	0	-1	0
1	-1	0	0	1	0	-1	0
-1	-1	0	0	1	0	1	0
1	1	0	0	1	0	1	0
0	0	0	0	0	0	0	0

Block-VI

A	B	C	D	E	F	G	H
0	0	-1	-1	0	-1	0	1
0	0	-1	-1	0	1	0	-1
0	0	-1	1	0	-1	0	-1
0	0	-1	1	0	1	0	1
0	0	1	-1	0	-1	0	-1
0	0	1	-1	0	1	0	1
0	0	1	1	0	-1	0	1
0	0	1	1	0	1	0	-1
-1	1	0	0	-1	0	-1	0
1	-1	0	0	-1	0	-1	0
-1	-1	0	0	-1	0	1	0
1	1	0	0	-1	0	1	0
-1	-1	0	0	1	0	-1	0
1	1	0	0	1	0	-1	0
-1	1	0	0	1	0	1	0
1	-1	0	0	1	0	1	0
0	0	0	0	0	0	0	0

Block - VII

A	B	C	D	E	F	G	H
0	0	0	-1	-1	0	-1	-1
0	0	0	-1	-1	0	1	1
0	0	0	-1	1	0	-1	1
0	0	0	-1	1	0	1	-1
0	0	0	1	-1	0	-1	1
0	0	0	1	-1	0	1	-1
0	0	0	1	1	0	-1	-1
0	0	0	1	1	0	1	1
-1	-1	-1	0	0	-1	0	0
-1	1	1	0	0	-1	0	0
1	-1	1	0	0	-1	0	0
1	1	-1	0	0	-1	0	0
-1	-1	1	0	0	1	0	0
-1	1	-1	0	0	1	0	0
1	-1	-1	0	0	1	0	0
1	1	1	0	0	1	0	0
0	0	0	0	0	0	0	0

Block-VIII

A	B	C	D	E	F	G	H
0	0	0	-1	-1	0	-1	1
0	0	0	-1	-1	0	1	-1
0	0	0	-1	1	0	-1	-1
0	0	0	-1	1	0	1	1
0	0	0	1	-1	0	-1	-1
0	0	0	1	-1	0	1	1
0	0	0	1	1	0	-1	1
0	0	0	1	1	0	1	-1
-1	-1	1	0	0	-1	0	0
-1	1	-1	0	0	-1	0	0
1	-1	-1	0	0	-1	0	0
1	1	1	0	0	-1	0	0
-1	-1	-1	0	0	1	0	0
-1	1	1	0	0	1	0	0
1	-1	1	0	0	1	0	0
1	1	-1	0	0	1	0	0
0	0	0	0	0	0	0	0

Block - IX

A	B	C	D	E	F	G	H
-1	0	0	0	-1	-1	0	-1
1	0	0	0	-1	-1	0	1
-1	0	0	0	-1	1	0	1
1	0	0	0	-1	1	0	-1
-1	0	0	0	1	-1	0	1
1	0	0	0	1	-1	0	-1
-1	0	0	0	1	1	0	-1
1	0	0	0	1	1	0	1
0	-1	-1	-1	0	0	-1	0
0	-1	1	1	0	0	-1	0
0	1	-1	1	0	0	-1	0
0	1	1	-1	0	0	-1	0
0	-1	-1	1	0	0	1	0
0	-1	1	-1	0	0	1	0
0	1	-1	-1	0	0	1	0
0	1	1	1	0	0	1	0
0	0	0	0	0	0	0	0

Block-X

A	B	C	D	E	F	G	H
-1	0	0	0	-1	-1	0	1
1	0	0	0	-1	-1	0	-1
-1	0	0	0	-1	1	0	-1
1	0	0	0	-1	1	0	1
-1	0	0	0	1	-1	0	-1
1	0	0	0	1	-1	0	1
-1	0	0	0	1	1	0	1
1	0	0	0	1	1	0	-1
0	-1	-1	1	0	0	-1	0
0	-1	1	-1	0	0	-1	0
0	1	-1	-1	0	0	-1	0
0	1	1	1	0	0	-1	0
0	-1	-1	-1	0	0	1	0
0	-1	1	1	0	0	1	0
0	1	-1	1	0	0	1	0
0	1	1	-1	0	0	1	0
0	0	0	0	0	0	0	0

Block - XI

A	B	C	D	E	F	G	H
0	-1	0	0	0	-1	-1	-1
0	1	0	0	0	-1	-1	1
0	-1	0	0	0	-1	1	1
0	1	0	0	0	-1	1	-1
0	-1	0	0	0	1	-1	1
0	1	0	0	0	1	-1	-1
0	-1	0	0	0	1	1	-1
0	1	0	0	0	1	1	1
-1	0	-1	-1	-1	0	0	0
-1	0	-1	1	1	0	0	0
-1	0	1	-1	1	0	0	0
-1	0	1	1	-1	0	0	0
1	0	-1	-1	1	0	0	0
1	0	-1	1	-1	0	0	0
1	0	1	-1	-1	0	0	0
1	0	1	1	1	0	0	0
0	0	0	0	0	0	0	0

Block-XII

A	B	C	D	E	F	G	H
0	-1	0	0	0	-1	-1	1
0	1	0	0	0	-1	-1	-1
0	-1	0	0	0	-1	1	-1
0	1	0	0	0	-1	1	1
0	-1	0	0	0	1	-1	-1
0	1	0	0	0	1	-1	1
0	-1	0	0	0	1	1	1
0	1	0	0	0	1	1	-1
-1	0	-1	-1	1	0	0	0
-1	0	-1	1	-1	0	0	0
-1	0	1	-1	-1	0	0	0
-1	0	1	1	1	0	0	0
1	0	-1	-1	-1	0	0	0
1	0	-1	1	1	0	0	0
1	0	1	-1	1	0	0	0
1	0	1	1	-1	0	0	0
0	0	0	0	0	0	0	0

Block - XIII

A	B	C	D	E	F	G	H
-1	0	-1	0	0	0	-1	-1
-1	0	1	0	0	0	-1	1
1	0	-1	0	0	0	-1	1
1	0	1	0	0	0	-1	-1
-1	0	-1	0	0	0	1	1
-1	0	1	0	0	0	1	-1
1	0	-1	0	0	0	1	-1
1	0	1	0	0	0	1	1
0	-1	0	-1	-1	-1	0	0
0	-1	0	-1	1	1	0	0
0	-1	0	1	-1	1	0	0
0	-1	0	1	1	-1	0	0
0	1	0	-1	-1	1	0	0
0	1	0	-1	1	-1	0	0
0	1	0	1	-1	-1	0	0
0	1	0	1	1	1	0	0
0	0	0	0	0	0	0	0

Block-XIV

A	B	C	D	E	F	G	H
-1	0	-1	0	0	0	-1	1
-1	0	1	0	0	0	-1	-1
1	0	-1	0	0	0	-1	-1
1	0	1	0	0	0	-1	1
-1	0	-1	0	0	0	1	-1
-1	0	1	0	0	0	1	1
1	0	-1	0	0	0	1	1
1	0	1	0	0	0	1	-1
0	-1	0	-1	-1	1	0	0
0	-1	0	-1	1	-1	0	0
0	-1	0	1	-1	-1	0	0
0	-1	0	1	1	1	0	0
0	1	0	-1	-1	-1	0	0
0	1	0	-1	1	1	0	0
0	1	0	1	-1	1	0	0
0	1	0	1	1	-1	0	0
0	0	0	0	0	0	0	0

Block - XV

A	B	C	D	E	F	G	H
2	0	0	0	0	0	0	0
-2	0	0	0	0	0	0	0
0	2	0	0	0	0	0	0
0	-2	0	0	0	0	0	0
0	0	2	0	0	0	0	0
0	0	-2	0	0	0	0	0
0	0	0	2	0	0	0	0
0	0	0	-2	0	0	0	0
0	0	0	0	2	0	0	0
0	0	0	0	-2	0	0	0
0	0	0	0	0	2	0	0
0	0	0	0	0	-2	0	0
0	0	0	0	0	0	2	0
0	0	0	0	0	0	-2	0
0	0	0	0	0	0	0	2
0	0	0	0	0	0	0	-2
0	0	0	0	0	0	0	0

CHAPTER IV

ROBUSTNESS AGAINST ONE MISSING OBSERVATION

4.1 Introduction

Classical designs were developed keeping in view the symmetry of designs and ease in calculations. With the advent of high-speed computers the emphasis was shifted to optimal/efficient designs relevant to purpose of experimentation. Mere ease in calculations is no longer a criterion for developing/selecting a design. Optimal design theory has been developed under very strict restrictions and ideal conditions. The ideal conditions may sometimes be disturbed on account of aberrations like outliers, missing data presence of systematic trend in the blocks of a block design, etc. Such disturbance(s) may render even an optimal design poor. In such situations, it is logical to look for designs that are insensitive or robust to such kind of disturbance(s). Box and Draper (1975) introduced the concept of robust designs in the presence of single outlier in response surface designs. This led to construction of designs that minimizes the effect of single outlier. Gopalan and Dey (1976) extended this study to designs where the design matrix is not of full rank.

Literature search on missing value estimation shows that missing observation can occur even in well-planned experiments. Lot of work has been done in the area of robust designs against missing observation(s). Herzberg and Andrews (1976) introduced two measures of the robustness of designs, namely, the probability of breakdown and the expected precision. Andrews and Herzberg (1979) showed that the expected precision might be easily calculated.

Ghosh (1979) introduced criterion of connectedness of designs, *i.e.*, a design is robust against missing observations if all the parameters are still estimable under an assumed model when a given number of observations are missing. Ghosh (1982) further observed that even in robust designs in the above sense, some observations are more informative than others and, consequently, if a more informative observation is lost accidentally, the overall loss in efficiency is larger than that in the case when a less informative observation is lost.

Srivastava, Gupta and Dey (1991) extended the above study to several types of designs. They studied the robustness of orthogonal resolution III designs and second-order rotatable designs obtained through central composite designs when single observation is missing.

Akhtar and Prescot (1986) investigated the ‘loss’ due to single missing observation in five factor central composite designs (CCD) with different configurations of half and complete replicate of factorial part, one or two replicate of axial part and some center points. The variances of parameter estimates were also studied. Minimax criterion was used to develop designs that are robust to a single missing observation. These designs were then compared with existing CCD of same configuration. In order to illustrate the damage missing observation(s) cause to the experiment, we take the following example:

Example 5.1: Consider the following design comprising of 4 factors (A, B, C, D) each at 5 levels (-2, -1, 0, 1, 2) in 25 design points

A	B	C	D
1	1	1	1
1	1	1	-1
1	1	-1	1
1	1	-1	-1
1	-1	1	1
1	-1	1	-1
1	-1	-1	1
1	-1	-1	-1
-1	1	1	1
-1	1	1	-1
-1	1	-1	1
-1	1	-1	-1
-1	-1	1	1
-1	-1	1	-1
-1	-1	-1	1
-1	-1	-1	-1
2	0	0	0
-2	0	0	0
0	2	0	0
0	-2	0	0
0	0	2	0
0	0	-2	0
0	0	0	2
0	0	0	-2
0	0	0	0

Here, $\det(\mathbf{X}'\mathbf{X})$ = 1.751E+19

There is only one central point and if by chance this is lost during experimentation then the observation from first 24 design points are available.

Now $\det(\mathbf{X}'\mathbf{X})=0$. This leads to the situation where Rank (**X)** is less than the number of columns leading to situation when some of the parameters cannot be estimated.

John (1979) has discussed the consequences of one or two missing points in 2^v factorial experiments and also some fractions of it. He showed that the increase in the variances of the estimates of some factorial effects due to missing plots can be as high as 50%. Response surface designs use factorial experiments as part of their design and are being increasingly used. A design that is found very useful, due to its versatility, is CCD in which one part consists of a factorial portion and the other parts correspond to some center points and axial points. It is, therefore, important to investigate the effect of one or two missing values in such a design. These days, missing values are not a problem to worry about due to the availability of electronic computers. If we have numerical data, the computer will be able to handle the analysis even if there are missing values, and will be able to give best estimates and their variances for response surface coefficients. On the other hand, the computer will not be able to provide general information about the extent of damage due to one or two missing values like increase in the variance of the predicted response, percentage loss in information, etc. Only algebraic treatment will be able to yield this information while computers will require extensive Monte Carlo trials to provide this information.

These considerations led McKee and Kshirsagar (1982) to investigate the consequences of missing plots in a central composite designs algebraically. Draper (1961) has done some such work for designs not arranged in blocks and when the linear model is of full rank. But results of McKee and Kshirsagar (1982) are more general. They are for designs arranged in blocks and for models not of full rank. Also the results are extended to equiradial designs.

In this study the above, robustness aspects of modified and/or rotatable second order response surface designs obtainable through central composite designs and BIB designs have been investigated with special emphasis on the designs when various factors are with equispaced doses. A new criterion of robustness viz. percent loss in information is introduced. Other criteria used in this investigation are information contained in an observation, D-efficiency and A-efficiency.

4.2 Robustness of Response Surface Designs against Single Missing Observation

Consider a general linear model for a response surface design, *d* (of any order)

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}_d + \mathbf{e} \tag{4.2.1}$$

where $\mathbf{y}$ is the $N \times 1$ observation vector, $\mathbf{X}$ is the $N \times p$ design matrix, $\boldsymbol{\beta}_d$ is the *p*-component vector of parameters, $\mathbf{e}$ is the $N \times 1$ vector of random errors assumed to be independently and identically distributed normally with mean *0* and variance σ^2. In the present context $\mathbf{X}$ has a full column rank *p* of design *d*. When all the observations $\mathbf{y}$ are available, the usual least square estimates of the normal equations are

$$\hat{\boldsymbol{\beta}}_d = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \tag{4.2.2}$$

and the variance covariance matrix of $\hat{\boldsymbol{\beta}}_d$ is

$$\mathrm{D}(\hat{\boldsymbol{\beta}}_d) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1} \tag{4.2.3}$$

Now consider that the observation pertaining to one of the design points is lost. Let the resulting design be denoted by d_1. Clearly, there will be N possible designs $\{d_1\}$. Without loss of generality, let us assume that $\mathbf{g}'$ represent the row in $\mathbf{X}$ corresponding to the missing observation. Then writing

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1' \\ \mathbf{g}' \end{bmatrix}.$$

We have
$$\mathbf{X}'_1 \mathbf{X}_1 = \mathbf{X}'\mathbf{X} - \mathbf{g}\mathbf{g}' \tag{4.2.4}$$

$$\Rightarrow \det\left(\mathbf{X}_1'\mathbf{X}_1\right) = \det\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{g} \\ \mathbf{g}' & \mathbf{I} \end{bmatrix}$$

$$\Rightarrow \det(\mathbf{X}'_1 \mathbf{X}_1) = \{1 - \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}\}\det(\mathbf{X}'\mathbf{X}) \tag{4.2.5}$$

We know that determinant of $\mathbf{A}^{-1}$ is reciprocal of the determinant of $\mathbf{A}$. Therefore,

$$\det[D(\hat{\boldsymbol{\beta}}_{d_1})] = \{1 - \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}\}^{-1}\det[D(\hat{\boldsymbol{\beta}}_d)] \tag{4.2.6}$$

If $\hat{\boldsymbol{\beta}}_d\,[\hat{\boldsymbol{\beta}}_{d_1}]$ denotes the best linear unbiased estimator of $\boldsymbol{\beta}$ using $d[d_1]$, then

$$D(\hat{\boldsymbol{\beta}}_{d_1}) = \sigma^2(\mathbf{X}_1'\mathbf{X}_1)^{-1}$$

$$\Rightarrow \frac{1}{\sigma^2}D(\hat{\boldsymbol{\beta}}_{d_1}) = (\mathbf{X}_1'\mathbf{X}_1)^{-1}$$

where
$$(\mathbf{X}_1'\mathbf{X}_1)^{-1} = (\mathbf{X}'\mathbf{X})^{-1} + \frac{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}'\mathbf{g}(\mathbf{X}'\mathbf{X})^{-1}}{1 - \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}}.$$

This has been obtained by making use of the following Lemma:

Lemma 4.2.1: Let $\mathbf{A}$ be a non-singular matrix and $\mathbf{U}$ and $\mathbf{V}$ be two column vectors then

$$\left(\mathbf{A} + \mathbf{U}\mathbf{V}\right)^{-1} = \mathbf{A}^{-1} - \frac{\left(\mathbf{A}^{-1}\mathbf{U}\right)\left(\mathbf{V}'\mathbf{A}^{-1}\right)}{1 + \mathbf{V}'\mathbf{A}^{-1}\mathbf{U}} \tag{4.2.7}$$

Now using (4.2.7) and taking $-\mathbf{g} = \mathbf{U}$ and $\mathbf{g}' = \mathbf{V}'$ we get the expression for $(\mathbf{X}_1'\mathbf{X}_1)^{-1}$.

The increase in the variance of BLUE of an estimable function of $\mathbf{x}'\hat{\boldsymbol{\beta}}_d$ (predicted response at point $\mathbf{x}$) due to the single missing observation pertaining to the point $\mathbf{g}$ is

$$\frac{\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}'\mathbf{g}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}}{1 - \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}}$$

The ratio of increase in variance of the predicted response at the point $\mathbf{x}$ when the missing point is $\mathbf{g}$ to that of the original variance at point $\mathbf{x}$ can be obtained and used as an indicator of robustness.

The amount of information contained in the unavailable observation in *d* is, therefore,

$$I(\mathbf{g}) = \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g} \tag{4.2.8}$$

It is easy to see that

$$\sum_{g} I(\mathbf{g}) = \text{trace}[\mathbf{X}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}] = p \tag{4.2.9}$$

It should be noted that for a robust design d, $0 < I(\mathbf{g}) < 1$. Clearly a good design should have a small $I(\mathbf{g})$ for all $\mathbf{g}$ so that the loss of an observation does not result in a large loss in efficiency of the resulting design. This result is due to Ghosh (1982). The value contained in an observation is small or large is a subjective decision. Therefore, we introduce another criterion *viz.* percent loss in information due to one missing observation given by

$$\text{Loss (\%)} = \frac{I(\mathbf{g})}{\text{p}} \times 100 \tag{4.2.10}$$

Using the expression of $(\mathbf{X}_1'\mathbf{X}_1)^{-1}$, we can obtain the trace of $(\mathbf{X}_1'\mathbf{X}_1)^{-1}$ as

$$\therefore \text{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1} = \text{trace}(\mathbf{X}'\mathbf{X})^{-1} + \frac{\text{trace}\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}'\mathbf{g}(\mathbf{X}'\mathbf{X})^{-1}\right]}{1 - \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}}$$

$$= \text{trace}(\mathbf{X}'\mathbf{X})^{-1} + \frac{\text{trace}\left[\mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}\right]}{1 - \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}}$$

$$[\because \text{trace}(\mathbf{AB}) = \text{trace}(\mathbf{BA})]$$

$$\text{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1} = \text{trace}(\mathbf{X}'\mathbf{X})^{-1} + \frac{\text{trace}\left[\mathbf{g}'\left((\mathbf{X}'\mathbf{X})^{-1}\right)^2\mathbf{g}\right]}{1 - \mathbf{g}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}} \tag{4.2.11}$$

Knowing the above, A- and D- efficiencies of the resulting design with respect to the original design are given by

$$\text{A-efficiency} = \frac{\text{trace}(\mathbf{X}'\mathbf{X})^{-1}}{\text{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}} \tag{4.2.12}$$

$$\text{D-efficiency} = \frac{[\det(\mathbf{X}_1'\mathbf{X}_1)]^{1/p}}{[\det(\mathbf{X}'\mathbf{X})]^{1/p}} \tag{4.2.13}$$

4.3 Robustness of Modified and/ or Rotatable Second Order Response Surface Designs

Using the results given in Section 3.2 of Chapter III, we know that for a second order response surface designs satisfying the conditions of symmetry (3.3.1)

$$\det(\mathbf{X}'\mathbf{X}) = R^v L^{v(v-1)/2}[(C-1)L]^{v-1} D \tag{4.3.1}$$

$$\begin{aligned}\text{trace}[(\mathbf{X}'\mathbf{X})^{-1}] &= \frac{(C+v-1)L}{D} + \frac{v}{R} + \frac{v}{(C-1)L}\left[1 + \frac{(R^2 - NL)}{D}\right] + \frac{v(v-1)}{2L} \\ &= T_X \text{ (say)}\end{aligned} \tag{4.3.2}$$

$$\sum_g I(\mathbf{g}) = \text{trace}[\mathbf{X}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}] = p = \frac{(v+1)(v+2)}{2} \tag{4.3.3}$$

where $D = NL(v+2) - vR^2$.

Now using (4.2.5) and (4.2.11), det $(\mathbf{X}_1'\mathbf{X}_1)$ and trace$(\mathbf{X}_1'\mathbf{X}_1)^{-1}$ can be obtained. Using (4.2.9), (4.2.12) and (4.2.13), the percentage loss in information, A-efficiency and D-efficiency can be obtained. In the context of response surface designs the percentage loss in information and D-efficiency should be preferred over A-efficiency. In the present investigation, we have made an attempt to obtain expressions for the percentage loss in information, A-efficiency and D-efficiency for the designs obtained from central composite designs and BIB designs.

4.3.1 Central Composite Designs

For Central Composite designs $\mathbf{g}$ can be of the following types

Factorial Point: $\mathbf{g}_1' = \begin{pmatrix} 1 & \alpha\mathbf{1}_v' & \alpha^2\mathbf{1}_v' & \alpha^2\mathbf{1}'_{\frac{v(v-1)}{2}} \end{pmatrix}$

Axial Point: $\mathbf{g}_2' = \begin{pmatrix} 1 & \beta\, 0...0 & \beta^2\, 0...0 & 0...0 \end{pmatrix}$

Center Point: $\mathbf{g}_3' = \begin{pmatrix} 1 & \mathbf{0}_v' & \mathbf{0}_v' & \mathbf{0}'_{\frac{v(v-1)}{2}} \end{pmatrix}$

For Factorial Point: $\mathbf{g}_1'$

$$\mathbf{g}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_1 = \begin{pmatrix} 1 & \alpha\mathbf{1}_v' & \alpha^2\mathbf{1}_v' & \alpha^2\mathbf{1}'_{\frac{v(v-1)}{2}} \end{pmatrix}\begin{pmatrix} A_1 \\ \frac{\alpha}{R}\mathbf{1} \\ B_1\mathbf{1} \\ \frac{\alpha^2}{L}\mathbf{1} \end{pmatrix}$$

$$= A_1 + \frac{v\alpha^2}{R} + v\alpha^2 B_1 + \frac{v(v-1)}{2L}\alpha^4$$

$$\Rightarrow \mathbf{g}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_1 = T_{g_{c1}} \text{(say)} \tag{4.3.4}$$

where $A_1 = \frac{(C+v-1)L - v\alpha^2 R}{D}$ and $B_1 = \frac{-R}{D} + \frac{\alpha^2}{(C-1)L}\left[1 - v\frac{(NL-R^2)}{D}\right]$.

Now det ($\mathbf{X}_1'\mathbf{X}_1$) =(1- $T_{g_{c1}}$) det$(\mathbf{X}'\mathbf{X})$ (4.3.5)

Therefore, $\left(\mathbf{X}_1'\mathbf{X}_1\right)^{-1} = (\mathbf{X}'\mathbf{X})^{-1} + \frac{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_1\mathbf{g}_1'(\mathbf{X}'\mathbf{X})^{-1}}{1-T_{g_{c1}}} = \begin{bmatrix} \mathbf{P}_1 & \mathbf{Q}_1 \\ \mathbf{Q}_1' & \mathbf{R}_1 \end{bmatrix}$

Where $\mathbf{P}_1 = \begin{bmatrix} \frac{(C+v-1)L}{D} + \frac{A_1^2}{(1-T_{g_{c1}})} & \frac{\alpha}{R}\frac{A_1}{(1-T_{g_{c1}})}\mathbf{1}' \\ \frac{\alpha}{R}\frac{A_1}{(1-T_{g_{c1}})}\mathbf{1} & \frac{1}{R}\mathbf{I} + \frac{\alpha^2}{R^2(1-T_{g_{c1}})}\mathbf{11}' \end{bmatrix}$,

$$\mathbf{Q}_1 = \begin{bmatrix} \left(\frac{-R}{D} + \frac{A_1B_1}{(1-T_{g_{c1}})}\right)\mathbf{1}' & \frac{\alpha^2 A_1}{L(1-T_{g_{c1}})}\mathbf{1}' \\ \frac{\alpha B_1}{R(1-T_{g_{c1}})}\mathbf{11}' & \frac{\alpha^3}{RL(1-T_{g_{c1}})}\mathbf{11}' \end{bmatrix},$$

$$\mathbf{R}_1 = \begin{bmatrix} \frac{1}{(C-1)L}\left[\mathbf{I} - \frac{(NL-R^2)}{D}\mathbf{11}'\right] + \frac{B_1^2}{(1-T_{g_{c1}})}\mathbf{11}' & \frac{\alpha^2 B_1}{L(1-T_{g_{c1}})}\mathbf{11}' \\ \frac{\alpha^2 B_1}{L(1-T_{g_{c1}})}\mathbf{11}' & \frac{1}{L}\mathbf{I} + \frac{\alpha^2}{L(1-T_{g_{c1}})}\mathbf{11}' \end{bmatrix}$$

Using (4.2.11), we have,

$$\operatorname{trace}\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_1'\mathbf{g}_1(\mathbf{X}'\mathbf{X})^{-1}\right] = A_1^2 + \frac{v\alpha^2}{R^2} + vB_1^2 + \frac{v(v-1)}{2}\frac{\alpha^4}{L^2} = T_{1c} \text{ (say)}$$

$$\therefore\ T_{Xc_1} = T_X + \frac{T_{1c}}{1-T_{gc1}} \tag{4.3.6}$$

For Axial Point: $\mathbf{g}_2'$

$$\mathbf{g}_2'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_2 = A_2 + \frac{\beta^2}{R} + \beta^2 B_2 = T_{g_{c2}} \text{ (say)} \tag{4.3.7}$$

where $A_2 = \dfrac{(C+v-1)L - R\beta^2}{D}$, $\quad B_2 = \dfrac{-R}{D} + \dfrac{\beta^2}{(C-1)L}\left[1 - \dfrac{(NL-R^2)}{D}\right]$

Now det ($\mathbf{X}_1'\mathbf{X}_1$) =(1- T_{gc_2}) det$(\mathbf{X}'\mathbf{X})$ (4.3.8)

Therefore, $\left(\mathbf{X}_1'\mathbf{X}_1\right)^{-1} = (\mathbf{X}'\mathbf{X})^{-1} + \dfrac{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_2\mathbf{g}_2'(\mathbf{X}'\mathbf{X})^{-1}}{1-T_{g_{c2}}} = \begin{bmatrix} \mathbf{P}_2 & \mathbf{Q}_2 \\ \mathbf{Q}_2' & \mathbf{R}_2 \end{bmatrix}$

where $\mathbf{P}_2 = \begin{bmatrix} A + A_2^2 h & \dfrac{A\beta}{R}h & \mathbf{0}_{v-1}' \\ \dfrac{A\beta}{R}h & \dfrac{1}{R} + \dfrac{\beta^2}{R^2}h & \mathbf{0}_{v-1}' \\ \mathbf{0}_{v\text{-}1} & \mathbf{0}_{v\text{-}1} & \dfrac{1}{R}\mathbf{I} \end{bmatrix}$,

$$\mathbf{Q}_2 = \begin{bmatrix} \left(\dfrac{-R}{D} + A_2B_2h\right) & \left(\dfrac{-R}{D} + A_2C_2h\right)\mathbf{1}_{v-1}' & \mathbf{0} \\ \dfrac{\beta B_2}{R}h & \dfrac{\beta C_2}{R}h\mathbf{1}_{v-1}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix},$$

$$\mathbf{R}_2 = \begin{bmatrix} e + f + B_2^2 h & (f + B_2C_2h)\mathbf{1}_{v-1}' & \mathbf{0} \\ (f + B_2C_2h)\mathbf{1}_{v-1} & (e\mathbf{I} + f\mathbf{11}' + C_2^2\mathbf{11}') & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \dfrac{1}{L}\mathbf{I} \end{bmatrix}$$

where $C_2 = \dfrac{-R}{D} + \dfrac{\beta^2}{(C-1)L}\left[\dfrac{-(NL-R^2)}{D}\right]$, $\quad A = \dfrac{(C+v-1)L}{D}$

$$e = \frac{1}{(C-1)L},\quad f = \frac{1}{(C-1)L}\left[\frac{-(NL-R^2)}{D}\right] \text{ and } \quad h = \frac{1}{(1-T_{g_{c2}})}$$

Using (4.2.11) we have,

$$\text{trace}\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_2'\mathbf{g}_2(\mathbf{X}'\mathbf{X})^{-1}\right] = A_2^2 + \frac{\beta^2}{R^2} + B_2^2 + (v-1)C_2^2 = T_{2c} \text{ (say)}$$

$$\therefore \quad T_{Xc_2} = T_X + \frac{T_{2c}}{1 - T_{gc2}} \tag{4.3.9}$$

For center point: $\mathbf{g}_3'$

$$\mathbf{g}_3'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_3 = A = T_{g_{c3}} \text{ (say)} \tag{4.3.10}$$

Now det ($\mathbf{X}_1'\mathbf{X}_1$) =(1- $T_{g_{c3}}$) det($\mathbf{X}'\mathbf{X}$) (4.3.11)

$$\left(\mathbf{X}_1'\mathbf{X}_1\right)^{-1} = (\mathbf{X}'\mathbf{X})^{-1} + \frac{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_3\mathbf{g}_3'(\mathbf{X}'\mathbf{X})^{-1}}{1 - T_{g_{c3}}}$$

Therefore

$$= \begin{bmatrix} A + \dfrac{A^2}{1-A} & \mathbf{0}' & \left(\dfrac{-R}{D} - \dfrac{RA}{D(1-A)}\right)\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & \dfrac{1}{R}\mathbf{I} & \mathbf{0} & \mathbf{0} \\ \left(\dfrac{-R}{D} - \dfrac{RA}{D(1-A)}\right)\mathbf{1} & \mathbf{0} & a\mathbf{I} + \left(b + \dfrac{R^2}{D^2(1-A)}\right)\mathbf{1}\mathbf{1}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dfrac{1}{L}\mathbf{I} \end{bmatrix}$$

Using (4.2.11), we have

$$\text{trace}\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_3'\mathbf{g}_3(\mathbf{X}'\mathbf{X})^{-1}\right] = A^2 + \frac{vR^2}{D^2} = T_{3c} \text{ (say)}$$

$$\therefore \quad T_{Xc_3} = T_X + \frac{T_{3c}}{1 - T_{gc3}} \tag{4.3.12}$$

The expressions for the information contained in observation given in (4.3.4), (4.3.7) and (4.3.10) can further be simplified as

$$I(\mathbf{g}_1) = \frac{(C+v-1)L - 2vR\alpha^2}{D} + \frac{v\alpha^2}{R} + \frac{v\alpha^4}{(C-1)L} - \frac{v^2(NL-R^2)\alpha^4}{(C-1)LD} + \frac{v(v-1)\alpha^4}{2L} \quad (4.3.13)$$

$$I(\mathbf{g}_2) = \frac{(C+v-1)L - 2R\beta^2}{D} + \frac{\beta^2}{R} + \frac{\beta^4}{(C-1)L} - \frac{(NL-R^2)\beta^4}{(C-1)LD} \quad (4.3.14)$$

$$I(\mathbf{g}_3) = \frac{(C+v-1)L}{D} \quad (4.3.15)$$

For a second order rotatable design, by substituting $C=3$ in (4.3.13), (4.3.14) and (4.3.15), we get

$$I(\mathbf{g}_1) = \frac{(v+2)L - 2vR\alpha^2}{D} + \frac{v\alpha^2}{R} + \frac{v^2\alpha^4}{2L} - \frac{v^2(NL-R^2)\alpha^4}{2LD} \quad (4.3.16)$$

$$I(\mathbf{g}_2) = \frac{(v+2)L - 2R\beta^2}{D} + \frac{\beta^2}{R} + \frac{\beta^4}{2L} - \frac{(NL-R^2)\beta^4}{2LD} \quad (4.3.17)$$

$$I(\mathbf{g}_3) = \frac{(v+2)L}{D} \quad (4.3.18)$$

For a modified and rotatable second order response surface design, substitute $R^2 = NL$ in (4.3.16), (4.3.17) and (4.3.18).

$$I(\mathbf{g}_1) = \frac{(v+2)L - 2vR\alpha^2}{2NL} + \frac{v\alpha^2}{R} + \frac{v^2\alpha^4}{2L} \quad (4.3.19)$$

$$I(\mathbf{g}_2) = \frac{(v+2)L - 2R\beta^2}{2NL} + \frac{\beta^2}{R} + \frac{\beta^4}{2L} \quad (4.3.20)$$

$$I(\mathbf{g}_3) = \frac{(v+2)}{2N} \quad (4.3.21)$$

For a modified second order response surface design alone, substituting $R^2 = NL$ in (4.3.13), (4.3.14) and (4.3.15), we get

$$I(\mathbf{g}_1) = \frac{(C+v-1)L - 2vR\alpha^2}{(C-1)NL} + \frac{v\alpha^2}{R} + \frac{v\alpha^4}{(C-1)L} + \frac{v(v-1)\alpha^4}{2L} \quad (4.3.22)$$

$$I(\mathbf{g}_2) = \frac{(C+v-1)L - 2R\beta^2}{(C-1)NL} + \frac{\beta^2}{R} + \frac{\beta^4}{(C-1)L} \quad (4.3.23)$$

$$I(\mathbf{g}_3) = \frac{(C+v-1)}{(C-1)N} \quad (4.3.24)$$

Now substituting $\alpha = 1$ and $\beta = 2$, in the expressions (4.3.13) to (4.3.24), we can get the corresponding expressions for central composite designs for symmetrical factorials when the factors are with equispaced doses. The corresponding expressions are given as

For any central composite design

$$I(\mathbf{g}_1) = \frac{(C+v-1)L - 2vR}{D} + \frac{v}{R} + \frac{v}{(C-1)L} - \frac{v^2(NL - R^2)}{(C-1)LD} + \frac{v(v-1)}{2L} \tag{4.3.25}$$

$$I(\mathbf{g}_2) = \frac{(C+v-1)L - 8R}{D} + \frac{4}{R} + \frac{16}{(C-1)L} - \frac{16(NL - R^2)}{(C-1)LD} \tag{4.3.26}$$

$$I(\mathbf{g}_3) = \frac{(C+v-1)L}{D} \tag{4.3.27}$$

For a second order rotatable response surface design obtained from CCD

$$I(\mathbf{g}_1) = \frac{(v+2)L - 2vR}{D} + \frac{v}{R} + \frac{v^2}{2L} - \frac{v^2(NL - R^2)}{2LD} \tag{4.3.28}$$

$$I(\mathbf{g}_2) = \frac{(v+2)L - 8R}{D} + \frac{4}{R} + \frac{8}{L} - \frac{8(NL - R^2)}{LD} \tag{4.3.29}$$

$$I(\mathbf{g}_3) = \frac{(v+2)L}{D} \tag{4.3.30}$$

For a modified and rotatable second order response surface design

$$I(\mathbf{g}_1) = \frac{(v+2)L - 2vR}{2NL} + \frac{v}{R} + \frac{v^2}{2L} \tag{4.3.31}$$

$$I(\mathbf{g}_2) = \frac{(v+2)L - 8R}{2NL} + \frac{4}{R} + \frac{8}{L} \tag{4.3.32}$$

$$I(\mathbf{g}_3) = \frac{(v+2)}{2N} \tag{4.3.33}$$

For a modified second order response surface design

$$I(\mathbf{g}_1) = \frac{(C+v-1)L - 2vR}{(C-1)NL} + \frac{v}{R} + \frac{v}{(C-1)L} + \frac{v(v-1)}{2L} \tag{4.3.34}$$

$$I(\mathbf{g}_2) = \frac{(C+v-1)L - 8R}{(C-1)NL} + \frac{4}{R} + \frac{16}{(C-1)L} \tag{4.3.35}$$

$$I(\mathbf{g}_3) = \frac{(C+v-1)}{(C-1)N} \tag{4.3.36}$$

Using these expressions, the corresponding expressions of $\det(\mathbf{X}_1'\mathbf{X}_1)$ can directly be obtained from (4.3.5), (4.3.8) and (4.3.11). The $\text{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}$ can also easily be obtained by making the appropriate substitutions in (4.3.6), (4.3.9) and (4.3.12).

The information contained in an observation, percent loss in information and D-efficiencies of the modified and rotatable second order response surface designs obtainable from central composite designs and catalogued in Table 3.3.2 are computed and are presented in Table 4.3.1. Similar computations can easily be made for modified or rotatable designs obtainable from central composite designs.

Table 4.3.1: The information contained in an observation, percent loss in information and D-efficiencies of the modified and rotatable second order response surface designs given in Table 3.3.2.

v	p	s	t	n_0	N	Factorial Point			Axial Point			Center Point		
						$I(\mathbf{g})$	Loss %	D-eff	$I(\mathbf{g})$	Loss %	D-eff	$I(\mathbf{g})$	Loss %	D-eff
3	3	2	1	14	36	0.351	3.507	0.958	0.569	5.694	0.919	0.069	0.694	0.993
4	4	1	1	12	36	0.583	3.889	0.943	0.583	3.889	0.943	0.083	0.556	0.994
5	4	1	1	10	36	0.878	4.183	0.905	0.597	2.844	0.958	0.097	0.463	0.995
5	5	1	2	20	72	0.439	2.092	0.973	0.299	1.422	0.983	0.049	0.231	0.998
6	5	1	2	16	72	0.618	2.207	0.966	0.306	1.091	0.987	0.056	0.198	0.998
6	6	1	4	32	144	0.309	1.104	0.987	0.153	0.546	0.994	0.028	0.099	0.999
7	6	1	4	24	144	0.414	1.150	0.985	0.156	0.434	0.995	0.031	0.087	0.999
7	7	1	8	48	288	0.207	0.575	0.994	0.078	0.217	0.998	0.016	0.043	1.000*
8	6	1	4	16	144	0.535	1.188	0.983	0.160	0.355	0.996	0.035	0.077	0.999
8	7	1	8	32	288	0.267	0.594	0.993	0.080	0.177	0.998	0.017	0.039	1.000*
9	7	1	8	16	288	0.336	0.610	0.993	0.082	0.148	0.998	0.019	0.035	1.000*

*denotes that the D-efficiency is greater than 0.9995.

From the Table 4.3.1, it is observed that the percent loss in information is marginal and D-efficiencies are reasonably high. Therefore, we can say that these designs are robust against unavailability of a single observation.

4.3.2 Designs Obtainable from BIB Designs

For the second order response surface designs obtainable from BIB design, the design points $\mathbf{g}$ can be of the following type

Incidence Matrix point:

$$\mathbf{g}_1' = (1 \quad \alpha\ 0\ \alpha\ 0\ldots0\alpha \quad \alpha^2\ 0\ \alpha^2\ 0\ldots0\ \alpha^2 \quad \alpha^2\ 0\ \alpha^2\ 0\ldots0\alpha^2)$$

Axial Point: $\mathbf{g}_2' = (1 \quad \beta\ 0\cdots0 \quad \beta^2\ 0\ldots0 \quad 0\ 0\ldots0)$

Factorial Point: $\mathbf{g}_3' = (1 \quad \beta...\beta \quad \beta^2...\beta^2 \quad \beta^2...\beta^2\ )$

Center Point: $\mathbf{g}_4' = (1 \quad 0\cdots0 \quad 0\ldots0 \quad 0\ldots0)$.

If $r = 3\lambda$, then points will be of the type $\mathbf{g}_1$ and $\mathbf{g}_4$. When $r < 3\lambda$, the points will be of the type $\mathbf{g}_1$, $\mathbf{g}_2$ and $\mathbf{g}_4$. When $r > 3\lambda$, the points will be of the type $\mathbf{g}_1$, $\mathbf{g}_3$ and $\mathbf{g}_4$.

Now for the point generated from incidence matrix $\mathbf{g}_1' = (1 \quad \alpha\ 0\ \alpha\ 0 \ldots 0 \alpha \quad \alpha^2\ 0\ \alpha^2\ 0 \ldots 0\ \alpha^2 \quad \alpha^2\ 0\ \alpha^2\ 0 \ldots 0 \alpha^2)$, without loss of generality we assume that first k elements are α and the remaining $v-k$ points are 0. Therefore, $\mathbf{g}_1$ can be rewritten as

$$\mathbf{g}_1' = \left(1 \quad \alpha \mathbf{1}_k' \ \ \mathbf{0}_{v-k}' \ \ \alpha^2 \mathbf{1}_k' \ \ \mathbf{0}_{v-k}' \ \ \alpha^2 \mathbf{1}_{k(k-1)/2}' \ \ \mathbf{0}'_{\left(\frac{v(v-1)}{2} - \frac{k(k-1)}{2}\right)}\right)$$

Now taking

$$A = \frac{(C+v-1)L}{D}, \qquad e = \frac{1}{(C-1)L}, \qquad f = \frac{-(NL-R^2)}{D(C-1)L}$$

$$U_1 = A - \frac{k\alpha^2 R}{D}, \qquad V_1 = \frac{-R}{D} + \alpha^2 (e + kf), \qquad W_1 = \frac{-R}{D} + \alpha^2 (v-k) f$$

we have

$$\mathbf{g}_1' (\mathbf{X}'\mathbf{X})^{-1} \mathbf{g}_1 = U_1 - \frac{k\alpha^2 R}{D} + \frac{k\alpha^2}{R} + k\alpha^4 e + fk^2 \alpha^4 + \frac{k(k-1)\alpha^4}{2L} = T_{g_{b1}} \text{ (say)} \quad (4.3.37)$$

Using (4.2.5), $\det(\mathbf{X}_1'\mathbf{X}_1) = (1 - T_{gb_1}) \det(\mathbf{X}''\mathbf{X})$ (4.3.38)

Therefore, $\left(\mathbf{X}_1'\mathbf{X}_1\right)^{-1} = \begin{bmatrix} \mathbf{P}_3 & \mathbf{Q}_3 \\ \mathbf{Q}_3' & \mathbf{R}_3 \end{bmatrix}$

$$\mathbf{P}_3 = \begin{bmatrix} A + U_1^2 h_1 & \frac{U_1 \alpha h_1}{R} \mathbf{1}' & \mathbf{0}' \\ \frac{U_1 \alpha h_1}{R} \mathbf{1} & \frac{1}{R}\mathbf{I} + \frac{\alpha^2 h_1}{R^2} \mathbf{11}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{1}{R}\mathbf{I} \end{bmatrix},$$

$$\mathbf{Q}_3 = \begin{bmatrix} \left(U_1 V_1 h_1 - \frac{R}{D}\right)\mathbf{1}' & \left(U_1 W_1 h_1 - \frac{R}{D}\right)\mathbf{1}' & \frac{\alpha^2 U_1 h_1}{L}\mathbf{1}' & \mathbf{0}' \\ \frac{\alpha h_1}{R} V_1 \mathbf{11}' & \frac{\alpha h_1}{R} W_1 \mathbf{11}' & \frac{\alpha^3 h_1}{RL}\mathbf{11}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}$$

Here $h_1 = \dfrac{1}{1-T_{gb_1}}$. Using (4.2.11), we have,

$$\text{trace}\left[(\mathbf{X}'\,\mathbf{X})^{-1}\mathbf{g}_1'\mathbf{g}_1(\mathbf{X}'\,\mathbf{X})^{-1}\right] = U_1^2 + \frac{k\alpha^2}{R^2} + kV_1^2 + (v-k)W_1^2 + \frac{k(k-1)\alpha^4}{2L^2} = T_{1b}$$

$$\therefore \quad T_{Xb1} = T_X + \frac{T_{1b}}{1-T_{gb1}} \tag{4.3.40}$$

For axial point: $\mathbf{g}_2' = (1 \quad \beta \;\, 0\cdots0 \quad \beta^2 \;\, 0\ldots0 \quad 0\;0\ldots0)$. $\mathbf{g}_2'$ can be rewritten as $\mathbf{g}_2' = (1 \quad \beta \;\, \mathbf{0}_{v-1}' \quad \beta^2 \;\, \mathbf{0}' \quad \mathbf{0}_{v(v-1)/2})$

Now taking, $U_2 = A - \dfrac{R\beta^2}{D}$, $\quad V_2 = \dfrac{-R}{D} + \beta^2(e+f)$, $\quad W_2 = \dfrac{-R}{D} + \beta^2 f$

we have $\quad \mathbf{g}_2'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_2 = U_2 + \dfrac{\beta^2}{R} + \beta^2 V_2 = T_{g_{b2}}$ (say) $\quad$ (4.3.41)

Using (4.2.5), $\det(\mathbf{X}_1'\mathbf{X}_1) = (1-T_{gb_2})\det(\mathbf{X}''\mathbf{X})$ $\quad$ (4.3.42)

Therefore

$$\left(\mathbf{X}_1'\mathbf{X}_1\right)^{-1} = \begin{bmatrix} A+U_2^2h_2 & \mathbf{0}' & \dfrac{-R}{D}+U_2V_2h_2 & \left(\dfrac{-R}{D}+U_2W_2h_2\right)\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & \dfrac{1}{R}\mathbf{I} & \mathbf{0} & & \mathbf{0} \\ \begin{matrix} \dfrac{-R}{D}+U_2V_2h_2 \\ \left(\dfrac{-R}{D}+U_2W_2h_2\right)\mathbf{1} \end{matrix} & \mathbf{0} & \begin{matrix} e+f+V_2^2h_2 \\ (f+V_2W_2h_2)\mathbf{1} \end{matrix} & \begin{matrix} (f+V_2W_2h_2)\mathbf{1}' \\ e\mathbf{I}+f\mathbf{1}\mathbf{1}'+W_2^2h_2\mathbf{1}\mathbf{1}' \end{matrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & & \dfrac{1}{L}\mathbf{I} \end{bmatrix}$$

where $\quad h_2 = \dfrac{1}{1-T_{gb_2}}$

Using (4.2.11), we have,

$$\text{trace}\left[(\mathbf{X}'\,\mathbf{X})^{-1}\mathbf{g}_2'\mathbf{g}_2(\mathbf{X}'\,\mathbf{X})^{-1}\right] = U_2^2 + \frac{\beta^2}{R^2} + V_2^2 + (v-1)W_2^2 = T_{2b}$$

$$\therefore\; T_{Xb2} = T_X + \frac{T_{2b}}{1-T_{gb2}} \tag{4.3.43}$$

For factorial point: $\mathbf{g}_3' = (1 \quad \beta\ldots\beta \quad \beta^2\ldots\beta^2 \quad \beta^2\ldots\beta^2\,)$. $\mathbf{g}_3'$ can further be rewritten as $\mathbf{g}_3' = \left(1 \quad \beta\mathbf{1}_v' \quad \beta^2\mathbf{1}_v' \quad \beta^2\,\mathbf{1}_{v(v-1)/2}'\right)$.

Now taking $U_3 = A - \dfrac{vR\beta^2}{D}$, $\quad V_3 = \dfrac{-R}{D} + (e+vf)\beta^2$, we have

$$\mathbf{g}_3'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_3 = U_3 + \frac{v\beta^2}{R} + v\beta^2 V_3 + \frac{v(v-1)}{2L}\beta^4 = T_{g_{b3}} \text{ (say)} \tag{4.3.44}$$

Using (4.2.5), $\det(\mathbf{X}_1'\mathbf{X}_1) = (1-T_{gb_3})\det(\mathbf{X}''\mathbf{X})$ (4.3.45)

Therefore

$$\left(\mathbf{X}_1^{'}\mathbf{X}_1\right)^{-1} = \begin{bmatrix} A+U_3^2h_3 & \dfrac{\beta h_3U_3}{R}\mathbf{1}' & \left(\dfrac{-R}{D}+U_3V_3h_3\right)\mathbf{1}' & \dfrac{\beta^2h_3U_3}{R}\mathbf{1}' \\ \dfrac{\beta h_3U_3}{R}\mathbf{1} & \dfrac{1}{R}\mathbf{I}+\dfrac{\beta^2h_3}{R}\mathbf{11}' & \dfrac{\beta h_3V_3}{R}\mathbf{11}' & \dfrac{\beta^3h_3}{RL}\mathbf{11}' \\ \left(\dfrac{-R}{D}+U_3V_3h_3\right)\mathbf{1} & \dfrac{\beta h_3V_3}{R}\mathbf{11}' & e\mathbf{I}+\left(f+V_3^2h_3\right)\mathbf{11}' & \dfrac{\beta^2V_3h_3}{L}\mathbf{11}' \\ \dfrac{\beta^2h_3U_3}{R}\mathbf{1} & \dfrac{\beta^3h_3}{RL}\mathbf{11}' & \dfrac{\beta^2V_3h_3}{L}\mathbf{11}' & \dfrac{1}{L}\mathbf{I}+\dfrac{\beta^4h_3}{L^2}\mathbf{11}' \end{bmatrix}$$

where $h_3 = \dfrac{1}{1-T_{gb_3}}$

Using (4.2.11) we have,

$$\text{trace}\left[(\mathbf{X}'\,\mathbf{X})^{-1}\mathbf{g}_3'\mathbf{g}_3(\mathbf{X}'\,\mathbf{X})^{-1}\right] = U_3^2 + \frac{v\beta^2}{R^2} + vV_3^2 + \frac{v(v-1)}{2}\frac{\beta^4}{L^2} = T_{3b}$$

$$\therefore\ T_{Xb3} = T_X + \frac{T_{3b}}{1-T_{gb3}} \tag{4.3.46}$$

For Center Point: $\mathbf{g}'_4 = (1 \quad 0\cdots0 \quad 0\ldots0 \quad 0\ldots0)$. $\mathbf{g}_4$ can be rewritten as $\mathbf{g}'_4 = \left(1 \quad \mathbf{0}'_v \quad \mathbf{0}'_v \quad \mathbf{0}'_{\frac{v(v-1)}{2}}\right)$.

We have

$$\mathbf{g}'_4(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}_4 = A = T_{g_{b4}} \text{ (say)} \tag{4.3.47}$$

Using (4.2.5), $\det(\mathbf{X}'_1\mathbf{X}_1) = (1-T_{gb_4})\det(\mathbf{X}''\mathbf{X})$ (4.3.48)

Therefore
$$\left(\mathbf{X}'_1\mathbf{X}_1\right)^{-1} = \begin{bmatrix} A+\dfrac{A^2}{1-A} & \mathbf{0}' & \left(\dfrac{-R}{D}-\dfrac{RA}{D(1-A)}\right)\mathbf{1}' & \mathbf{0}' \\ \mathbf{0} & \dfrac{1}{R}\mathbf{I} & \mathbf{0} & \mathbf{0} \\ \left(\dfrac{-R}{D}-\dfrac{RA}{D(1-A)}\right)\mathbf{1} & \mathbf{0} & e\mathbf{I}+\left(f+\dfrac{R^2}{D^2(1-A)}\right)\mathbf{11}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dfrac{1}{L}\mathbf{I} \end{bmatrix}$$

Using (4.2.11), we have,

$$\operatorname{trace}\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{g}'_4\mathbf{g}_4(\mathbf{X}'\mathbf{X})^{-1}\right] = A^2 + \frac{vR^2}{D^2} = T_{4b}$$

$$\therefore\ T_{Xb4} = T_X + \frac{T_{4b}}{1-T_{gb_4}} \tag{4.3.49}$$

The expressions for the information contained in an observation given in (4.3.37), (4.3.41), (4.3.44) and (4.3.47) can further be simplified as

$$I(\mathbf{g}_1) = \frac{(C+v-1)L-2k\alpha^2R}{D} + \frac{k\alpha^2}{R} + \frac{k\alpha^4}{(C-1)L} + \frac{k^2\alpha^4(R^2-NL)}{L(C-1)D} + \frac{k(k-1)\alpha^4}{2L} \tag{4.3.50}$$

$$I(\mathbf{g}_2) = \frac{(C+v-1)L-2R\beta^2}{D} + \frac{\beta^2}{R} + \frac{\beta^4}{(C-1)L} + \frac{\beta^4(R^2-NL)}{L(C-1)D} \tag{4.3.51}$$

$$I(\mathbf{g}_3) = \frac{(C+v-1)L-2vR\beta^2}{D} + \frac{v\beta^2}{R} + \frac{v\beta^4}{(C-1)L} + \frac{v^2\beta^4(R^2-NL)}{L(C-1)D} + \frac{v(v-1)\beta^4}{2L} \tag{4.3.52}$$

$$I(\mathbf{g}_4) = \frac{(C+v-1)L}{D} \tag{4.3.53}$$

We can see that $I(\mathbf{g}_2)$ and $I(\mathbf{g}_4)$ are same as that of $I(\mathbf{g}_2)$ (4.3.14) and $I(\mathbf{g}_3)$(4.3.15) of Central composite designs, respectively. $I(\mathbf{g}_3)$ is same as that of $I(\mathbf{g}_1)$(4.3.13) of Central composite designs with α replaced by β. $I(\mathbf{g}_1)$ is same as that of $I(\mathbf{g}_1)$(4.3.13) of Central composite designs with *v* replaced by *k*. For a second order rotatable design obtained through BIB designs, substituting $C=3$ in (4.3.50), (4.3.51), (4.3.52) and (4.3.53), we get

$$I(\mathbf{g}_1) = \frac{(v+2)L-2k\alpha^2R}{D} + \frac{k\alpha^2}{R} + \frac{k^2\alpha^4}{2L} + \frac{k^2\alpha^4(R^2-NL)}{2LD} \tag{4.3.54}$$

$$I(\mathbf{g}_2) = \frac{(v+2)L-2R\beta^2}{D} + \frac{\beta^2}{R} + \frac{\beta^4}{2L} + \frac{\beta^4(R^2-NL)}{2LD} \tag{4.3.55}$$

$$I(\mathbf{g}_3) = \frac{(v+2)L-2vR\beta^2}{D} + \frac{v\beta^2}{R} + \frac{v^2\beta^4}{2L} + \frac{v^2\beta^4(R^2-NL)}{2LD} \tag{4.3.56}$$

$$I(\mathbf{g}_4) = \frac{(v+2)L}{D} \tag{4.3.57}$$

For a modified and rotatable second order response surface design, substitute $R^2 = NL$ in (4.3.54), (4.3.55), (4.3.56) and (4.3.57).

$$I(\mathbf{g}_1) = \frac{(v+2)L-2k\alpha^2R}{2NL} + \frac{k\alpha^2}{R} + \frac{k^2\alpha^4}{2L} \tag{4.3.58}$$

$$I(\mathbf{g}_2) = \frac{(v+2)L-2R\beta^2}{2NL} + \frac{\beta^2}{R} + \frac{\beta^4}{2L} \tag{4.3.59}$$

$$I(\mathbf{g}_3) = \frac{(v+2)L-2vR\beta^2}{2NL} + \frac{v\beta^2}{R} + \frac{v^2\beta^4}{2L} \tag{4.3.60}$$

$$I(\mathbf{g}_4) = \frac{(v+2)}{2N} \tag{4.3.61}$$

For a modified second order response surface design alone, substituting $R^2 = NL$ in (4.3.50), (4.3.51), (4.3.52) and (4.3.53), we get

$$I(\mathbf{g}_1) = \frac{(C+v-1)L-2k\alpha^2R}{(C-1)NL} + \frac{k\alpha^2}{R} + \frac{k\alpha^4}{(C-1)L} + \frac{k(k-1)\alpha^4}{2L} \tag{4.3.62}$$

$$I(\mathbf{g}_2) = \frac{(C+v-1)L-2R\beta^2}{(C-1)NL} + \frac{\beta^2}{R} + \frac{\beta^4}{(C-1)L} \tag{4.3.63}$$

$$I(\mathbf{g}_3) = \frac{(C+v-1)L-2vR\beta^2}{(C-1)NL} + \frac{v\beta^2}{R} + \frac{v\beta^4}{(C-1)L} + \frac{v(v-1)\beta^4}{2L} \tag{4.3.64}$$

$$I(\mathbf{g}_4) = \frac{(C+v-1)}{(C-1)N} \qquad (4.3.65).$$

Now substituting $\alpha = 1$ and $\beta = 2$, in the expressions (4.3.50) to (4.3.65), we can get the corresponding expressions for second order response surface designs obtainable through BIB designs when the various factors are with equispaced doses. The corresponding expressions for modified and rotatable second order response surface designs are given below. The other expressions can be obtained on the similar lines.

$$I(\mathbf{g}_1) = \frac{(v+2)L - 2kR}{2NL} + \frac{k}{R} + \frac{k^2}{2L} \qquad (4.3.66)$$

$$I(\mathbf{g}_2) = \frac{(v+2)L - 8R}{2NL} + \frac{4}{R} + \frac{8}{L} \qquad (4.3.67)$$

$$I(\mathbf{g}_3) = \frac{(v+2)L - 8vR}{2NL} + \frac{4v}{R} + \frac{8v^2}{L} \qquad (4.3.68)$$

$$I(\mathbf{g}_4) = \frac{v+2}{2N} \qquad (4.3.69)$$

Using these expressions, the corresponding expressions of $\det(\mathbf{X}_1'\mathbf{X}_1)$ can directly be obtained from (4.3.38), (4.3.42), (4.3.45) and (4.3.48). The $\mathrm{trace}(\mathbf{X}_1'\mathbf{X}_1)^{-1}$ can also easily be obtained using (4.3.40), (4.3.43), (4.3.46) and (4.3.49) respectively.

The information contained in an observation, percent loss in information and D-efficiencies of the modified and rotatable designs obtainable from BIB designs with $r = 3\lambda$ and $r < 3\lambda$ catalogued in Tables 3.3.4 and (3.3.6) respectively and are presented in Tables 4.3.2 and 4.3.3.

Table 4.3.2: The information contained in an observation, percent loss in information and D-efficiencies of the modified and rotatable second order response surface designs given in Table 3.3.4.

v	p	n_0	N	Factorial Point			Center Point		
				$I(\mathbf{g})$	Loss %	D-eff	$I(\mathbf{g})$	Loss %	D-eff
4	2	12	36	0.583	3.889	0.943	0.083	0.556	0.994
7	3	16	72	0.625	1.736	0.973	0.063	0.174	0.998
10	4	48	288	0.271	0.410	0.995	0.021	0.032	1.000*

*denotes that the D-efficiency is greater than 0.9995.

Table 4.3.3a: The information contained in an observation, percent loss in information and D-efficiencies of the modified and rotatable second order response surface designs given in Table 3.3.6.

v	p	s	t	n_0	N	Factorial Point			Axial Point			Center Point		
						$I(\mathbf{g})$	Loss %	D-eff	$I(\mathbf{g})$	Loss %	D-eff	$I(\mathbf{g})$	Loss %	D-eff
4	3	4	3	136	288	0.086	0.575	0.994	0.143	0.951	0.990	0.010	0.069	0.999
5	3	4	3	304	654	0.056	0.266	0.997	0.093	0.445	0.995	0.005	0.025	1.000*
6	3	4	1	144	476	0.080	0.286	0.997	0.135	0.483	0.995	0.008	0.030	1.000*
6	4	2	7	456	732	0.115	0.410	0.996	0.077	0.276	0.997	0.005	0.020	1.000*
6	5	1	7	456	732	0.115	0.410	0.996	0.077	0.276	0.997	0.005	0.020	1.000*
7	4	1	1	64	190	0.282	0.783	0.991	0.282	0.783	0.991	0.024	0.066	0.999

*denotes that the D-efficiency is greater than 0.9995.

From Table 4.3.3.a, it is observed that the percent loss in information is marginal and D-efficiencies are reasonably high. Therefore, we can say that modified and rotatable designs obtained through BIB designs with $r = 3\lambda$ are robust against the unavailability of one observation. However, to satisfy the property of $R^2 = NL$, n_0 is very high. Therefore, we have also computed the percent loss in information and D-efficiencies for rotatable designs obtained through BIB designs by taking $n_0 = 2$ in the above table and presented in Table 4.3.3b.

Table 4.3.3b: The information contained in an observation, percent loss in information and D-efficiencies of the modified and rotatable second order response surface designs given in Table 3.3.6 with n_0=2.

v	p	s	t	n_0	N	Factorial Point			Axial Point			Center Point		
						$I(\mathbf{g})$	Loss %	D-eff	$I(\mathbf{g})$	Loss %	D-eff	$I(\mathbf{g})$	Loss %	D-eff
4	3	4	3	2	154	0.085	0.564	0.994	0.153	1.021	0.989	0.250	1.667	0.981
5	3	4	3	2	352	0.054	0.259	0.997	0.107	0.508	0.995	0.206	0.980	0.989
6	3	4	1	2	334	0.079	0.284	0.997	0.163	0.583	0.994	0.308	1.099	0.987
6	4	2	7	2	278	0.109	0.390	0.996	0.078	0.280	0.997	0.216	0.772	0.991
6	5	1	7	2	278	0.109	0.390	0.996	0.078	0.280	0.997	0.216	0.772	0.991
7	4	1	1	2	128	0.278	0.772	0.991	0.278	0.772	0.991	0.500	1.389	0.981

Similar computations can easily be made for modified designs obtainable from BIB design.

CHAPTER V

RESPONSE SURFACE DESIGNS FOR QUALITATIVE CUM QUANTITATIVE FACTORS

5.1 Introduction

Response Surface studies often involve quantitative factors only and as such much of work in the response surface studies has been undertaken for quantitative factors only. A brief account of the results available in the literature and obtained in the present investigation on response surface designs for quantitative factors is given in Chapters II, III and IV. There are, however, many situations in agricultural experimentation where both the qualitative and quantitative variables are involved. For example, in fertilizer trials, the response or yield of a crop not only depends on various doses of fertilizers but also on the method of its application viz. foliar application, behind the plough, broadcasting, etc. Here the method of application is a qualitative variable while the amount of fertilizer applied is a quantitative variable. Another example could be the differences in response (s) to fertilizer application due to its various sources. Here the source of fertilizer is a qualitative variable while the amount of fertilizer applied is quantitative variable. To improve the agricultural productivity there is continuous research activity for the development of new varieties of crop and often the agronomy for the crop vary from variety to variety in some of the aspects of crop production and management. Thus it is essential to conduct the experiment to find out the influence of various agronomic practices to the newly developed varieties and consequently evolve optimum combinations of nitrogen, phosphorus and potassium doses for maximizing the varieties productivity. All those experiments where variety of the crop is a factor along with other factors like fertilizer, etc. constitute a qualitative-cum-quantitative experiment. A close scrutiny of the experiments available in the Agricultural Field Experiments Information System (AFEIS) maintained at Indian Agricultural Statistics Research Institute, New Delhi revealed that more than 10% of the experiments conducted in the country have variety as one of the factors. Most of these experiments have been conducted either in randomized complete block design or Split plot design. It is, therefore, required to undertake response surface studies involving these trials.

The qualitative-cum-quantitative experiments differ from experiments involving only quantitative factors in the sense that we may often have dummy treatments. Here the experimenter is mainly interested in the types or forms that are more responsive as well as in the interaction of different qualities with quantities. The important feature of these experiments which make them different from ordinary factorials is that some of the level combinations, namely those where the quantitative factor is at zero level, are indistinguishable. To be clearer, consider the following example.

Consider that we have three forms of nitrogenous fertilizers say, ammonium sulphate (AS), calcium ammonium nitrate (CAN) and urea. Each of these forms are being tested at 3 levels viz. 0,1 and 2. Further, suppose that the other factor being tested is phosphorus with levels 0, 1 and 2. Here we get the following three sets of identical treatments combinations.

Set I	$n_0 q_0 p_0$	$n_0 q_1 p_0$	$n_0 q_2 p_0$
Set II	$n_0 q_0 p_1$	$n_0 q_1 p_1$	$n_0 q_2 p_1$
Set III	$n_0 q_0 p_2$	$n_0 q_1 p_2$	$n_0 q_2 p_2$

where $n_{\#}$ denotes the level of nitrogen, $q_{\#}$ source of nitrogen and $p_{\#}$ as level of phosphorus. Thus in this we get three sets of identical treatments which are called dummy treatments. This is so because there is no meaning of any quality being applied at zero level of nitrogen. Thus any differences between these combinations are due to uncontrolled factors and hence, they form a part of error component. Thus the construction of the confounded designs and their analysis for qualitative-cum-quantitative becomes different from that of quantitative type of designs.

Fisher (1935) described a few such experiments in the context of agricultural experiments where zero, single and double doses of certain fertilizers were applied and yield was studied. Subsequently Sardana (1961) and Narayana and Sardana (1967) investigated the designs for such experimental situations. Lal and Das (1973) proposed a method of construction of confounded designs for qualitative-cum-quantitative experiments. Bose and Mukerjee (1987) pointed out that substantial modifications are required in the standard calculus for factorial arrangements (see e.g. Kurkjian and Zelen (1963)) and obtained necessary and sufficient conditions for inter and intra effect orthogonality for qualitative-cum-quantitative experiments. They also gave some methods of construction of such designs. In the above literature, the designs for qualitative cum quantitative experiments were developed keeping in view the standard factorial experiments analysis, *i.e.,* evaluating of main effects and interaction of various factors involved in the experiment. It was Cox (1984) who pointed out the need for the development of response surface designs for qualitative-cum-quantitative experiments. Such experiments are quite common in food processing experiments as well.

For example, consider an experimental situation where it is desired to prepare a best recipe for a cakemix to be sold in a box at the supermarket. In this example, experiment is to be run with four design factors, flour (x_1), shortening (x_2), eggpowder (x_3), shape of the baked cake (w). First three factors are quantitative while the fourth can take only two shapes: round and square, so it is a qualitative factor.

In response surface studies goal of the experiments for inclusion of qualitative variable(s) is same as that of quantitative variables, *i.e.,*

(i) they must be included in the model,
(ii) they must be involved in response prediction or optimization using model,
(iii) the nature of interaction between quantitative and qualitative variables determines the complexities of both the design and analysis.

The designs that are optimal for fitting first or second order response surfaces when all factors are quantitative in nature may not be so when some of the factors are qualitative and effect the response. This may be due to the constraints in the level of qualitative factors or due to the terms involving the interactions of terms. The most common optimal design for fitting second order response surface is Central Composite Design (CCD) and involves five levels of each of the factor being investigated. An experimenter, say, is interested in studying the effects of nitrogen from two sources (urea and calcium ammonium nitrate), he./she cannot be told that there must be five sources of nitrogen. Even if there are five sources of nitrogen, it is very difficult to associate them with the five levels of a central composite design viz. $-\beta, -\alpha, 0, \alpha, \beta$ as for $\alpha = 1$, β is generally not an integer. Thus it may not be suitable and when one or more factors are qualitative in nature *e.g.* in a trial involving sources of nitrogen fertilizer as a qualitative factor, it is not desirable to insist on five sources of nitrogen for adopting CCD for experimentation. Further, one may think of using a second order response surface design such as the central composite design, the design obtainable from BIB designs for cyclic permutations of factors for each level of the qualitative factor. This, however, will require a large number of runs. Thus there is a need to develop designs for experiments involving both quantitative and qualitative factors.

Draper and John (1988) were the first to tackle the problem of obtaining response surface designs for qualitative-cum quantitative factors. They discussed the relations between designs and models and gave designs for some specific situations. Wu and Ding (1998) have cited the following example requiring response surface designs for given some designs for qualitative-cum quantitative factors.

Consider a machining process for slab caster rolls in a steel plant. The experiment was conducted to improve the machining time keeping a low rating of surface roughness. Four factors viz. (i) feed (the distance the tool advances in one revolution), (ii) speed at which the surface moves past the cutting tool, (iii) lead angle at which the tool meets the work piece, and (iv) insert (a replaceable part of the cutting tool), are identified as potentially important. The first three factors are quantitative, while the fourth can take only two shapes: round and square.

Wu and Ding (1998) have given a systematic method of construction of such designs of economical size and discuss the underlying objectives and models. Aggarwal and Bansal (1998) further extended this method of construction for the situations where some of the quantitative factors are uncontrollable or noise factors.

The special care is required for defining the levels of qualitative factors in the model. A brief account of this is given in Section 5.2. For more details on this, one may refer to Draper and John (1988). The first and second order response surface designs for qualitative-cum-quantitative experiments are given in Sections 5.3 and 5.4 respectively.

5.2 Inclusion of Terms Involving Qualitative Factor in the Model

Qualitative factors are included in response surfaces using Indicator or Dummy variables. For example, suppose that one of the factors in fertilizer response studies is a source of nitrogen. Assuming that only two sources are involved, we wish to assign different levels to the two sources to account for the possibility that each source may have different effect on the response. Thus to introduce the effect of two different sources into a model, we define a dummy variable z as follows

$z = 1$, if the observation is from source I
$z = -1$, if the observation is from source II

In fact any two levels, (0,1); (-1,1) or (-3,7) would work perfectly well and, in general, there are infinite number of ways for allocating the levels of the dummy variables.

In general, a qualitative factor with *t* levels is represented by $t-1$ dummy variables that are assigned the values either –1 or 1. Thus, if there were three sources of nitrogen, the different level would be accounted for by two dummy variables defined as follows:

z_1	z_2	
-1	-1	if the observation is from source I
1	-1	if the observation is from source II
-1	1	if the observation is from source III

5.3 Design Considerations in First Order Response Surfaces

Design choice is dependent upon the model postulated by experimenter and following situations are of interest. Here we shall consider a system that is affected by *v* quantitative variables $(x_i;\ i=1,...,v)$ and single qualitative variable (z) each at two levels.

Situation I: It is postulated that only change in the intercept is required at the level of qualitative factor changes, *i.e*., the model is

$$y=\beta_0+\beta_1x_1+\beta_2x_2+...+\beta_vx_v+\phi_1z+\varepsilon \tag{5.3.1}$$

Situation II: In addition to whatever is postulated is situation I, whether or not linear coefficient of $x_1, x_2,..., x_v$ vary from one level to anther of qualitative variable, thus the model to fit is

$$y=\beta_0+\sum_{i=1}^{v}\beta_ix_i+\phi_1z+\sum_{i=1}^{v}\delta_ix_iz+\varepsilon \tag{5.3.2}$$

Clearly 2^v factorials would allow for estimation of model in equations (5.3.1) and (5.3.2). In addition to 2^v factorial combinations some extra runs (may be of center points) allow for testing to determine if quadratic terms are needed. Since the number of runs in 2^v is quite large as compare to terms in model to be estimated (particularly for large value of *v*), therefore, the experimenter is interested in designs that are smaller than full 2^v factorial that can be used to fit a model (5.3.1) or (5.3.2). For 2 quantitative factors, Draper and John (1988) have shown that the design consisting of five points $(-1,\ -1,\ -1);\ (1,\ -1,\ -1);\ (-1,\ 1,\ 1);\ (-1,\ 1,\ 1);\ (0,\ 0,\ -1)$ can be used to fit the model (5.3.1) along with an extra term, only one of x_1x_2, x_1z or x_2z. For this five point design replication would be necessary to obtain a test for lack of fit.

For more than two quantitative variables and qualitative variables that are at two levels fractional factorials that all two factor interactions involving the qualitative and quantitative factors are estimable. In other words, one may also think of using designs of mixed resolution that allow a smaller resolution that applies in the case of quantitative variables then that which applies in dealing with interaction involving quantitative and qualitative variables. This is explained through the following example.

Example 5.3.1: Consider 2^6 experiments involving 5 quantitative variables and one qualitative variable and model (5.3.2) is of interest. Rewriting model (5.3.2) for $v=5$

$$y=\beta_0+\sum_{i=1}^{5}\beta_ix_i+\phi_1z+\sum_{i=1}^{5}\delta_ix_iz+\varepsilon \tag{5.3.3}$$

we can fit model (5.3.3) with 2^{6-2} factorial with defining contrast

$$I = x_1x_2x_3 = x_1x_3x_4x_5z = x_2x_4x_5z\ .$$

It will allow fitting of (5.3.3) leaving 4 degrees of freedom for lack of fit.

Further, Hedayat and Pesotan (1992, 1997) gave two factor fractional factorial designs for main effects and selected two factor of interaction when all other interactions are assumed to be negligible. It is conjectured that these designs can be used for response surface studies involving the qualitative cum quantitative variables by designating the interaction between qualitative and quantitative factors as interaction of interest and interactions between qualitative cum quantitative factor as zero.

5.4 Designs for Fitting of Second Order Response Surfaces

In this section, we discuss the procedure of obtaining designs for fitting response surfaces in qualitative-cum-quantitative experiments. We begin with a brief review of the work done by Draper and John (1988) and Wu and Ding (1998). It will be followed by some remarks on the use of response surface designs when various factors are with equispaced doses, second order response surface designs with orthogonal blocking and asymmetric rotatable designs.

Draper and John (1988) considered that if a second-order response surface is under consideration with coded quantitative variables $x_1, x_2,..., x_v$ and qualitative variables $z_1, z_2,..., z_r$, whose effects also have to be incorporated in the model and we wish to choose a design, which will allow to:

1. Fit a linear model in the v quantitative variables $x_1, x_2,..., x_v$ of first or second order response surface, as selected, to the response variables.
2. Take account of the effects that changes in the qualitative variables $z_1, z_2,..., z_r$ have on the form of the linear model.
3. To test whether or not a simpler model might adequately explain the data, given a model.

Restricting to second order models only, the most general formulation is

$$E(y) = \sum_{z=1}^{m} w_z f_z(\mathbf{x}, \beta_z) \qquad (5.4.1)$$

where f is a polynomial of second order.

$$f_z(\mathbf{x}, \beta_z) = \beta_{0z} + \sum_{i=1}^{v} \beta_{iz} x_i + \sum_{i=1}^{v}\sum_{i'=1}^{v} \beta_{ii'z} x_i x_{i'}$$

and the z subscript indicates a different set of β's for each choice of z levels. The $w_z\ (z = 1,..., m)$ represent the selected levels of m dummy variables, chosen in such a way as to distinguish between all possible combinations of qualitative variables. For example, if there is one qualitative variable with two levels, we can set $w_z = -1$ for first level and $w_z = 1$ for second level. If we had two qualitative variables, say $z_1 = (-1,1)$ and $z_2 = (-1,1)$, then the w_z representation can be as shown below:

Category	w_1	$w_2 = z_1$	$w_3 = z_2$	$w_4 = z_1 z_2$
1	1	-1	-1	1
2	1	1	-1	-1
3	1	-1	1	-1
4	1	1	1	1

This representation not only separates the four categories but also has the advantage that it can be immediately related to the specific z - levels.

In designing an experiment to fit a particular model of the form (5.4.1), it is necessary to choose a design that will allow testing of lack of fit. It other words, it should allow the examination of the goodness of fit of this model relative to a model given by the addition of further higher order terms in the quantitative variables or of interactions between the quantitative and qualitative variables.

Wu and Ding (1998) gave a systematic method for constructing designs of economical size. The main idea is to start with an efficient design for the quantitative factors and then partition its points into groups. Each group corresponds to level combinations of the qualitative factors. From these designs, designs are selected with high overall efficiencies as measured by the determinant criterion.

They use the determinant criterion (D-criterion) for efficiency comparison

$$\text{D-efficiency} = |\mathbf{X}'\mathbf{X}|^{1/p} \Big/ N$$

The other criterion that can be used for efficiency comparison are

$$\text{A-efficiency} = p \Big/ \left(N * trace(\mathbf{X}'\mathbf{X})^{-1}\right)$$

$$\text{G-efficiency} = p / \max(V(x))$$

where $max(V(x))$ is the maximum scaled prediction variance of the design.

Wu and Ding (1998) constructed the designs to meet the following objectives.

A. The overall design is efficient for a model that is second order in $x_1, x_2, ..., x_v$ and has the main effects of $z_1, z_2, ..., z_r$ and the interactions between x_i and z_j.

B. At each combination of the quantitative factor or each level of a qualitative factor z_j, it is an efficient first order design in $x_1, x_2, ..., x_v$.

C. The design in A consists of two parts: the first part is a first-order design for both $x_1, x_2, ..., x_v$ and $z_1, z_2, ..., z_r$, and the second part can be viewed as a sequential addition to the first part so that the expanded design is second-order.

D. When collapsed over the levels of $z_1, z_2, ..., z_r$, it is an efficient second-order design for $x_1, x_2, ..., x_v$.

Objective A is the most important. It ensures that the first and second order effects of x_i, the main effects of z_j and the interactions between x_i and z_j can all be estimated with high overall efficiency.

The effects of x_i may vary with the levels of z_j. It is desirable to have the design at each combination of $z_1, z_2, ..., z_r$ (or at each level of z_j) that allows separate estimation of the first-order effects of x_i. The goal is met by implementing Objective B.

Objective C enables the experiment to be conducted in two stages. The initial experiment allows the estimation of the main effects of x_i, z_j and some of their interactions.

Objective D ensures that, when there is no significant difference among the z_j's the combined design is a second-order design with good overall properties.

If the objectives cannot be met simultaneously priority should be given to A and B. Objective D is emphasized only if the effects of the qualitative factors are believed to be small.

Now stating these objectives with the aid of regression models, for $r = 1$, the case of one qualitative factor, a second-order model for x_i and z is given by

$$E(y) = \sum_{z=1}^{m} W_z \left(\beta_{0z} + \sum_{i=1}^{v} \beta_{iz} x_i \right) + \sum_{i=1}^{v-1} \sum_{i'=i+1}^{v} \beta_{ii'} x_i x_{i'} \tag{5.4.2}$$

where m = number of levels of qualitative factor

W_z = 1, when y is taken at level 1 of the variable z

= 0, otherwise.

β_{0z} = constant term, dependent on the choice of z

β_{iz} = slope of x_i, dependent on the choice of z.

If the run size is small, the following sub models of equation (5.4.2) may be fitted

$$E(y) = \sum_{z=1}^{m} W_z \left(\beta_{0z} + \sum_{i=1}^{v} \beta_{iz} x_i \right) + \sum_{i=1}^{v} \beta_{ii} x_i^2 + \text{some of } \beta_{ii'} x_i x_{i''} \qquad (i < i') \tag{5.4.3}$$

$$E(y) = \sum_{z=1}^{m} W_z \beta_{0z} + \sum_{i=1}^{v} \left(\beta_i x_i + \beta_{ii} x_i^2 \right) + \text{some of } W_z \beta_{iz} x_i \text{ and } \beta_{ii'} x_i x_{i'} \quad (i < i') \tag{5.4.4}$$

Model (5.4.3) excludes some interaction terms $\beta_{ii'} x_i x_{i'}$, $i < i'$ in the model (5.4.2). Model (5.4.4) further excludes some $\beta_{iz} x_i$ terms.

Objective A stipulates that the overall design allows one of these models to be fitted with high efficiency.

Objective B requires that the coefficients in the model

$$E(y) = \beta_0 + \sum_{i=1}^{v} \beta_i x_i + \text{some of } \beta_{ii'} x_i x_{i'} \quad (i < i') \tag{5.4.5}$$

be estimated with high efficiency from the design at each level of the qualitative factor. By excluding the x_i^2 terms in (5.3.3) and (5.3.4) one gets the following submodels

$$E(y) = \sum_{z=1}^{m} W_z \left(\beta_{0z} + \sum_{i=1}^{v} \beta_{iz} x_i \right) + \text{some of } \beta_{ii'} x_i x_{i'} \quad (i < i') \tag{5.4.6}$$

$$E(y) = \sum_{z=1}^{m} W_z \beta_{0z} + \sum_{i=1}^{v} \beta_i x_i + \text{some of } W_z \beta_{iz} x_i \text{ and } \beta_{ii'} x_i x_{i'} \quad (i < i') \tag{5.4.7}$$

Objective C requires that the coefficients in (5.4.6) and (5.4.7) be estimated with high efficiency from the first-order equation.

The method of construction given by Wu and Ding (1998) is based on central composite designs. To be clearer, consider the experimental situation when there is one qualitative variable with two levels, *i.e.*, for $r = 1$. The design for the above experimental situation can be constructed as follows

Run	x_1	x_2	$\cdots$	x_v	z
1 2 $\vdots$ $t\left(= 2^{v-p}\right)$	± 1 according to a 2^{v-p} design				$z = 1 \text{ or } -1$ by (i) equating column z to an interaction column among the x_i's, or (ii) search over different combinations of ± 1 according to some criteria.
$t+1$	0	0	$\ldots$	0	1 or -1
$t+2$	0	0	$\ldots$	0	-1 or 1
$t+3$	β	0	$\ldots$	0	Search over different combinations of ± 1 according to some criteria.
$t+4$	$-\beta$	0	$\ldots$	0	
$t+5$	0	β	$\ldots$	0	
$t+6$	0	$-\beta$	$\ldots$	0	
$\vdots$	$\vdots$	$\vdots$			
$t+2v+1$	0	0	$\ldots$	β	
$t+2v+2$	0	0	$\ldots$	$-\beta$	

For $x_1,\ldots,x_v$, the first $t\left(= 2^{v-p}\right)$ runs are chosen according to a 2^{v-p} fractional factorial design with high resolution and $x_i = \pm 1$.

The $(t+1)^{\text{th}}$ and $(t+2)^{\text{th}}$ runs are at the center point. The last $2v$ runs are the axial points whose distance from the origin is α. The value of α be chosen so that the design for $x_1,...,x_v$ are rotatable.

They have used the determinant criteria (D-criteria) for efficiency comparison, $|\mathbf{X}'\mathbf{X}|^{1/p}$ where the model is described by $E(\mathbf{y}) = \mathbf{X\beta}$, $\mathbf{y}$ is the vector of observations, $\boldsymbol{\beta}$ is the vector of parameters, of dimension p, *i.e.*, the number of parameters in the model, and $\mathbf{X}$ is the model matrix consisting of all the important effects stipulated in the objectives and the intercept term.

According to A, the overall design with $t+2v+2$ runs should allow the parameters in model (5.4.2) and (5.4.33) to be estimated with high efficiency in terms of D-efficiency.

According to B, the runs at each level of z should allow the parameters in model (5.4.5) to be estimated with high D-efficiency.

According to C, the first $(t+1)$ runs, including one center point, should allow the parameters in model (5.4.6) or (5.4.7) to be estimated with high D-efficiency.

When there are two or more qualitative factors, construction of designs becomes more complicated because Objective B can take several forms. Wu and Ding (1998) gave an example for the case of $r=2$ and $v=2$.

In defining a model involving both qualitative and quantitative there is also uncertainty in including various terms involving the interaction of qualitative and quantitative factors in the model based only on quantitative factors. Thus, the structure of interaction of qualitative factors and the response surface model in the terms such as $x_i z$ is essential. (Here x_i and z denote the quantitative and qualitative factors respectively.

It can easily be seen that the above method provides design when the levels of various factors are unequispaced. *The above method can easily be extended for obtaining designs when the quantitative factors have equispaced levels by choosing $\beta = 2$ in the above method*. In the sequel, we establish a relationship between some of the existing designs and designs for qualitative-cum-quantitative factors.

Remark 5.4.1: If we recall, in Section 5.1, we have argued that the standard designs for fitting linear or quadratic response surfaces when all factors are quantitative in nature may not be suitable when some of the factors are qualitative and influence the response. As it was difficult to associate the levels of qualitative factor with the levels that are non-integers. However, this problem can be taken care of by using the designs for various factors with equispaced doses obtained from central composite designs and BIB designs in Section 3.3 of Chapter III.

Remark 5.4.2: In Section 5.1, we have discussed that the standard designs for fitting second order response surfaces when all factors are quantitative are not suitable for qualitative-cum-quantitative experiments as the number of levels of the qualitative factor may not be same as that of the quantitative factors. This problem to some extent can be taken care of through the use of asymmetric rotatable designs when various factors are with equispaced doses obtained in Section 3.3 of Chapter III.

Remark 5.4.3: Draper and Stoneman (1968) gave response surface designs which are subsets of points of the 2^p3^q or the 2^p4^q factorial design according to the levels specified. In these designs, the response surface cannot include quadratic terms in the factors that are at 2 levels each but all second order terms for the factors to be examined at 3 or 4 levels can be permitted. Now if we associate the qualitative factors with the factors at 2 level each and quantitative factors at 3 or 4 levels each, we can get designs for qualitative-cum-quantitative factors.

Remark 5.4.4: Herzberg (1966) introduced cylindirically rotatable designs that are rotatable with respect to all factors except one. If we consider, the factor with respect to which the design is not rotatable as qualitative factor, then we may get the designs for qualitative-cum-quantitative factors.

Remark 5.4.5: In Chapter III, Section 3.5, we have obtained and catalogued several second order response surface designs with orthogonal blocking. If we consider qualitative factor as blocking factor, then the design that allows orthogonal blocking can be used for fitting model (5.4.1) by superimposing level of qualitative variable with blocks. For catalogues of these designs, please refer to Section 3.5 of Chapter III. The procedure of obtaining response surface designs for qualitative-cum-quantitative factors from second order rotatable designs with equispaced doses is explained through the following example.

Example 5.4.1: Consider an agricultural experiment where it is desired to obtain an optimum combination of 4 quantitative factors A, B, C and D. Each of these factors were tried at 5 levels. There is one qualitative factor, Z with three levels in the experiments. The layout of design obtained using a second order rotatable design with orthogonal blocking with block contents as

Block-I				Block-II				Block-III			
A	B	C	D	A	B	C	D	A	B	C	D
-1	-1	-1	-1	-1	-1	-1	1	2	0	0	0
-1	-1	1	1	-1	-1	1	-1	-2	0	0	0
-1	1	-1	1	-1	1	-1	-1	0	2	0	0
1	-1	-1	1	1	-1	-1	-1	0	-2	0	0
1	-1	1	-1	-1	1	1	1	0	0	2	0
1	1	-1	-1	1	-1	1	1	0	0	-2	0
-1	1	1	-1	1	1	-1	1	0	0	0	2
1	1	1	1	1	1	1	-1	0	0	0	-2
0	0	0	0	0	0	0	0	0	0	0	0

By associating, the blocks with the levels of qualitative factor, we get

z	A	B	C	D
-1	-1	-1	-1	-1
-1	-1	-1	1	1
-1	-1	1	-1	1

-1	1	-1	-1	1
-1	1	-1	1	-1
-1	1	1	-1	-1
-1	-1	1	1	-1
-1	1	1	1	1
-1	0	0	0	0
0	-1	-1	-1	1
0	-1	-1	1	-1
0	-1	1	-1	-1
0	1	-1	-1	-1
0	-1	1	1	1
0	1	-1	1	1
0	1	1	-1	1
0	1	1	1	-1
0	0	0	0	0
1	2	0	0	0
1	-2	0	0	0
1	0	2	0	0
1	0	-2	0	0
1	0	0	2	0
1	0	0	-2	0
1	0	0	0	2
1	0	0	0	-2
1	0	0	0	0

This design can now be used to fit the model

$$y = \beta_0 + \phi_1 z + \sum_{i=1}^{4} \beta_i x_i + \sum_{i=1}^{4} \beta_{ii} x_i^2 + \sum_{i=1}^{3} \sum_{i'=i+1}^{4} \beta_{ii'} x_i x_{i'} + \varepsilon$$

and is useful when the experimenter feels that only the change in intercept is required as the level of qualitative variable changes. However, this particular design is also useful for fitting the complete model with interaction of qualitative and quantitative factors.

Some hit and trial solutions can also be obtained. One such design is given in the following example:

Example 5.4.2: Consider an agricultural experiment involving three quantitative factor N, P and K each at 3 levels and one qualitative factor named as sources of N (S) at two levels, *i.e.*, $3 \times 3 \times 3 \times 2$ design. The layout of design obtained using a second order rotatable design with orthogonal blocking with block contents as

Block-I			Block-II			Block-III		
N	P	K	N	P	K	N	P	K
-1	-1	0	-1	0	-1	0	-1	-1
-1	1	0	-1	0	1	0	-1	1
1	-1	0	1	0	-1	0	1	-1
1	1	0	1	0	1	0	1	1
0	0	1	0	1	0	1	0	0
0	0	1	0	1	0	1	0	0
0	0	-1	0	-1	0	-1	0	0
0	0	-1	0	-1	0	-1	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0

Now if we associate the levels of two sources within blocks in such a fashion that the sum of the entries in the column of qualitative factor and its cross products with quantitative factors is zero, we get the following design:

S	N	P	K
1	-1	-1	0
-1	-1	1	0
-1	1	-1	0
1	1	1	0
1	0	0	1
-1	0	0	1
1	0	0	-1
-1	0	0	-1
1	0	0	0
-1	0	0	0
1	-1	0	-1
-1	-1	0	1
-1	1	0	-1
1	1	0	1
1	0	1	0
-1	0	1	0
1	0	-1	0
-1	0	-1	0
1	0	0	0
-1	0	0	0
1	0	-1	-1
-1	0	-1	1
-1	0	1	-1
1	0	1	1
1	1	0	0
-1	1	0	0
1	-1	0	0

-1	-1	0	0
1	0	0	0
-1	0	0	0

If we consider the fitting of the model with 14 parameters as

$$y = \beta_0 + \phi_1 z + \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{3} \beta_{ii} x_i^2 + \sum_{i=1}^{2} \sum_{i'=i+1}^{3} \beta_{ii'} x_i x_{i'} + \sum_{i=1}^{3} \delta_i x_i z + \varepsilon$$

then the matrix $\mathbf{X'X}$, is given by

30	0	0	0	0	12	12	12	0	0	0	0	0	0
0	30	0	0	0	0	0	0	4	4	4	0	0	0
0	0	12	0	0	0	0	0	0	0	0	0	4	4
0	0	0	12	0	0	0	0	0	0	0	4	0	4
0	0	0	0	12	0	0	0	0	0	0	4	4	0
12	0	0	0	0	12	4	4	0	0	0	0	0	0
12	0	0	0	0	4	12	4	0	0	0	0	0	0
12	0	0	0	0	4	4	12	0	0	0	0	0	0
0	4	0	0	0	0	0	0	4	0	0	0	0	0
0	4	0	0	0	0	0	0	0	4	0	0	0	0
0	4	0	0	0	0	0	0	0	0	4	0	0	0
0	0	0	4	4	0	0	0	0	0	0	12	0	0
0	0	4	0	4	0	0	0	0	0	0	0	12	0
0	0	4	4	0	0	0	0	0	0	0	0	0	12

The matrix $(\mathbf{X'X})^{-1}$ is

β_0	ϕ_1	β_1	β_2	β_3	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	δ_1	δ_2	δ_3
0.119	0.000	0.000	0.000	0.000	-0.071	-0.071	-0.071	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.056	0.000	0.000	0.000	0.000	0.000	0.000	-0.056	-0.056	-0.056	0.000	0.000	0.000
0.000	0.000	0.113	0.019	0.019	0.000	0.000	0.000	0.000	0.000	0.000	-0.013	-0.044	-0.044
0.000	0.000	0.019	0.113	0.019	0.000	0.000	0.000	0.000	0.000	0.000	-0.044	-0.013	-0.044
0.000	0.000	0.019	0.019	0.113	0.000	0.000	0.000	0.000	0.000	0.000	-0.044	-0.044	-0.013
-0.071	0.000	0.000	0.000	0.000	0.143	0.018	0.018	0.000	0.000	0.000	0.000	0.000	0.000
-0.071	0.000	0.000	0.000	0.000	0.018	0.143	0.018	0.000	0.000	0.000	0.000	0.000	0.000
-0.071	0.000	0.000	0.000	0.000	0.018	0.018	0.143	0.000	0.000	0.000	0.000	0.000	0.000
0.000	-0.056	0.000	0.000	0.000	0.000	0.000	0.000	0.306	0.056	0.056	0.000	0.000	0.000
0.000	-0.056	0.000	0.000	0.000	0.000	0.000	0.000	0.056	0.306	0.056	0.000	0.000	0.000
0.000	-0.056	0.000	0.000	0.000	0.000	0.000	0.000	0.056	0.056	0.306	0.000	0.000	0.000
0.000	0.000	-0.013	-0.044	-0.044	0.000	0.000	0.000	0.000	0.000	0.000	0.113	0.019	0.019
0.000	0.000	-0.044	-0.013	-0.044	0.000	0.000	0.000	0.000	0.000	0.000	0.019	0.113	0.019
0.000	0.000	-0.044	-0.044	-0.013	0.000	0.000	0.000	0.000	0.000	0.000	0.019	0.019	0.113

It can easily be observed that most of the parameters are estimated without correlation. Hence, this may be a good design for qualitative-cum-quantitative experiments.

Meyers and Montgomery (1995) have used SAS-QC for construction of response surface designs involving both qualitative and quantitative variables. These designs may allow two or more than two qualitative variables. One of the designs obtained by them using G, A and D-optimality criterion is given in the following example.

Example 5.4.3: Consider a situation in which there are four quantitative variables and one qualitative variable at two levels. It is assumed that second order model in quantitative variables and terms of the type z and $x_i z$ $(i = 1,...,4)$ to account for possible changes in structure of response surface due to change in quantitative variables shall be appropriate. As such the model to be fitted shall contain 20 terms

$$y = \beta_0 + \sum_{i=1}^{4} \beta_i x_i + \sum_{i=1}^{4} \beta_{ii} x_i^2 + \sum_{j<k}\sum \beta_{jk} x_j x_k + \phi z + \sum_{i=1}^{4} \delta_i x_i z + \varepsilon$$

The possible candidate for the design points in a grid involving full central composite design with levels –2, -1, 0, 1, 2 and x's crossed with –1 and +1, the two levels of the qualitative variables. The experiments can afford only 24 total runs. The SAS system gave the following design using G-efficiency, A-efficiency & D-efficiency criterion.

Design I: G-efficiency Criterion

observation	x_1	x_2	x_3	x_4	z
1	-2	0	0	0	-1
2	-1	-1	-1	-1	-1
3	-1	-1	-1	-1	1
4	-1	-1	1	-1	1
5	-1	-1	1	1	1
6	-1	1	-1	-1	-1
7	-1	1	-1	1	1
8	-1	1	1	-1	1
9	-1	1	1	1	-1
10	0	-2	0	0	1
11	0	0	-2	0	-1
12	0	0	0	0	1
13	0	0	0	2	-1
14	0	0	2	0	1
15	0	2	0	0	1
16	1	-1	-1	-1	-1
17	1	-1	1	-1	-1
18	1	-1	1	1	-1
19	1	-1	1	1	1
20	1	1	-1	-1	1
21	1	1	-1	1	1
22	1	1	1	-1	-1
23	1	1	1	-1	1
24	2	0	0	0	-1

Design II: A-efficiency Criterion

observation	x_1	x_2	x_3	x_4	z
1	-1	-1	-1	-1	-1
2	-1	-1	-1	1	1
3	-1	-1	1	-1	1
4	-1	-1	1	1	-1
5	-1	1	-1	-1	1
6	-1	1	-1	1	-1
7	-1	1	1	-1	-1
8	-1	1	1	1	1
9	0	-2	0	0	-1
10	0	-2	-2	0	-1
11	0	0	0	-2	-1
12	0	0	0	0	-1
13	0	0	0	0	1
14	0	0	0	2	-1
15	0	0	2	0	-1
16	0	2	0	0	-1
17	1	-1	-1	-1	1
18	1	-1	1	-1	-1
19	1	-1	1	1	1
20	1	1	-1	-1	-1
21	1	1	-1	1	1
22	1	1	1	-1	1
23	1	1	1	1	-1
24	2	0	0	0	-1

Design III: D-efficiency Criterion

observation	x_1	x_2	x_3	x_4	z
1	-2	0	0	0	-1
2	-1	-1	-1	-1	1
3	-1	-1	-1	1	1
4	-1	-1	1	-1	1
5	-1	-1	1	1	1
6	-1	1	-1	-1	1
7	-1	1	-1	1	1
8	-1	1	1	-1	1
9	-1	1	1	1	1
10	0	-2	0	0	-1
11	0	0	-2	0	-1
12	0	0	0	-2	-1
13	0	0	0	0	1
14	0	0	0	2	-1
15	0	0	2	0	-1
16	0	2	0	0	-1
17	1	-1	-1	-1	1

18	1	-1	1	-1	1
19	1	-1	1	1	1
20	1	1	-1	-1	1
21	1	1	-1	1	1
22	1	1	1	-1	1
23	1	1	1	1	1
24	2	0	0	0	-1

The most of the designs for qualitative-cum-quantitative experiments obtained in this investigation are obtained through heuristic approach and are restricted to one qualitative factor only. Therefore, the problem of obtaining a general method of construction of response surface designs for qualitative-cum-quantitative experiments when the quantitative factors are with equispaced doses is still an open problem.

CHAPTER VI

EXTENSION OF RESEARCH FINDINGS

One of the significant features of the study is that three designs reported in the project were actually used by the experimenters in National Agricultural Research System. The applications are mainly in food processing experiments conducted for value addition to the agriculture produce. In these experiments, the major objective of the experimenter is to obtain the optimum combination of levels of several factors that are required for the product. The details of the experimental situations and the designs used are given in the sequel:

Experimental Situation 6.1: An experiment related to osmotic dehydration of the banana slices was planned to obtain the optimum combination of levels of concentration of sugar solution, solution to sample ratio and temperature of osmosis at Division of Agricultural Engineering, Indian Agricultural Research Institute, New Delhi. The factors and levels are as given below:

	Factors	Levels
1.	Concentration of sugar solution	40%, 50%, 60%, 70% and 80%
2.	Solution to sample ratio	1:1, 3:1, 5:1, 7:1 and 9:1
3.	Temperature of osmosis	25^0C, 35^0C, 45^0C, 55^0C and 65^0C

A modified second order rotatable response surface design for 3 factors each at 5 equispaced levels in 36 design points have been suggested. Layout of the design with levels coded as -2a, -a, 0, a ,2a and factors coded as A,B,C is as given below:

Design Point Number	A	B	C	Design Point Number	A	B	C
1	-a	-a	-a	19	0	-2a	0
2	-a	-a	a	20	0	2a	0
3	-a	a	-a	21	0	0	-2a
4	a	-a	-a	22	0	0	2a
5	-a	a	a	23	0	0	0
6	a	-a	a	24	0	0	0
7	a	a	-a	25	0	0	0
8	a	a	a	26	0	0	0
9	-a	-a	-a	27	0	0	0
10	-a	-a	a	28	0	0	0
11	-a	a	-a	29	0	0	0
12	a	-a	-a	30	0	0	0
13	-a	a	a	31	0	0	0
14	a	-a	a	32	0	0	0
15	a	a	-a	33	0	0	0
16	a	a	a	34	0	0	0
17	-2a	0	0	35	0	0	0
18	2a	0	0	36	0	0	0

The experiment was conducted using this design. The data obtained from this experiment was analyzed as per procedure of response surface methodology. Based on this experiment, following paper has been published:

- Abhijit Kar, Pitam Chandra and **Rajender Parsad** (2001). Osmotic dehydration of banana (*Dwarf Cavendish*) slices. *Journal of Agricultural Engineering*, **38(3),** 12-21.

Experimental Situation 6.2: This experiment is related to production of low fat meat products using fat replacers planned at Division of Bio-Technology, Indian Veterinary Research Institute, Izzatnagar. The experimenter was interested in obtaining the optimum combination of fat replacers. The details of fat replacers (factors) and levels are given below:

S.No.	Factor	Levels
1.	Whey protein	2%, 3%, 4%, 5% and 6%
2.	Guar Gum	0.50%, 0.75%, 1.00%, 1.25% and 1.50%.
3.	Starch	2.0%, 2.5%, 3.0%, 3.5% and 4.0%.

A second order rotatable response surface design for 3 factors each at 5 equi-spaced levels in 28 design points was recommended. The 28 design points were essentially the same as that of design points 1-28 in Experimental Situation 6.1.

Experimental Situation 6.3: A modified second order response surface design (Box-Behnken with 4 center points, the number of center points have been decided on the basis of the modified second order response surface designs introduced in the present investigation) for three factors each at three levels in 16 points was recommended for the experiment related to finding the optimum storability conditions of Instant Pigeon Pea Dal conducted at Division of Agricultural Engineering, Indian Agricultural Research Institute, New Delhi. The details of the factors and their levels are given as under.

S.No.	Factors	Levels
1.	Soaking Solution Concentration	0.5, 1.0, 1.5%
2.	Cooking Time	8, 10, 12 minutes
3.	Flaking Thickness	0.5, 0.75, 1.0 mm

The design points with coded levels as –1, 0, 1 are given as under:

X1	**X2**	**X3**	**X1**	**X2**	**X3**
1	1	0	0	1	1
1	-1	0	0	1	-1
-1	1	0	0	-1	1
-1	-1	0	0	-1	-1
1	0	1	0	0	0
1	0	-1	0	0	0
-1	0	1	0	0	0
-1	0	-1	0	0	0

SUMMARY

To deal with the evolution and methods of analysis for probing onto mechanism of system of variables, the experiments involving several factors simultaneously are being conducted in agricultural, horticultural and allied sciences. Data from experiments with levels or level combinations of one or more factors are generally investigated to compare level effects of factors along-with their interactions. Even though such investigations are useful to have objective assessment of the effects of the levels actually tried in the experiment, they fail to throw any light on the possible effects of the intervening levels especially when the factors are quantitative in nature. In such cases, therefore, it is realistic to carry out the investigations with the twin purposes viz. (i) to determine and quantify the relationship between the response and the settings of experimental factors and (ii) to find the settings of the experimental factor(s) that produce the best value or best set of values of the response (s). For the factors that are quantitative in nature, it is natural to think the response as a function of the factor levels. The data from the experiment involving quantitative factors can be utilized for fitting the response surfaces over the region of interest. Response surfaces besides inferring on these twin purposes can provide information on the rate of change of the response variable and can throw light on interactions between quantitative factors.

Response surface methodology has been extensively used in industrial experimentation but appear to be not so popular in research areas in agricultural and allied sciences. This is due to the fact that experimental situations in agricultural sciences are different from those in industry. Broadly, there are mainly five distinctions that are identified namely: (i) time and factor range (ii) factor levels (iii) blocking (iv) accuracy of observations' (v) shape of response surface.

Keeping in view the importance and relevance of response surface methodology in agriculture this study was undertaken. In this investigation, we have presented a comprehensive account of response surface methodology in Chapter II. The methodology includes fitting of both first and second order response surfaces with and without intercept, the procedure of performing canonical analysis of the second order response surface and the method of exploration of the response surface in the vicinity of the stationary point. The codes have been written using Statistical Analysis System (SAS) and Statistical Package for Social Sciences (SPSS) for fitting second order response surfaces both with and without intercept, perform canonical analysis and exploration of the response surface in the vicinity of stationary point. These codes are presented in Chapter II for the benefit of the users. A computer software "Response" has also been developed for fitting first and second order response surfaces both with and without intercept, performing the canonical analysis of the second order response surface and the exploration of the response surface in the vicinity of the stationary point. The response surface methodology is also illustrated with the help of examples.

Some series of response surface designs for both symmetric and asymmetric factorial experiments when the various factors are at equispaced levels that provide estimates of response at specific points with a reasonably high precision have been obtained in Chapter III. A new criterion in terms of second order moments and mixed fourth order moments is also introduced. This criterion helps in minimizing the variance of the estimated response to a

reasonable extent. The designs satisfying this property have been termed as modified second order response surface designs. Catalogues of the modified and/or rotatable second order response surface designs with number of factor (v) and number of design points (N) satisfying $3 \le v \le 10$ and $N \le 500$ have been developed and presented in Chapter III. The rotatable designs ensure that the variance of the predicted response remains constant at all points that are equidistant from the design center. However, it may not always be achievable for all the factors or if achievable may require a large number of runs. For such situations, a new series of group divisible rotatable designs has been introduced. The method of construction is based on group divisible designs. A catalogue of group divisible rotatable designs obtainable for 3 level factors and 5 level factors obtainable from group divisible designs has been prepared for $3 \le v \le 10$ and $N \le 500$.

Several experiments are being conducted where the experimenter is interested in the rate of change of response rather than the absolute response. If the difference in responses at points close together in the factor space is involved, then the estimation of local slope of the response surface is of interest. An attempt has also been made to obtain efficient designs for slope estimation for the situations in which various factors have equispaced doses. Further, in agricultural experiments, the use of elaborate blocking systems is essential to control environmental variability. Orthogonal blocking aspects of second order response surface designs have been investigated. A catalogue along with block contents of second order rotatable designs with orthogonal blocking for $3 \le v \le 8$ factors each at 3 or 5 equispaced doses has been prepared and presented in Chapter III. In some cases, the number of center points in a block are more than one, they can be used for estimation for pure error. Hence, appropriately identified blocks can be used for fitting of first order response surface and testing the lack of fit and rest of the blocks can be used for sequential build up of second order response surface design.

The above results have been obtained under very strict restrictions and ideal conditions. The ideal conditions may sometimes be disturbed due to missing observations. The robustness aspects of modified and/or rotatable second order response surface designs for response optimization obtainable through central composite designs and BIB designs have been investigated in Chapter IV with special emphasis on the designs when various factors are with equispaced doses. A new criterion of robustness viz. percent loss in information is introduced. Other criteria used in this investigation are information contained in an observation, D-efficiency and A-efficiency of the resulting design.

A large number of agricultural and food processing experiments are conducted that involve some qualitative factors along with the quantitative factors. The designs that are optimal for fitting first or second order response surfaces when all factors are quantitative in nature may not be so when some of the factors are qualitative and influence the response. The designing aspects of such experiments for response optimization have been discussed in Chapter V. Several procedures of obtaining designs for qualitative-cum-quantitative factors have been discussed. These procedures are essentially based on the designs for various factors with equispaced doses, asymmetric rotatable designs, cylindrically rotatable designs and second order response surface designs with orthogonal blocking. The procedures have been illustrated through examples.

One of the significant features of the study is that two designs obtained during the present investigation were used at the Division of Agricultural engineering, Indian Agricultural Research Institute, New Delhi. In one experiment modified and rotatable response surface design with 3 factor having 5 levels each in 36 design points was used. Another design used was modified second order response surface design with 3 factor each at 3 levels in 16 design points. At the Division of Bio-Technology, Indian Veterinary Research Institute, Izatnagar, second order rotatable design with 3 factors at 5 levels each in 28 design points was used. This clearly indicates that response surface methodology can be gainfully employed in agricultural and food processing experiments. We hope that the findings of this study will be of great help to both researcher and practicing statisticians.

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