OPTIMALITY CRITERIA FOR THIRD ORDER ROTATABLE DESIGNS CONSTRUCTED THROUGH BALANCED INCOMPLETE BLOCK DESIGN

BY

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DECLARATION

Declaration by Candidate

This thesis is my original work and has not been presented for a Degree in any other University.

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DEDICATION

I would like to dedicate this thesis to my family.

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ABSTRACT

In the design and analysis of experiments for estimating statistical models, optimal designs allow parameters to be estimated with minimum variance. These designs are generated based on a particular optimality criterion and are generally optimal only for a specific statistical model. The purpose of this study was to investigate the optimality criteria for third order rotatable designs (TORD) constructed from balanced incomplete block design (BIBD). Specifically, the study obtained alphabetic optimality criteria for specific TORD in three, four, five and six factors. A general method of evaluating alphabetic optimality for TORD constructed using BIBD in k-factors was determined. Further a compound optimality for D- and T- was evaluated for TORD constructed from BIBD. From the existing TORD constructed using BIBD, the design matrix, and moment matrix considering full parameter system were used. The existing methods were utilized to evaluate alphabetic optimality and DT-optimality for the designs from their information matrices. Evaluation of alphabetic optimality was done and D-, A-, T-, E-, I- and G- optimal designs were obtained. The study evaluated DT- compound optimality and determined DT- optimal design. A general method of evaluating alphabetic optimality for TORD constructed from BIBD in k-factors was also determined. In conclusion, the study showed that the designs' optimal values decreased with the increase in the number of factors for D-, G- and T- optimality. However, all the designs under investigation were found to be E-optimal. The values of DT-optimality increases as the number of factors increase implying that DT-compound optimality is appropriate for design with few factors. The study recommends the application of optimum designs in the design and analysis of field experiments

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LIST OF ABBREVIATIONS

A-	Average variance criterion
B.I.B.D	Balanced incomplete block design
D-	Determinant criterion
DOE	Design of experiments
E-	Eigenvalue criterion
RSM	Response Surface Methodology
T-	Trace criterion
TORD	Third order rotatable design
X	Design Matrix
X'	Transpose of a matrix X

CHAPTER ONE

INTRODUCTION

1.1 Background Information

Response surface methodology (RSM) is a collection of statistical and mathematical techniques used to develop, improve and optimize processes. Despite the arguments put forward by Mead and Pike (1975), there seems to be a general agreement that the concept of response surfaces and designs for their exploration began in the chemical industry.

Classical experimental designs are concerned with comparative experiments, that is, experiments in which the primary objective is to compare the effects of various treatments and, especially, to estimate treatment contrasts. An exception is the more recently developed field of response surface designs in which treatments are various combinations of different levels of the factors that are quantitative. Here the main objective of the experimenter is usually to estimate the absolute response or the parameters of a model providing the relationship between the response and the factors. In this context, rotatable designs were introduced by Box and Hunter (1957) in order to explore the response surface. Rotatable designs have the nice property that the variance of the estimated response is constant at points equidistant from the Centre of the design, conventionally taken to be the origin of the factor space. Rotatable designs generate information about the response surface equally in all directions and are therefore useful when no or little prior knowledge is available about the nature of the response surface. In the design of experiments, optimal designs are a class of experimental designs that are optimal with respect to some statistical criterion. In practical terms, optimal experiments can reduce the costs of experimentation. The optimality of a design depends on the statistical model and is assessed with respect to a statistical criterion, which is related to the variance matrix of the estimator. Specifying an appropriate model and specifying a suitable criterion function both require an understanding of statistical theory and practical knowledge with designing experiments. Designed experiments allow the analyst to control the factors thought to be important in characterizing or explaining the response variable(s) of the experiment. In the recent years there has been dramatic growth in the use of designed experiments, not just in the classical industrial, life sciences, and agricultural settings, but in many areas of business, such as marketing and financial services. This interest in the design of experiments has led to much new research on the subject. There are many types of experimental designs in the literature, and there are also many criteria on which experimental designs are based. It is critical for an experimenter to understand the characteristics and features that should be taken into account when a design is chosen.

1.2 Basic Concepts

1.2.1 Rotatability

The concept of rotatability as a desirable quality of an experimental design was first put forward by Box and Hunter in 1957. This property is that the variances of estimates of the response made from the least squares estimates of the Taylors series are constant on circles, spheres or hyper-spheres about the center of the design. Thus, a rotatable design, that is, a design which satisfies this property, could be rotated through any angle around its center and the variances of responses estimated from it would be unchanged.

1.2.2 Balanced incomplete block design

According to Das and Giri (1986), the precision of the estimate of a treatment effect depends on the number of replications of the experiment. That is, the larger the number of replications, the more is the precision. If in a block the number of units or plots is smaller than the number of treatments, then the block is said to be incomplete and a design constituted of such blocks is called an incomplete block design.

Different patterns of values of the numbers of replicates of different pairs of treatments in a design, have given rise to different types of incomplete block designs. When the number of replications of all pairs of treatments in a design is the same, then an important series of designs known as balanced incomplete block design is obtained. This series of designs ensures equal precisions of the estimates of all pairs of treatments effects and it was first devised for agricultural experiments.

According to Kempthorne and Hinkelmann (2005), an incomplete block design is said to be a balanced incomplete block (BIB) design if it satisfies the following conditions:

(i) The experimental material is divided into b blocks of s units each, different treatments being applied to the units in the same block.

(ii) There are v treatments each of which occurs in r blocks.

(iii) Any two treatments occur together in exactly λ blocks.

The quantities v, b, r, s and λ are called the parameters of BIB design.

The following relations hold among the parameters and even these are only necessary conditions for the existence of a BIB design:

(i) $rv=sb$

(ii) $\lambda(v-1)=r(s-1)$

(iii) $r > \lambda$

(iv) $b \geq v$

Also according to Calvin (1954) a doubly balanced incomplete block (DBIB) design is an incomplete block design in which each triple of treatments occurs together the same number of times in a block.

1.2.3 Sequential designs and non-sequential designs

Third order rotatable designs can be grouped into sequential and non-sequential designs. Sequential designs are performed in parts or blocks while non-sequential experimentation all the runs must be run at one time to make a rotatable least square fitting possible. Draper, (1960) stated that sequential experiments are more useful in practice and are economical. Therefore third order rotatable designs may be run sequentially in three stages with three or four blocks depending on the model adequacy. Normally, the first part consisting of first order is run and the response function is approximated using a first order model. If the first order model is found to be adequate, as the representation of the unknown function by noting evidence of the goodness of fit, the experiment may be terminated at this stage. However, if the first model is found to be inadequate, the trials of second order are run and ultimately, proceed to fit a third order if a second order model is also found to be inadequate. The first block may contain the k+1 runs, second block containing the second order runs and third block containing third order runs.

1.2.4 Optimal design

In the designs of experiments, optimal designs are a class of experimental designs that are optimal with respect to some statistical criterion. In the design of experiments for estimating statistical models, optimal designs allow the parameters to be estimated without bias and with minimum variance. A non-optimal design requires a greater number of experimental runs to estimate the parameters with the same precision as an optimal design. The optimality of a design depends on statistical model and is assessed with respect to statistical criterion, which is related to variance-matrix of the estimator. Some of the advantages of optimal designs include; reducing the cost of experimentation by allowing models to be estimated with fewer experimental runs and optimal designs can accommodate multiple types of factors.

1.3 Statement of the Problem

Second order rotatable designs have been studied extensively where construction and evaluation of their optimality criteria have been done. A second-order polynomial can be used as a local approximation of the response in a small region where, hopefully, optimal operating conditions exist. It is appropriate in most of the cases applicable in industry, though there are instances when quadratic fit is not sufficiently flexible to explain a given response. In such cases, the experimenter needs a third order model that involves cubic effects. Construction of the TORD has also been considered widely, however, little has been done on evaluation of optimality This study therefore considered the existing third order designs constructed through BIBDs to evaluate their alphabetic optimality criteria.

1.4 Objectives of the Study

1.4.1 General objective

To obtain optimality criteria for third order rotatable designs constructed through balanced incomplete block design.

1.4.2 Specific objectives

1. To obtain alphabetic optimality for specific third order rotatable designs constructed through balanced incomplete block design.
2. To determine a general method of obtaining alphabetic optimality for third order rotatable designs constructed through balanced incomplete block design.
3. To evaluate DT- compound optimality criterion for third order rotatable designs constructed through balanced incomplete block design.

1.5 Significance of the Study

There is need to obtain third order optimal designs in order to deal with inadequacy suffered by second order designs. This study focused on obtaining optimal third order rotatable designs constructed through BIBDs. Optimal designs obtained will allow parameters to be estimated with minimum variance. This study also allows the researcher to determine the alphabetic optimality criteria for TORD constructed from BIBD at any level of factors.

CHAPTER TWO

LITERATURE REVIEW

2.1 Introduction

Several third order designs have been constructed from the concept of rotatability. Das and Narasimham (1962) constructed many third order rotatable designs by taking appropriate combinations of the symmetric point set or the suitably balanced subset obtained through balanced incomplete block designs and fractional replication. Petersen (1993), Box and Draper (1963) employed this aspect to construct the designs for 2^{nd} and 3^{rd} order response models. Similarly, Koske (1984) constructed 4^{th} order rotatable designs by utilizing the same aspect. Mutiso (1998) developed theory for the optimum estimation of the free parameters in the rotatable design point sets first considered by Draper (1960) for which Kosgei (2002) obtained alphabetic optimality criteria. Victorbabu (2006) suggested new methods of construction of three and five-level modified second order rotatable designs (SORD) and modified second order slope rotatable designs (SOSRD) using suitably chosen balanced incomplete block designs. Victorbabu (2009) examined in detail different methods of construction of modified second order response surface designs, modified second order rotatable designs (SORD), modified SORD with equispaced doses (levels) using central composite designs, balanced incomplete block designs (BIBD), pairwise balanced designs (PBD) and symmetrical unequal block arrangements (SUBA) with two unequal block sizes. Victorbabu (2011) studied a new method of construction of second order slope rotatable design using balanced incomplete block designs. Some new four dimensional third order rotatable designs through balanced incomplete block design were constructed by Mutai et al (2012).

2.2 Alphabetic Optimality Criteria

Under design of experiments for estimating statistical models, optimal designs allow parameter to be estimated without bias and with minimum variance. A non-optimal design requires a greater number of experimental runs to estimate the parameter with the same precision as an optimal design. The optimality of a design depends on statistical model and is assessed with respect to a statistical criterion, which is related to the variance matrix of the estimator.

Kiefer (1960) stated that the class of rotatable designs is very rich in the sense that under many commonly used criteria, such as D-optimality, the optimal designs for polynomial regression models over hyper spherical regions may be found within this class. It has been recognized in recent years, that even in response surface designs the main interest of the experimenter may not always be in the response at individual locations. Sometimes, the differences between responses at various locations may be of greater interest (Herzberg, 1967).

G–optimality criterion is "a prediction criterion" introduced by Smith (1918). She gave a paper, which states a criterion, and obtains optimal designs for regression problems. D–optimality is the most important and popular design criterion in the life applications, which was introduced by Wald (1943), it emphasis on the quality of the parameter estimates. D-optimality criterion is also known as the determinant criterion. The aim of D-optimality is essentially a parameter estimation criterion.

A–optimality criterion introduced by Chernoff (1953), showed the employed criterion of optimality which is the one that involves the use of Fisher's information matrix.

E–optimality was introduced by Ehrenfeld (1955). The aim of E-optimality is to minimize the maximum variance of all possible normalized linear combinations of parameter estimates.

I–optimality criterion "integrated variance" which is also known as Q–optimality criterion was introduced by Fedorov (1972). Q–optimality is also called V or Iv–optimality and it minimizes the normalized average or integrated prediction variance.

Kiefer (1975) introduced convex optimality function $\emptyset$ on the information matrices and proved that balanced incomplete block designs (BIBD) are universally optimal. Mukerjee and Huda (1985) also contributed towards optimality design of experiments for estimating slopes.

According to Pukelsheim (2006), real optimality criteria are functions with such properties as are appropriate to measure largeness of information matrices. These functions have properties that include positively homogenous, super additive, non-negative, non-constant and upper semi continuous. Such criteria are called information functions. Morgan (2007) has been working on design optimality for various classes of designs with blocking. When restricting the response surface problem to response optimization, we want to select a design that will provide a good fitting model to the data, and, in particular, provide reliable parameter estimates, which then can be used for precise predictions. Huda (2007) did a study on A- and D- rotatability of two dimensional third order designs. He obtained the expression for variance-covariance matrix of the estimated axial slopes at a point in the factor space for a symmetric balanced two dimensional third order design. Huda went ahead to derive the trace and the determinant of the matrix to show that symmetry and balance are not sufficient for either A-rotatability or D-rotatability of the design.

Keny (2014) constructed optimal second order rotatable designs using balanced incomplete block designs (BIBD). She went ahead to examine optimality criteria, optimal weights and optimal values of parameter estimates for second order rotatable designs. This study focused on obtaining alphabetic optimality criteria for existing third order rotatable designs constructed from balanced incomplete block design.

2.3 Compound Optimality

There are many statistical aspects to consider in the design of an empirical study. The problems include the control of unwanted variation and the internal validity of the study. This is among the questions raised by (Cox, 1958 and Cox and Reid, 2000). In the context of nested regression models which differ by only one parameter, Dette (1993) proposed to use the D1-criterion for model discrimination and the D-criterion for precise estimation of the parameters. The resulting compound criterion (a weighted geometric mean of D1- and D-efficiencies) is called DD1-criterion. Atkinson (2008) introduced DT–optimality which is a combination of D–optimality and T–optimality for discriminating between models. It provides a specified balance between model discrimination and parameter estimation. Tommasi (2009) proposed the DKL-optimality criterion, which is a compound criterion given by the weighted geometric mean of KL- and D-efficiencies considering the D-criterion as a measure of precision in parameter estimation. As a measure of discrimination, however, she has used the KL-criterion which is useful for model discrimination in a more general context than nested regression models with Gaussian homoscedastic errors. The main advantage of the DKL-optimality criterion over the other compound criteria is its general applicability. The DKL-optimality criterion can be used for any kind of regression models, nested or not, with homoscedastic or heteroscedastic errors, which may be Gaussian or not. The purpose of the experiment is to find the model and its adequacy. To address the issue of model discrimination and to provide specified balance between model discrimination and parameter estimation, the study resolved to obtain compound DT- optimality criteria for third order rotatable designs constructed through BIBD.

CHAPTER THREE

METHODOLOGY

3.1 Introduction

This chapter outlines the methods used in calculating optimality criteria. The third order rotatable designs constructed through BIBD by Mutai (2012) are extended to determine optimality. The moment matrices derived from the specific TORD were used to determine alphabetic optimality. Matrix laboratory (MATLAB) was used in manipulation of matrices.

3.1.1: Third order moment condition

These are conditions that must be satisfied by a set of points to form a third order rotatable arrangement. They are as follows in (3.1.1)

$$\sum_{u=1}^{N} x^2{}_{iu} = A \quad \text{(i=1,2,…k)}$$

$$\sum_{u=1}^{N} x^4{}_{iu} = 3\sum_{u=1}^{N} x^2{}_{iu} x^2{}_{ju} = 3B$$

(3.1.1)

$$\sum_{u=1}^{N} x^6{}_{iu} = 5\sum_{u=1}^{N} x^2{}_{iu} x^4{}_{ju} = 15\sum_{u=1}^{N} x^2{}_{iu} x^2{}_{ju} x^2{}_{lu} = 15C \qquad \begin{array}{l} i \neq j \neq l = 1,2,...,k \\ u = 0,1,...,N \end{array}$$

and all other sums of powers and products up to order six are zero, where $A = N\lambda_2$, $B = N\lambda_4$, and $C = N\lambda_6$

3.1.2: Non–singularity conditions

Let X be an $(N \times L)$ matrix defined as follows

$$X = \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \\ . \\ . \\ . \\ \underline{x}_N \end{bmatrix}$$

$L = \dfrac{(k+3)!}{k!3!}$, is the number of terms in the model

If X' is the transpose of X then $N^{-1}(X'X)$ is the moment matrix of the arrangement of N points in K-dimensional factor space.

Gardiner et al, (1959) derived the following non-singularity conditions of the moment matrix.

$$\frac{\lambda_4}{\lambda_2^2} > \frac{K}{K+2}$$

$$\frac{\lambda_6 \lambda_2}{\lambda_4^2} > \frac{K+2}{K+4} \qquad (3.1.2)$$

These are conditions required for a third order arrangement of points to form a TORD.

3.2 Alphabetic Optimality criteria for TORD constructed through BIBD

The study utilized the moment matrices in three, four, five and six factors to obtain alphabetic optimality criteria for specific third order rotatable designs constructed through BIBD.

3.2.1 The moment matrix of TORD constructed through BIBD in three factors

From an existing $BIBD(v=3, b=3, r=2, s=2, \lambda=1, \mu=0)$ a third order rotatable design in three dimensions with 60 points was obtained as;

$$D_1 = S(a \;\; a \;\; 0) + S(b \;\; b \;\; b) + S\left(\frac{\rho}{\sqrt{2}} \;\; \frac{\rho}{\sqrt{2}} \;\; 0\right) + 2S(d \;\; d \;\; d) + 2S(\rho \;\; 0 \;\; 0)$$

where $a^2 = 0.421716\rho^2$, $b^2 = 0.367743686\rho^2$, $d^2 = 0.064475339\rho^2$ and $\rho = 1$

The third order model in three factors is given by

$$\begin{aligned} y(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{22} x_2^2 + \beta_{23} x_2 x_3 \\ + \beta_{33} x_3^2 + \beta_{111} x_1^3 + \beta_{112} x_1^2 x_2 + \beta_{113} x_1^2 x_3 + \beta_{122} x_2^2 x_1 + \beta_{123} x_1 x_2 x_3 \\ + \beta_{133} x_3^2 x_1 + \beta_{222} x_2^3 + \beta_{223} x_2^2 x_3 + \beta_{233} x_3^2 x_2 + \beta_{333} x_3^3 \end{aligned}$$

The third order model with three factors has 20 terms and

$X' = [1, x_1^2, \dots, x_3^2, x_1 x_2, \dots, x_1 x_2 x_3, x_1, x_1^3, x_1 x_2^2, x_1 x_3^2, \dots, x_3^3, x_3 x_1^2, x_3 x_2^2]$

Thus, the moment matrix, $M = N^{-1}(X'X)$, of a TORD in three factors is as follows;

$$M_{3(20\times 20)} = \begin{bmatrix} G & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_4 I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_6 I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & K_{31} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & K_{32} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & K_{33} \end{bmatrix} \quad (3.2.1)$$

The sub-matrices of M_3 are as follows

$$\boldsymbol{G}_{(4\times 4)} = \begin{bmatrix} 1 & 0.2558 & 0.2558 & 0.2558 \\ 0.2558 & 0.1428 & 0.0476 & 0.0476 \\ 0.2558 & 0.0476 & 0.1428 & 0.0476 \\ 0.2558 & 0.0476 & 0.0476 & 0.1428 \end{bmatrix}$$

$$\lambda_4 I_{(\mathbf{3}\times\mathbf{3})} = \begin{bmatrix} 0.0476 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.0476 \end{bmatrix}$$

$$\lambda_6 I_{(\mathbf{1}\times\mathbf{1})} = [0.0067]$$

$$K_{31(\mathbf{4}\times\mathbf{4})} = K_{32(\mathbf{4}\times\mathbf{4})} = K_{33(\mathbf{4}\times\mathbf{4})} = \begin{bmatrix} 0.2558 & 0.1429 & 0.0476 & 0.0476 \\ 0.1429 & 0.1005 & 0.0201 & 0.0201 \\ 0.0476 & 0.0201 & 0.0201 & 0.0067 \\ 0.0476 & 0.0201 & 0.0067 & 0.0201 \end{bmatrix}$$

The moment matrix $(M_3)(3.2.1)$ was utilized in determining the alphabetic optimality criteria for TORD constructed through BIBD for three factors.

3.2.2 The moment matrix of TORD constructed through BIBD in four factors

From an existing $BIBD(v = 4, b = 6, r = 3, s = 2, \lambda = 1, \mu = 0)$ a third order rotatable design in four dimensions with 120 points was obtained as;

$$D_2 = S(a\ \ a\ \ 0\ \ 0) + S(b\ \ b\ \ b\ \ b) + S\left(\frac{\rho}{\sqrt{2}}\ \ \frac{\rho}{\sqrt{2}}\ \ 0\ 0\right) + 2S(d\ \ d\ \ d\ \ d) + 3S(\rho\ \ 0\ \ 0\ \ 0)$$

where $a^2 = 0.629960524\,\rho^2$, $b^2 = 0.359780535\rho^2$, $d^2 = 0.067259838\rho^2$ and $\rho = 1$

The third order model in four factors is given by

$$\begin{aligned} y = \beta_0 &+ \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{14} x_1 x_4 \\ &+ \beta_{22} x_2^2 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 + \beta_{33} x_3^2 + \beta_{34} x_3 x_4 + \beta_{44} x_4^2 + \beta_{111} x_1^3 \\ &+ \beta_{112} x_1^2 x_2 + \beta_{113} x_1^2 x_3 + \beta_{114} x_1^2 x_4 + \beta_{122} x_2^2 x_1 + \beta_{123} x_1 x_2 x_3 \\ &+ \beta_{124} x_1 x_2 x_4 + \beta_{133} x_3^2 x_1 + \beta_{134} x_1 x_3 x_4 + \beta_{144} x_4^2 x_1 + \beta_{222} x_2^3 \\ &+ \beta_{223} x_2^2 x_3 + \beta_{224} x_2^2 x_4 + \beta_{233} x_3^2 x_2 + \beta_{234} x_2 x_3 x_4 + \beta_{244} x_4^2 x_2 \\ &+ \beta_{333} x_3^3 + \beta_{334} x_3^2 x_4 + \beta_{344} x_4^2 x_3 + \beta_{444} x_4^3 \end{aligned}$$

Where the terms are 35 in the model and

$X' =$

$[1, x_1^2, \ldots, x_4^2, x_1x_2, \ldots, x_3x_4, x_1x_2x_3, \ldots, x_2x_3x_4, x_1, x_1^3, x_1x_2^2, \ldots, x_1x_4^2, \ldots, x_4, x_4^3, x_4x_1^2, \ldots, x_4x_3^2]$

Thus, the moment matrix, $M = N^{-1}(X'X)$, of a TORD in four factors is as follows;

$$M_{4(35\times35)}=\begin{bmatrix} G & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_4 I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_6 I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & K_{41} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & K_{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & K_{43} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_{44} \end{bmatrix}$$

(3.2.2)

The sub-matrices of M_4 are;

$$G_{(5\times5)}=\begin{bmatrix} 1.0000 & 0.2289 & 0.2289 & 0.2289 & 0.2289 \\ 0.2289 & 0.1332 & 0.0444 & 0.0444 & 0.0444 \\ 0.2289 & 0.0444 & 0.1332 & 0.0444 & 0.0444 \\ 0.2289 & 0.0444 & 0.0444 & 0.1332 & 0.0444 \\ 0.2289 & 0.0444 & 0.0444 & 0.0444 & 0.1332 \end{bmatrix}$$

$$\lambda_4 I_{(6\times6)} = \begin{bmatrix} 0.0444 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.0444 \end{bmatrix}$$

$$\lambda_6 I_{(4\times4)} = \begin{bmatrix} 0.0063 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.0063 \end{bmatrix}$$

$$K_{41} = K_{42} = K_{43} = K_{44}=\begin{bmatrix} 0.2289 & 0.1332 & 0.0444 & 0.0444 & 0.0444 \\ 0.1332 & 0.0945 & 0.0189 & 0.0189 & 0.0189 \\ 0.0444 & 0.0189 & 0.0189 & 0.0063 & 0.0063 \\ 0.0444 & 0.0189 & 0.0063 & 0.0189 & 0.0063 \\ 0.0444 & 0.0189 & 0.0063 & 0.0063 & 0.0189 \end{bmatrix}$$

The moment matrix (M_4)(3.2.2) was utilized in determining the alphabetic optimality criteria for TORD constructed through BIBD for four factors.

3.2.3 The moment matrix of TORD constructed through BIBD in five factors

From an existing $BIBD(v=5, b=10, r=4, s=2, \lambda=1, \mu=0)$ a third order rotatable design in five dimensions with 248 points was obtained as;

$$D_3 = S(a \;\; a \;\; 0\;0\;0) + S(b \;\; b \;\; b \;\; b\; b) + S\left(\frac{\rho}{\sqrt{2}} \;\; \frac{\rho}{\sqrt{2}} \;\; 0\;0\;0\right) +$$

$$3S(d \;\; d \;\; d \;\; d\; d) + 4S(\rho \;\; 0 \;\; 0 \;\; 0\; 0)$$

where $a^2 = 0.536893346\,\rho^2$, $b^2 = 0.\,.285053845\,\rho^2$, $d^2 = 0.183393832\,\rho^2$ and $\rho = 1$

The third order model in five factors is given by

$$\begin{aligned} y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 \\ + \beta_{14} x_1 x_4 + \beta_{15} x_1 x_5 + \beta_{22} x_2^2 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 + \beta_{25} x_2 x_5 \\ + \beta_{33} x_3^2 + \beta_{34} x_3 x_4 + \beta_{35} x_3 x_5 + \beta_{44} x_4^2 + \beta_{45} x_4 x_5 + \beta_{55} x_5^2 + \beta_{111} x_1^3 \\ + \beta_{112} x_1^2 x_2 + \beta_{113} x_1^2 x_3 + \beta_{114} x_1^2 x_4 + \beta_{115} x_1^2 x_5 + \beta_{122} x_2^2 x_1 \\ + \beta_{123} x_1 x_2 x_3 + \beta_{124} x_1 x_2 x_4 + \beta_{125} x_1 x_2 x_5 + \beta_{133} x_3^2 x_1 + \beta_{134} x_1 x_3 x_4 \\ + \beta_{135} x_1 x_3 x_5 + \beta_{144} x_4^2 x_1 + \beta_{145} x_1 x_4 x_5 + \beta_{155} x_5^2 x_1 + \beta_{222} x_2^3 \\ + \beta_{223} x_2^2 x_3 + \beta_{224} x_2^2 x_4 + \beta_{225} x_2^2 x_5 + \beta_{233} x_3^2 x_2 + \beta_{234} x_2 x_3 x_4 \\ + \beta_{235} x_2 x_3 x_5 + \beta_{244} x_4^2 x_2 + \beta_{245} x_2 x_4 x_5 + \beta_{255} x_5^2 x_2 + \beta_{333} x_3^3 \\ + \beta_{334} x_3^2 x_4 + \beta_{335} x_3^2 x_5 + \beta_{344} x_4^2 x_3 + \beta_{345} x_3 x_4 x_5 + \beta_{355} x_5^2 x_3 \\ + \beta_{444} x_4^3 + \beta_{445} x_4^2 x_5 + \beta_{455} x_5^2 x_4 + \beta_{555} x_5^3 \end{aligned}$$

The third order model with five factors has 56 terms and

$X' =$

$$\left[1, x_1^2, \dots, x_5^2, x_1x_2, \dots, x_4x_5, x_1x_2x_3, \dots, x_3x_4x_5, x_1, x_1^3, x_1x_2^2, \dots, x_1x_5^2, \dots, x_5, x_5^3, x_5x_1^2, \dots, x_5x_4^2\right]$$

Thus, the moment matrix, $M = N^{-1}(X'X)$, of a TORD in five factors is as follows;

$$M_{5(56*56)}=\begin{bmatrix} G & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_4 I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_6 I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & K_{51} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & K_{52} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & K_{53} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_{54} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_{55} \end{bmatrix} \tag{3.2.3}$$

The sub-matrices of M_5 are;

$$G_{(6\times6)}=\begin{bmatrix} 1.0000 & 0.2249 & 0.2249 & 0.2249 & 0.2249 & 0.2249 \\ 0.2249 & 0.1146 & 0.0382 & 0.0382 & 0.0382 & 0.0382 \\ 0.2249 & 0.0382 & 0.1146 & 0.0382 & 0.0382 & 0.0382 \\ 0.2249 & 0.0382 & 0.0382 & 0.1146 & 0.0382 & 0.0382 \\ 0.2249 & 0.0382 & 0.0382 & 0.0382 & 0.1146 & 0.0382 \\ 0.2289 & 0.0382 & 0.0382 & 0.0382 & 0.0382 & 0.1146 \end{bmatrix}$$

$$\lambda_4 I_{(10\times10)} = \begin{bmatrix} 0.0382 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.0382 \end{bmatrix}$$

$$\lambda_6 I_{(10\times10)} = \begin{bmatrix} 0.0054 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.0054 \end{bmatrix}$$

$$K_{51} = K_{52} = K_{53} = K_{54} = K_{55}=\begin{bmatrix} 0.2249 & 0.1146 & 0.0382 & 0.0382 & 0.0382 & 0.0382 \\ 0.1146 & 0.0806 & 0.0162 & 0.0162 & 0.0162 & 0.0162 \\ 0.0382 & 0.0162 & 0.0162 & 0.0054 & 0.0054 & 0.0054 \\ 0.0382 & 0.0162 & 0.0054 & 0.0162 & 0.0054 & 0.0054 \\ 0.0382 & 0.0162 & 0.0054 & 0.0054 & 0.0162 & 0.0054 \\ 0.0382 & 0.0162 & 0.0054 & 0.0054 & 0.0054 & 0.0162 \end{bmatrix}$$

The moment matrix $(M_5)(3.2.3)$ was utilized in determining the alphabetic optimality criteria for TORD constructed through BIBD for five factors.

3.2.4 The moment matrix of TORD constructed through BIBD in six factors

From an existing $BIBD(v=6, b=15, r=5, s=2, \lambda=1, \mu=0)$ a third order rotatable design in six dimensions with 372 points was obtained as;

$D_4 = S(a\ a\ 0\ 0\ 0\ 0) + S(b\ b\ b\ b\ b\ b) + S(\frac{\rho}{\sqrt{2}}\ \frac{\rho}{\sqrt{2}}\ 0\ 0\ 0\ 0) + 2S(d\ d\ d\ d\ d\ d) + 5S(\rho\ 0\ 0\ 0\ 0\ 0)$

where $a^2 = 1.040041912\rho^2$, $b^2 = 0.283229057\rho^2$, $d^2 = 0.201415924\rho^2$ and $\rho = 1$

The third order model in six factors is given by

$$
\begin{aligned}
y = \beta_0 &+ \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 \\
&+ \beta_{14} x_1 x_4 + \beta_{15} x_1 x_5 + \beta_{16} x_1 x_6 + \beta_{22} x_2^2 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 \\
&+ \beta_{25} x_2 x_5 + \beta_{26} x_2 x_6 + \beta_{33} x_3^2 + \beta_{34} x_3 x_4 + \beta_{35} x_3 x_5 + \beta_{36} x_3 x_6 \\
&+ \beta_{44} x_4^2 + \beta_{45} x_4 x_5 + \beta_{46} x_4 x_6 + \beta_{55} x_5^2 + \beta_{56} x_5 x_6 + \beta_{66} x_6^2 + \beta_{111} x_1^3 \\
&+ \beta_{112} x_1^2 x_2 + \beta_{113} x_1^2 x_3 + \beta_{114} x_1^2 x_4 + \beta_{115} x_1^2 x_5 + \beta_{116} x_1^2 x_6 \\
&+ \beta_{122} x_2^2 x_1 + \beta_{123} x_1 x_2 x_3 + \beta_{124} x_1 x_2 x_4 + \beta_{125} x_1 x_2 x_5 + \beta_{126} x_1 x_2 x_6 \\
&+ \beta_{133} x_3^2 x_1 + \beta_{134} x_1 x_3 x_4 + \beta_{135} x_1 x_3 x_5 + \beta_{136} x_1 x_3 x_6 + \beta_{144} x_4^2 x_1 \\
&+ \beta_{145} x_1 x_4 x_5 + \beta_{146} x_1 x_4 x_6 + \beta_{155} x_5^2 x_1 + \beta_{156} x_1 x_5 x_6 + \beta_{166} x_6^2 x_1 \\
&+ \beta_{222} x_2^3 + \beta_{223} x_2^2 x_3 + \beta_{224} x_2^2 x_4 + \beta_{225} x_2^2 x_5 + \beta_{226} x_2^2 x_6 \\
&+ \beta_{233} x_3^2 x_2 + \beta_{234} x_2 x_3 x_4 + \beta_{235} x_2 x_3 x_5 + \beta_{236} x_2 x_3 x_6 + \beta_{244} x_4^2 x_2 \\
&+ \beta_{245} x_2 x_4 x_5 + \beta_{246} x_2 x_4 x_6 + \beta_{255} x_5^2 x_2 + \beta_{256} x_2 x_5 x_6 + \beta_{266} x_6^2 x_2 \\
&+ \beta_{333} x_3^3 + \beta_{334} x_3^2 x_4 + \beta_{335} x_3^2 x_5 + \beta_{336} x_3^2 x_6 + \beta_{344} x_4^2 x_3 \\
&+ \beta_{345} x_3 x_4 x_5 + \beta_{346} x_3 x_4 x_6 + \beta_{355} x_5^2 x_3 + \beta_{356} x_3 x_5 x_6 + \beta_{366} x_6^2 x_3 \\
&+ \beta_{444} x_4^3 + \beta_{445} x_4^2 x_5 + \beta_{446} x_4^2 x_6 + \beta_{455} x_5^2 x_4 + \beta_{456} x_4 x_5 x_6 \\
&+ \beta_{466} x_6^2 x_4 + \beta_{555} x_5^3 + \beta_{556} x_5^2 x_6 + \beta_{566} x_6^2 x_5 + \beta_{666} x_6^3
\end{aligned}
$$

Where the number of terms in the model is 84 and

$X' =$

$[1, x_1^2, \dots, x_6^2, x_1 x_2, \dots, x_5 x_6, x_1 x_2 x_3, \dots, x_4 x_5 x_6, x_1, x_1^3, x_1 x_2^2, \dots, x_1 x_6^2, \dots, x_6, x_6^3, x_6 x_1^2, \dots, x_6 x_5^2]$

Thus, the moment matrix, $M = N^{-1}(X'X)$, of a TORD in six factors is as follows;

$$M_{6(84\times84)}=\begin{bmatrix} G & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_4 I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_6 I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & K_{61} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & K_{62} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & K_{63} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_{64} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_{65} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_{66} \end{bmatrix} \qquad (3.2.4)$$

The sub-matrices of M_6 are;

$$G_{(7\times7)}=\begin{bmatrix} 1.0000 & 0.2277 & 0.2277 & 0.2277 & 0.2277 & 0.2277 & 0.2277 \\ 0.2277 & 0.1263 & 0.0421 & 0.0421 & 0.0421 & 0.0421 & 0.0421 \\ 0.2277 & 0.0421 & 0.1263 & 0.0421 & 0.0421 & 0.0421 & 0.0421 \\ 0.2277 & 0.0421 & 0.0421 & 0.1263 & 0.0421 & 0.0421 & 0.0421 \\ 0.2277 & 0.0421 & 0.0421 & 0.0421 & 0.1263 & 0.0421 & 0.0421 \\ 0.2277 & 0.0421 & 0.0421 & 0.0421 & 0.0421 & 0.1263 & 0.0421 \\ 0.2277 & 0.0421 & 0.0421 & 0.0421 & 0.0421 & 0.0421 & 0.1263 \end{bmatrix}$$

$$\lambda_4 I_{\ (15\times15)} = \begin{bmatrix} 0.0421 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.0421 \end{bmatrix}$$

$$\lambda_6 I_{\ (20\times20)} = \begin{bmatrix} 0.0067 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.0067 \end{bmatrix}$$

$K_{61} = K_{62} = K_{63} = K_{64} = K_{65} =$

$$K_{66}=\begin{bmatrix} 0.2277 & 0.1263 & 0.0421 & 0.0421 & 0.0421 & 0.0421 & 0.0421 \\ 0.1263 & 0.1005 & 0.0201 & 0.0201 & 0.0201 & 0.0201 & 0.0201 \\ 0.0421 & 0.0201 & 0.0201 & 0.0067 & 0.0067 & 0.0067 & 0.0067 \\ 0.0421 & 0.0201 & 0.0067 & 0.0201 & 0.0067 & 0.0067 & 0.0067 \\ 0.0421 & 0.0201 & 0.0067 & 0.0067 & 0.0201 & 0.0067 & 0.0067 \\ 0.0421 & 0.0201 & 0.0067 & 0.0067 & 0.0067 & 0.0201 & 0.0067 \\ 0.0421 & 0.0201 & 0.0067 & 0.0067 & 0.0067 & 0.0067 & 0.0201 \end{bmatrix}$$

The moment matrix $(M_6)(3.2.4)$ was utilized in determining the alphabetic optimality criteria for TORD constructed through BIBD for six factors.

The alphabetic optimality criteria that were evaluated by this study are the Determinant criterion D-, the Average variance criterion A-, the Eigenvalue criterion, the E- , the trace, T-criterion, I-optimality criteria and G-optimality criteria. These are the methods proposed by Pukelshiem (2006). These alphabetic optimality criteria are variance related criteria. In obtaining the D-, A-, T- and E- , M is the moment matrix given by $M = N^{-1}(X'X)$ and S is the number of parameters of interest.

3.2.5 Determinant (D-criterion)

To determine D-optimality for the designs considered, the determinant criterion was evaluated as follows;

$$\phi_0(\mathrm{M}) = [\det(M)]^{1/s} \tag{3.2.5}$$

The determinant criterion $\emptyset(C)$ differs from the determinant det(C) by taking the s$^{\text{th}}$ root.

3.2.6 Average variance (A-criterion)

The average variance criterion $\phi_{-1}(\mathrm{M})$ is determined as;

$$\phi_{-1}(\mathrm{M}) = \left(\frac{1}{s} traceM^{-1}\right)^{-1} \text{ if C is positive definite} \tag{3.2.6}$$

This is the average of the standardized variances of the optimal estimators for the scalar parameter systems $c_1\theta, \ldots, c_s\theta$ formed from the columns of K.

3.2.7 The smallest eigenvalue (E- criterion)

The smallest eigenvalue criterion was obtained as follows

$$\phi_{-\infty}(\mathrm{M}) = \lambda_{(\min)}(M) \tag{3.2.7}$$

This criterion involves the evaluation of the smallest eigenvalue. It is the same as minimizing the largest eigenvalue of the moment matrix. This criterion plays a crucial role in the admissibility investigations.

3.2.8 Trace (T-criterion)

The evaluation of the trace criterion is given by

$$\phi_{-\infty}(\mathrm{M})=\frac{1}{s}trace(M) \qquad (3.2.8)$$

3.2.9 G-optimality criterion

This criterion is concerned with prediction variance. The aim of G-optimality is to have a good prediction at a particular location in the design. To attain this variance function, the scaled prediction variance (SPV) is defined as;

$$\mathrm{Nvar}\,\frac{[var\hat{y}]}{\sigma^2}=X(X^IX)^{-1}X^I \qquad (3.2.9)$$

Where X is vector of coordinates of points in the region of interest expanded to model form. That is

$$X^I = [1, x_1 \ldots x_k, x_1^2 \ldots x_k^2, x_1^3 \ldots x_k^3 x_1, x_1x_2 \ldots x_{k-1}x_k, x_1x_2x_3 \ldots x_{k-2}x_{k-1}x_k]$$

σ^2 is the process variance which is assumed to be 1.

The scaled prediction variance (SPV) provides a measure of precision of the estimated response at any point in the design space.

3.2.10 Integrated variance (IV) (I-optimality criteria)

I-optimality, which minimizes the normalized average or integrated prediction variances, is defined as follows;

I= $\frac{n}{\sigma^2}\int_R var\hat{y}(x)d\mu(x)$ (3.2.10)

Where R is the region of interest (modelling region)

μ is uniform measure on R with total measure=1.

This integral simplifies to give

I= trace$\{MM^{-1}\}$

3.3 The Generalized Alphabetic Optimality Criteria

To determine the general method of obtaining alphabetic optimality criteria for TORD constructed from BIBD, the study required a general moment matrix.

3.3.1 The moment matrix of TORD constructed from BIBD in k factors

From an existing BIBD (v=k, b, r=k-1, s, λ, μ) a third order rotatable design in k dimensions with $4[k(k+1)+2^k]$ points was obtained as;

D_k =S(a,a,0,. . .,0)+S(b, b, . . .,b)+S($\frac{\rho}{\sqrt{2}}, \frac{\rho}{\sqrt{2}}, 0, \ldots, 0$)+3S(d,d,. . .,d)+4S($\rho$,0,. . .,0),where

$$a^2 = \left(\frac{-3}{4}C\frac{(5k-12)}{k-8}\right)^{\frac{1}{3}}$$

$$b^2 = \left(\frac{12C(k-1)}{2^{k+1}(8-k)}\frac{1}{1+t^3}\right)^{\frac{1}{3}}$$

$$d^2 = t\left(\frac{12C(k-1)}{2^{k+1}(8-k)}\frac{1}{1+t^3}\right)^{\frac{1}{3}}$$

The value of t is evaluated as follows;

$$\frac{(1+t^2)^3}{(1+t^3)^2} = \left(\frac{3B(k-2)+4\left(\frac{-3}{4}C\left(\frac{5k-12}{k-8}\right)\right)^{\frac{2}{3}}}{2^{k+1}b^4}\right)^3\left(\frac{2^{k+1}(8-k)b^6}{12C(k-1)}\right)^2$$

The general third order design can be expressed as;

$$\eta_\mu = \beta_o + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i \le j=1}^{k} \beta_{ij} x_{iu} x_{ju} + \sum_{i \le j \le l=1}^{k} \beta_{ijl} x_{iu} x_{ju} x_{lu}$$, where u=1, 2,…, N

with parameters

$\beta_0, \beta_{11}, \beta_{22}, ..., \beta_{kk}, \beta_1, \beta_2, ..., \beta_k, \beta_{12}, ..., \beta_{k-1,k}$

$, \beta_{111}, \dots, \beta_{kkk,} \beta_{112}, \dots, \beta_{k-1k-1k}, \beta_{122}, \dots, \beta_{k-1kk}, \beta_{123}, \dots, \beta_{k-2k-1k}$

The model will be

$$\underline{y} = X \underline{\beta} + \underline{\varepsilon}$$

where y = ($y_1, y_2, \dots, y_N)^{/}$ is an N $\times 1$ vector of response values.

X = ($x_1, x_2, \dots, x_N)^{/}$ is an $n \times k$ model matrix or matrix of observation

β = is a $k \times 1$vector of parameter and

ε = is an $n \times 1$vector of errors and where the random errors ε_u's are independently and identically distributed with mean 0 and variance σ^2 , that is,

E($\varepsilon_u) = 0$, var ($\varepsilon_u) = \sigma^2$ and cov ($\varepsilon_u, \varepsilon_u{}^{/}) = 0$

The independent variables $x_1, x_2, \dots, x_k$ have been coded so that

$$\sum_{u=1}^{N} x_{1u}^2 = \sum_{u=1}^{N} x_{2u}^2 = \cdots = \sum_{u=1}^{N} x_{ku}^2 = N$$

To standardize the moment matrix for ease in further investigation, each term is a moment of independent variables i.e. the term in the column headed by x_2^2 and the row labeled x_2^2 is a fourth moment of x_2.

That is;

$$\frac{1}{N} \sum_{u=1}^{N} x_{2u}^4 = 3\,\lambda_4$$

And the term in the column headed by $x_1x_2^2$ and the row, x_1^3, is a sixth order mixed moment of both x_1 and x_2, i.e.

$$\frac{1}{N}\sum_{u=1}^{N} x_{1u}^4 x_{2u}^2 = 3\,\lambda_{\ 6}$$

Thus, the moment matrix $N^{-1}(X'X)$ (according to Gardiner et al (1959)), of a rotatable design of order 3 in k factors can be written as follows in (3.3.1)

Where

$$X' = \begin{bmatrix} 1, x_1^2, \dots, x_k^2, x_1x_2, \dots, x_{(k-1)}x_{(k)}, x_1x_2x_3, \dots, x_{(k-2)}x_{(k-1)}x_{(k)}, x_1, x_1^3, \\ x_1x_2^2, \dots, x_1x_{(k)}^2, \dots, x_{(k)}, x_{(k)}^3, x_{(k)}x_1^2, \dots, x_kx_{(k-1)}^2 \end{bmatrix}$$

$$M_{\left[\begin{smallmatrix}3+k\\k\end{smallmatrix}\right]\times\left[\begin{smallmatrix}3+k\\k\end{smallmatrix}\right]} = \begin{bmatrix} G & 0 & 0 & 0 & . & . & . & 0 & 0 \\ & \lambda_4 I & 0 & 0 & . & . & . & 0 & 0 \\ & & \underline{\lambda_6 I} & 0 & . & . & . & 0 & 0 \\ & & & \underline{K_{k1}} & . & . & . & 0 & 0 \\ & & & & K_{k2} & & & & . \\ & & & & & . & & & . \\ (symmetric) & & & & & & . & & . \\ & & & & & & & . & 0 \\ & & & & & & & & K_{kk} \end{bmatrix}$$

(3.3.1)

in which the submatrices are defined as follows

$$G_{(k+1)\times(k+1)} = \begin{bmatrix} 1 & \lambda_2 & \lambda_2 & . & . & . & \lambda_2 \\ & 3\lambda_4 & \lambda_4 & . & . & . & \lambda_4 \\ & & 3\lambda_4 & . & . & . & \lambda_4 \\ & & & . & & & . \\ & & & & . & & . \\ (symm) & & & & & . & . \\ & & & & & & 3\lambda_4 \end{bmatrix}$$

$$\lambda_4 I_{\left[\begin{smallmatrix} k \\ 2 \end{smallmatrix}\right]} = \begin{bmatrix} \lambda_4 & 0 & . & . & . & 0 \\ & \lambda_4 & . & . & . & 0 \\ & & . & & & 0 \\ & & & . & & 0 \\ (symm) & & & & . & 0 \\ & & & & & \lambda_4 \end{bmatrix}$$

$$\lambda_6 I_{\left(\left[\begin{smallmatrix} k \\ 3 \end{smallmatrix}\right]\right)} = \begin{bmatrix} \lambda_6 & 0 & . & . & . & 0 \\ & \lambda_6 & . & . & . & 0 \\ & & . & & & . \\ & & & . & & . \\ (symm) & & & & . & . \\ & & & & & \lambda_6 \end{bmatrix}$$

and

$$K_{ik(k+1)\times(k+1)} = \begin{bmatrix} \lambda_2 & 3\lambda_4 & \lambda_4 & . & . & . & \lambda_4 \\ & 15\lambda_6 & 3\lambda_6 & . & . & . & 3\lambda_6 \\ & & 3\lambda_6 & . & . & . & \lambda_6 \\ & & & . & & & . \\ & & & & . & & . \\ (symm) & & & & & . & . \\ & & & & & & 3\lambda_6 \end{bmatrix}$$

where i =1, 2,…,k,

The general third order moment matrix (M_k) (3.3.1) was used to determine the general alphabetic optimality criteria as follows;

1. The general determinant criterion is given by the product of the sub-matrices.

$$\emptyset_0 M_k = |G||I\lambda_4||I\lambda_6||K| \qquad (3.3.2)$$

2. The general smallest eigenvalue criterion

$$\emptyset_{-\infty} M_k = \lambda_{min}[M_k]$$

$$= \left| M_k - \lambda I_{\begin{bmatrix}3+k\\k\end{bmatrix} * \begin{bmatrix}3+k\\k\end{bmatrix}} \right| \qquad (3.3.3)$$

3. The general trace criterion

   Considering the general moment matrix (M_k), the trace of a matrix is given as the sum of all the elements in the principal diagonal, thus the generalized trace criterion will be given by;

$$\emptyset_{-\infty}(M_k) = \frac{1}{S}[trace\ M_k] \qquad (3.3.4)$$

4. The generalized average variance criterion is given by;

$$\emptyset_{-1}(M_k) = \left[\frac{1}{S} trace\ (M_k)^{-1}\right]^{-1} \qquad (3.3.5)$$

3.4 The DT- Optimality Criterion

This method was proposed by Atkinson (2008). It is a combination of D–optimality and T–optimality. It provides a specified balance between model discrimination and parameter estimation. The criterion to be maximized is

$$\phi^{DT}(\xi) = (1-k)\log \Delta_2(\xi) + \left(\frac{K}{p}\right)\log\ |M_1(\xi)| \qquad (3.4.1)$$

Where $\phi^{DT}(\xi)$ is a convex combination of two design criteria, the first criterion is $\log \Delta_2(\xi)$, the logarithm of the T–optimality and the second is D–optimality. Then the design which maximizes the above criterion is called DT–optimum and is denoted byξ^*_{DT} .

CHAPTER FOUR

RESULTS AND DISCUSSION

4.1 Introduction

In this chapter the alphabetic optimality criteria for specific TORD in three, four, five, six and k dimensions are presented. Further, the compound optimality comprising of D- and T-optimality criteria is evaluated for the designs in three, four, five and six dimensions.

4.2 Alphabetic optimality criteria

Alphabetic optimality criteria under the study are variance related criteria since they address the minimization of the variance associated with the estimation of the model. The smallest value is picked as it determines the optimality.

4.2.1 Particular criteria for three dimensional TORD constructed through BIBD

Utilizing the moment matrix (3.2.1), the alphabetic optimality criteria D-, A-, E-, T-, G- and I- for three dimensional TORD constructed from BIBD were obtained from the expressions in (3.2.5), (3.2.6), (3.2.7), (3.2.8), (3.2.9) and (3.2.1.1) respectively and presented in the table 4.2.1.

Table 4.2.1: Alphabetic optimality criteria for three dimensional TORD constructed through BIBD

Optimality criteria	D-criteria	A-criteria	E-criteria	T-criteria	G-criteria	I-criteria
values	0.03583	55.338	0.0031	0.1383	0.2263	49.5917

E- Criterion is the best criteria for TORD in three factors constructed through BIBD. That means E-criteria is more optimal since it addresses minimization of variance more than the other criteria. D- Criterion is the second best criterion.

4.2.2 Particular criteria for four dimensional TORD through BIBD

Utilizing the moment matrix (3.2.2), the alphabetic optimality criteria D-, A-, E-, T-, G- and I- for four dimensional TORD constructed from BIBD were obtained from the expressions in (3.2.5), (3.2.6), (3.2.7), (3.2.8), (3.2.9) and (3.2.1.1) respectively and presented in the table 4.2.2.

Table 4.2.2: Alphabetic optimality criteria for four dimensional TORD constructed through BIBD

Optimality criteria	D-criteria	A-criteria	E-criteria	T-criteria	G-criteria	I-criteria
values	0.02455	117.0680	0.0063	0.0956	0.1442	-51454.9846

E- Criterion is the best criteria for TORD in four factors constructed through BIBD. That means E-criterion is more optimal since it addresses minimization of variance more than the other criteria. D- Criterion is the second best criteria.

4.2.3 Particular criteria for five dimensional TORD constructed through BIBD

Utilizing the moment matrix (3.2.3), the alphabetic optimality criteria D-, A-, E-, T-, G- and I- for five dimensional TORD constructed from BIBD were obtained from the expressions in (3.2.5), (3.2.6), (3.2.7), (3.2.8), (3.2.9) and (3.2.1.1) respectively and presented in table 4.2.3 below.

Table 4.2.3: Alphabetic optimality criteria for five dimensional TORD constructed through BIBD.

Optimality criteria	D-criteria	A-criteria	E-criteria	T-criteria	G-criteria	I-criteria
values	0.01939	216.188	0.0033	0.0689	0.1273	176.014

E- Criterion is the best criteria for TORD in five factors constructed through BIBD. That means E-criterion is more optimal since it addresses minimization of variance more than the other criteria. D- Criterion is the second best criteria.

4.2.4 Particular criteria for six dimensional TORD constructed through BIBD

Utilizing the moment matrix (3.2.4), the alphabetic optimality criteria D-, A-, E-, T-, G- and I- for six dimensional TORD constructed from BIBD were obtained from the expressions in (3.2.5), (3.2.6), (3.2.7), (3.2.8), (3.2.9) and (3.2.1.1) respectively and presented in the table 4.2.4.

Table 4.2. 4 : Alphabetic optimality criteria for six dimensional TORD constructed from BIBD

Optimality criteria	D-criteria	A-criteria	E-criteria	T-criteria	G-criteria	I-criteria
values	0.0203	428.022	0.0033	0.0607	0.1005	205.639

E- Criterion is the best criteria for TORD in six factors constructed through BIBD. That means E-criterion is more optimal since it addresses minimization of variance more than the other criteria. D- Criterion is the second best criteria.

Table 4.2.5 gives the summary of particular criteria for the four designs. From the table E-Criterion is the best criteria for the four designs.

Table 4.2.5 : A summary of particular criteria for the four designs

Design	D	A	T	E	I	G
D_1	0.03583	55.338	0.1383	0.0031	49.5917	0.2263
D_2	0.02455	117.0680	0.0956	0.0063	-51454.9846	0.1442
D_3	0.01939	216.188	0.0689	0.0033	176.014	0.1273
D_4	0.0203	428.022	0.0607	0.0033	205.639	0.1005

The behavior of this the optimal values on different factors can be visualized well in figure 4.2

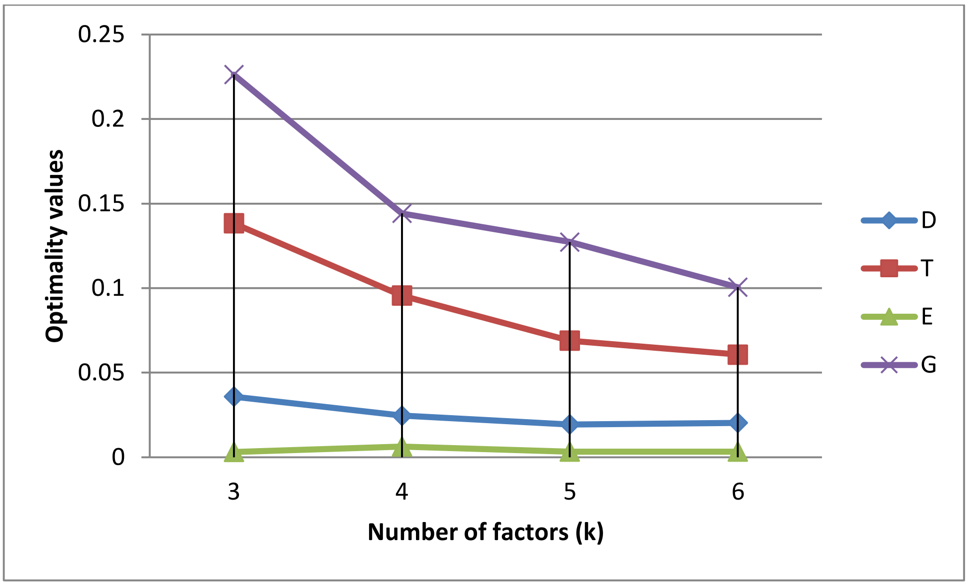

Figure 1 : Graph of optimal values vs number of factors

Evaluation of alphabetic optimality was done and D-, A-, T-, E-, I- and G- optimal designs were obtained. From the above results, it shows that at three factors all the designs are less optimal. All the designs are relatively optimal for E- and D- criterion. For G- and T- criteria the designs gets optimal at four factors and even more optimal as the number of factors increase. In general the designs becomes more optimal in all the criteria as the number of factors increase.

4.3 Optimality criteria for k- dimensional TORD constructed through BIBD

The general third order moment matrix given in (3.3.1) was utilized in determining the general alphabetic optimality criteria.

4.3.1 Generalized determinant criterion

The determinant $|\boldsymbol{M_k}|$ is given by the product of $|G||I\lambda_4||I\lambda_6||K|$

Having obtained the determinant for 3, 4, 5 and six factors, the study obtained the determinant for k-factors. To establish a trend the determinant for each sub-matrix in each factor is obtained as shown in table 4.3.1 below.

Table 4.3 1: General determinant of each sub-matrix for different factors

Sub-matrix	**3-factors**	**4-factors**	**5-factors**
G	$20\lambda_4^3 - 12\lambda_2^2\lambda_4^2$	$48\lambda_4^4 - 32\lambda_2^2\lambda_4^2$	$112\lambda_4^5 - 80\lambda_2^2\lambda_4^2$
$I\lambda_4$	λ_4^3	λ_4^6	λ_4^{10}
$I\lambda_6$	λ_6	λ_6^4	λ_6^{10}
K	$84\lambda_2\lambda_6^3 - 60\lambda_4^2\lambda_6^2$	$192\lambda_2\lambda_6^4 - 144\lambda_4^2\lambda_6^3$	$432\lambda_2\lambda_6^5 - 336\lambda_4^2\lambda_6^4$

The determinant for each sub-matrix for k-factors is obtained as shown in table 4.3.2 below

Table 4.3 2 : General determinant of each sub-matrix for k-factors

	k-factors
G	$(2\lambda_4)^{k-1}\left[(k+2)\lambda_4 - k\lambda_2^2\right]$
$I\lambda_4$	$\lambda_4^{\left[\frac{k}{2}\right]}$
$I\lambda_6$	$\lambda_6^{\left[\frac{k}{3}\right]}$
K	$\left\{3(2\lambda_6)^{k-1}\left[(k+4)\lambda_6\lambda_2 - (k+2)\lambda_4^2\right]\right\}^k$

The generalized determinant criterion is given by

$$\emptyset_0 \boldsymbol{C_k}(\boldsymbol{M}) = (2\lambda_4)^{k-1}\left[(k+2)\lambda_4 - k\lambda_2^2\right]\lambda_4^{\left[\frac{k}{2}\right]}\lambda_6^{\left[\frac{k}{3}\right]}\left\{3(2\lambda_6)^{k-1}\left[(k+4)\lambda_6\lambda_2 - (k+2)\lambda_4^2\right]\right\}^k$$

4.3.2 Generalized Trace-criterion

Considering the moment matrix M, the trace of a matrix is given as the sum of all the elements in the principal diagonal, thus the generalized trace criterion is be given by

$$\emptyset_1 C_k(M) = \frac{1}{S}\left[trace\ C_k(M)\right]$$

$$= \frac{1}{\left[\begin{matrix}K+3\\K\end{matrix}\right]}\left\{1 + k(3\lambda_4) + \lambda_4\left[\begin{matrix}k\\2\end{matrix}\right] + \lambda_6\left[\begin{matrix}k\\3\end{matrix}\right] + k\left[\lambda_2 + 15\lambda_6 + (k-1)3\lambda_6\right]\right\}$$

4.3.3 Generalized average variance criterion

The generalized variance criterion is given by

$$\emptyset_{-1} C_k(M) = \left[\frac{1}{S} trace\ C_k(M)^{-1}\right]^{-1}$$

$$= \left[\frac{1}{\left[\begin{matrix}K+3\\K\end{matrix}\right]}\left\{1 + k(3\lambda_4) + \lambda_4\left[\begin{matrix}k\\2\end{matrix}\right] + \lambda_6\left[\begin{matrix}k\\3\end{matrix}\right] + k\left[\lambda_2 + 15\lambda_6 + (k-1)3\lambda_6\right]\right\}^{-1}\right]^{-1}$$

4.3.4 Generalized smallest eigenvalue criterion

The smallest eigenvalue criterion is obtained as

$$\emptyset_{-\infty} C_k(M) = \lambda_{min}[C_k(M)]$$

$$= \left| C_k(M) - \lambda I_{\begin{bmatrix}3+k\\k\end{bmatrix}\times\begin{bmatrix}3+k\\k\end{bmatrix}} \right|$$

where it produces a kth-degree polynomial λ , called characteristic polynomial, where

$$k(\lambda) \equiv \det(\lambda I_n - A)$$

$$\equiv \lambda_n + k_1\lambda^{n-1} + k_2\lambda^{n-2} + \ldots + k_{n-1}\lambda + k_n = 0\,.$$

The k roots $\lambda_1, \lambda_2, ..., \lambda_k$ of this equation are called the eigenvalues of M.

$$\left\| \begin{bmatrix} \lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda \end{bmatrix}_{\begin{bmatrix}k+3\\k\end{bmatrix}\begin{bmatrix}k+3\\k\end{bmatrix}} - \begin{bmatrix} G & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_4 I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_6 I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & K_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & K_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_k \end{bmatrix}_{\begin{bmatrix}k+3\\k\end{bmatrix}\begin{bmatrix}k+3\\k\end{bmatrix}} \right\| = 0$$

The eigenvalues of each sub-matrix are obtained as follows

$$|\lambda I_{(k+1)(k+1)} - G_{(k+1)(k+1)}| = \begin{vmatrix} \lambda - 1 & -\lambda_2 & -\lambda_2 & . & . & . & -\lambda_2 \\ & \lambda - 3\lambda_4 & -\lambda_4 & . & . & . & -\lambda_4 \\ & & \lambda - 3\lambda_4 & . & . & . & -\lambda_4 \\ & & & . & & & . \\ & & & & . & & . \\ (symm) & & & & & . & . \\ & & & & & & \lambda - 3\lambda_4 \end{vmatrix} = 0$$

$$= [\lambda - 3\lambda_4 + \lambda^2{}_2 + (-\lambda_4 + \lambda^2{}_2)(k-1)][\lambda - 3\lambda_4 + \lambda^2{}_2 + \lambda_4 - \lambda^2{}_2]^{k-1} = 0$$

We have $\lambda_4 I$ as,

$$\left|\lambda I_{\left[\begin{smallmatrix}k\\2\end{smallmatrix}\right]} - \lambda_4 I_{\left[\begin{smallmatrix}k\\2\end{smallmatrix}\right]}\right| = \begin{vmatrix} \lambda-\lambda_4 & 0 & . & . & . & 0 \\ & \lambda-\lambda_4 & . & . & . & 0 \\ & & . & & & . \\ & & & . & & . \\ (symmetric) & & & & . & . \\ & & & & & \lambda-\lambda_4 \end{vmatrix} = 0$$

$$=(\lambda-\lambda_4)^{\left[\begin{smallmatrix}k\\2\end{smallmatrix}\right]}$$

We have $\lambda_6 I$ as,

$$\left|\lambda I_{\left[\begin{smallmatrix}k\\3\end{smallmatrix}\right]} - \lambda_6 I_{\left[\begin{smallmatrix}k\\3\end{smallmatrix}\right]}\right| = \begin{vmatrix} \lambda-\lambda_6 & 0 & . & . & . & 0 \\ & \lambda-\lambda_6 & . & . & . & 0 \\ & & . & & & . \\ & & & . & & . \\ (symmetric) & & & & . & . \\ & & & & & \lambda-\lambda_6 \end{vmatrix} = 0$$

$$=(\lambda-\lambda_6)^{\left[\begin{smallmatrix}k\\3\end{smallmatrix}\right]}$$

We have K as,

$$\left|\lambda I_{(k+1)(k+1)} - K_{(k+1)(k+1)}\right| = \begin{vmatrix} \lambda_2 & 3\lambda_4 & \lambda_4 & . & . & . & \lambda_4 \\ & 15\lambda_6 & 3\lambda_6 & . & . & . & 3\lambda_6 \\ & & 3\lambda_6 & . & . & . & \lambda_6 \\ & & & . & & & . \\ & & & & . & & . \\ (symm) & & & & & . & . \\ & & & & & & 3\lambda_6 \end{vmatrix} = 0$$

$$[\lambda^3 - \lambda^2(\lambda_2 + \lambda_6 k) + (15\lambda^2{}_6 k + \lambda_6\lambda_2 k - \lambda^2{}_4 k) - 15\lambda^2{}_6\lambda_2 k + 6\lambda^2{}_4\lambda_2 k][\lambda - 2\lambda_6] = 0$$

The generalized smallest eigenvalue criterion for third order in k-factors is given by

$$(\lambda-\lambda_4)^{\left[\begin{smallmatrix}k\\2\end{smallmatrix}\right]} = \left|C_k(M) - \lambda I_{\left[\begin{smallmatrix}3+k\\k\end{smallmatrix}\right]*\left[\begin{smallmatrix}3+k\\k\end{smallmatrix}\right]}\right|$$

$$= [\lambda - 3\lambda_4 + \lambda^2{}_2 + (-\lambda_4 + \lambda^2{}_2)(k-1)][\lambda - 3\lambda_4 + \lambda^2{}_2 + \lambda_4 - \lambda^2{}_2]^{k-1}(\lambda-\lambda_4)^{\left[\begin{smallmatrix}k\\2\end{smallmatrix}\right]}(\lambda-\lambda_6)^{\left[\begin{smallmatrix}k\\3\end{smallmatrix}\right]}$$

$$[\lambda^3 - \lambda^2(\lambda_2 + \lambda_6 k) + (15\lambda^2{}_6 k + \lambda_6\lambda_2 k - \lambda^2{}_4 k) - 15\lambda^2{}_6\lambda_2 k + 6\lambda^2{}_4\lambda_2 k][\lambda - 2\lambda_6] = 0$$

4.4 DT- optimality criterion for third order rotatable designs constructed from BIBD

The criterion to be maximized is given by expression (3.4.1).

DT- compound optimality criterion for third order rotatable designs constructed from balanced incomplete block design was evaluated. Results were obtained as shown in table 4.4.1.

Table 4.4. 1 : DT-compound optimality for the four designs

Design	DT-optimality
D_1	1.5015
D_2	2.8746
D_3	4.4942
D_4	5.9632

The values of the DT- compound optimality versus the number of factors can be visualized well in figure 2.

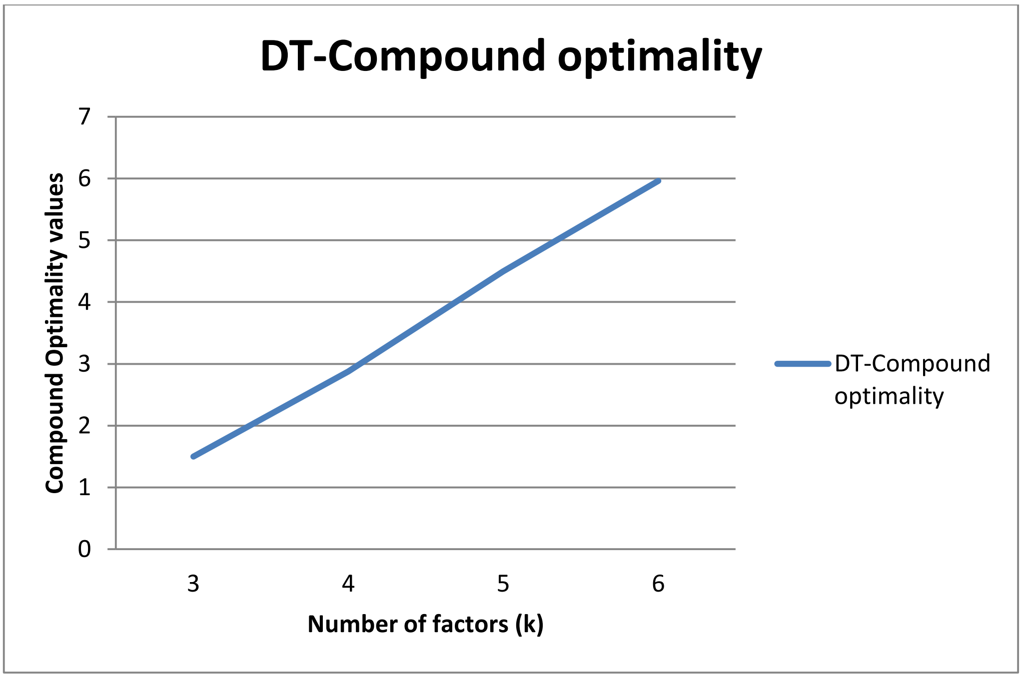

Figure 2 : DT-compound optimality values vs number of factors

DT- compound optimality was evaluated and a DT- optimal design determined. The values of DT-optimality increases as the number of factors increase. The design D_1 (three factors) is DT-optimum, that is, the design is ξ^*_{DT}. It is evident that compound DT- optimality is appropriate for designs with few factors, that is the fewer the factors the optimal the design.

4.5: Numerical Example

A central composite rotatable design with 6 center-point replications was set up to investigate the effects of three fertilizer ingredients on the yield of snap beans. The fertilizer ingredients and actual amounts applied were nitrogen (N), from 0.94 to 6.29 kg/plot; phosphoric acid (P2O5) , from 0.59 to 2.97 kg/plot; and potash (K2O) , from 0.60 to 4.22 kg/plot. The response of interest, y, is the average yield in pounds per plot of snap beans. The coded variables, x1, x2, x3, are given by

$$X1 = \frac{N-3.62}{1.59}, \quad X2 = \frac{P_2O_5-1.78}{0.71}, \quad X3 = \frac{K_2O-2.42}{1.07}$$

The values 3.62, 1.78 and 2.42 kg/plot represent the centres of the values of nitrogen, phosphoric and potash respectively.

The design settings (in coded form) and corresponding response values are given in Table 1 [15]: We note that the design is rotatable since the axial parameter value is α=F1/4=1.682,, where F=8 is the number of points in the factorial portion of this CCD. The region R is therefore spherical with a radius = 1.682.

In this example, the predicted response is

$$y = 10.61 + 0.43x_1 + 1.89x_2 + 1.23x_3 + 0.71x_1^2 + 0.94x_1x_2 + 0.87x_1x_3 + 0.21x_2^2 + 0.23x_2x_3 + 0.15x_3^2 - 2.11x_1^3 + 1.76x_1^2x_2 + 0.67x_1^2x_3 + 0.98x_2^2x_1 + 0.87x_1x_2x_3 - 1.47x_3^2x_1 + 2.33x_2^3 + 1.48x_2^2x_3 - 0.45x_3^2x_2 + 2.08x_3^3$$

x1	x2	x3	**N**	**P2O5**	**K2O**	**Yield**
-1	-1	-1	2.03	1.07	1.35	11.28
1	-1	-1	5.21	1.07	1.35	8.44
-1	1	-1	2.03	2.49	1.35	13.19
1	1	-1	5.21	2.49	1.35	7.71
-1	-1	1	2.03	1.07	3.49	8.94
1	-1	1	5.21	1.07	3.49	10.9
-1	1	1	2.03	2.49	3.49	11.85
1	1	1	5.21	2.49	3.49	11.03
-1.682	0	0	0.94	1.78	2.42	8.26
1.682	0	0	6.29	1.78	2.42	7.87
0	-1.682	0	3.62	0.59	2.42	12.08
0	1.682	0	3.62	2.97	2.42	11.06
0	0	-1.682	3.62	1.78	0.6	7.98
0	0	1.682	3.62	1.78	4.22	10.43
0	0	0	3.62	1.78	2.42	10.14
0	0	0	3.62	1.78	2.42	10.22
0	0	0	3.62	1.78	2.42	10.53
0	0	0	3.62	1.78	2.42	9.5
0	0	0	3.62	1.78	2.42	11.53
0	0	0	3.62	1.78	2.42	11.02

CHAPTER FIVE

SUMMARY, CONCLUSION AND RECOMENDATION

5.1 Introduction

This chapter gives conclusion and recommendations based on the objectives of the study. The implications of the main findings based on the study are also stated in this chapter. For further research this chapter gives what is considered to be gap left out by the study which would need further investigation through research.

5.2 Conclusion

The alphabetic optimality criteria are very useful in designing of experiment. The study shows that all designs optimal values decrease with the increase in the number of factors for D-, G- and T- optimality. All the designs under consideration in the study were found to be E optimal, therefore E- optimality criterion is the best for third order rotatable designs in three, four, five and six factors.

A general method of evaluating alphabetic optimality for TORD constructed through BIBD in *k* factors was determined.

Compound DT- optimality was obtained. The values of DT-optimality increases as the number of factors increase. The design D_1 (three factors) is DT-optimum, that is, the design is ξ_{DT}^{*}. It is evident that compound DT- optimality is appropriate for designs with few factors, that is the fewer the factors the optimal the design.

5.3 Recommendation

Rotatable designs constructed from BIBD for second and third order have been constructed and their optimality determined. The study also recommends the application of the designs in the design and analysis of field experiments.

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