THE COMPUTER SEARCH FOR THE OPTIMAL SETTINGS OF A MULTI-FACTORIAL EXPERIMENT USING RESPONSE SURFACES D-OPTIMALITY DESIGN CRITERION

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DECLARATION

I declare that the work in the dissertation entitled "THE COMPUTER SEARCH FOR THE OPTIMAL SETTINGS OF A MULTI-FACTORIAL EXPERIMENT USING RESPONSE SURFACES D-OPTIMALITY DESIGN CRITERION" has been performed by me in the department of Mathematics under the supervision of Prof. O.E. Asiribo and Dr K.N. Misra.

The information derived from literature has been duly acknowledged in the text and a list of references provided. No part of this dissertation was previously presented for another degree or diploma at any university.

Bamanga, Muhammad Ardo **May 25, 2006**

CERTIFICATION

This Dissertation titled “THE COMPUTER SEARCH FOR THE OPTIMAL SETTINGS OF A MULTI-FACTORIAL EXPERIMENT USING RESPONSE SURFACES D-OPTIMALITY DESIGN CRITERION” by Bamanga, Muhammad Ardo meets the regulation governing the award of the degree of Doctor of Philosophy of Ahmadu Bello University and is approved for its contribution to scientific knowledge and literary presentation.

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DEDICATION

This Dissertation is dedicated to my parents, family and friends.

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ABSTRACT

Most experimental situations call for standard designs that can be constructed with many statistical software packages. In some situations, however, standard designs are not appropriate or practicable.

Computer-aided designs are experimental designs that are generated based on a particular optimality criterion and are generally optimal only for a specified model.

In this work designs are generated for non-standard multifactor experiment using D-optimality criterion.

The experiment involves four factors, Nitrogen, Phosphorus, Sulphur, and Potassium each varied at 5, 5, 3, and 2 levels respectively. The total treatment combinations are 150, out of which only the best 21 treatment combinations are required. The factors were tested on maize, sorghum and millet.

The D-optimality criterion, which seeks to maximize the determinant of the information matrix of a design, was used to search for the best 21 treatment combinations (optimal settings). The interaction, quadratic and purequadratic models were used as prespecified models while generating the optimal settings. Also, control and without control levels of the factors were considered.

The spread of points and the number of design points generated by each model was studied. The quadratic model was found to be the most suitable and recommended for this type of experiment. A measure of rotatability was computed for the quadratic model and it was found that the design generated by the model is 83.55% rotatable, indicating that the design is near rotatable.

TABLE OF CONTENTS

Title i
Declaration ii
Certification iii
Dedication iv
Acknowledgement v
Abstract vii
List Of Tables x
List Of Figures xi
Chapter One 1
Introduction 1
1.1 Background Of The Study 1
1.2 Experimental Procedure 6
1.3 Objectives Of The Study 10
1.4 Purpose/Scope Of The Study 10
1.5 Significance Of The Study 11
1.6 Limitations 12
1.7 Definition Of Terms 12
Chapter Two 18
Literature Review 18
2.1 Introduction 18
2.2 The Emergence And Development Of Response Surface Methods 18
2.3 Standard Designs 21
2.3.1 Full Factorial Design 21
2.3.2 Central Composite Design 23
2.3.3 Box-Behnken Design 25
Chapter Three 31
RSM Optimization Procedure (Path Of Steepest Ascent) 31
3.1 Introduction 31
3.2 RSM Experimental Optimisation Procedure (PSA) 31
3.3 Illustration Of Rsm Procedure 33
Chapter Four 44
Computer-Aided Designs Methodology 44
4.1 Introducton 44
4.2 Design Regions 44
4.3 Restricted Design Region (Non-Standard Design) 46
4.4 Computer-Aided/ Optimum Designs 48
4.5 The D-Optimal Designs 50
4.6 The Least Squares Of D-Optimal Designs 52
4.7 Properties Of D-Optimum Designs 54
4.8 Algorithm For The Consruction Of D-Optimum Designs 56
4.8.1 Exchange Algorithms 56
4.8.2 Sequential Algorithms 57
4.9 Models 58
4.10 Measure Of Rotatability 59

Chapter Five 61
Matlab Software 61
5.1 Introducton 61
5.2 The D-Optimum Designs 62
5.3 Matlab Algorithm For D-Optimum Designs 63
5.3.1 Transforming Variables 63
5.3.2 Generating Treatment Combinations 63
5.3.3 Searching For The D-Optimal Designs 66
Chapter Six 69
Construction Of D-Optimum Designs 69
6.1 Introducton 69
6.2 An Illustration With A 2^2 Factorial Experiment 70
6.2.1 Final Settings 70
6.3 An Illustration With A 3^2 Factorial Experiment 71
6.3.1 Final Settings 72
6.4 Generation Of D-Optimal Designs For Maize 74
6.4.1 Interaction Model For Maize 77
6.4.2 Quadratic Model For Maize 80
6.4.3 Pure-Quadratic Model For Maize 89
6.5 Generation Of D-Optimal Designs For Sorghum & Millet 96
6.5.1 Interaction Model For Sorghum And Millet 100
6.5.2 Quadratic Model For Sorghum & Millet 102
6.5.3 Pure-Quadratic Model For Sorghum & Millet 111
6.6 Observations 118
6.6.1 Measure Of Rotatability 120
Chapter Seven 122
Summary, Conclusion And Recommendations 122
7.1 Introducton 122
7.2 Summary And Conclusion 122
7.3 Recommendations 123
7.3.1 The Settings For Main Experiment 123
7.3.2 The Recommended Settings For Maize With Control 124
7.3.3 The Recommended Settings For Maize Without Control 126
7.3.4 The Recommended Settings For Sorghum/Millet With Control 126
7.3.5 The Recommended Settings For Sorghum/Millet Without Control 128
7.4 Areas of Future Research 129
References 131
Apendix A 139
Apendix B 145

LIST OF TABLES

Table 1.1 Layout Of An Initial 2^2 Factorial Design. 3
Table 1.2 Result Of The 2^2 Factorial Design Of Froth Flotation Process. 3
Table 3.1 Layout Of An Initial 2^2 Factorial Design. 33
Table 3.2 Result Of The 2^2 Factorial Design Of Froth Flotation Process. 33
Table 3.3 Test Plan 1. 36
Table 3.4 Result Of The Second 2^2 Factorial Design Of Froth Flotation Process. 36
Table 3.5 Test Plan 2. 38
Tab1e 3.6 Test Plan 3. 39
Table 3.7 Predicted And Residual Values. 42
Table 6.1 Summary Of Results For With Control..... 118
Table 6.2 Summary Of Results For Without Control..... 118

LIST OF FIGURES

Fig. 2.1 2^3 Full Factorial Design (8 Points)..... 22
Fig. 2.2 Central Composite Rotatable Design In Two X-Variables..... 24
Fig. 3.1 Diagram Of Results Of The 2^2 Factorial Design Of Froth Flotation Process. 34
Fig. 3.2 Diagram Of Results Of The Second 2^2 Factorial Design Of Froth Flotation Process. 37
Fig. 3.3 Diagram Of Central Composite Design. 39
Fig. 3.4 The Three-Dimensional Predicted Froth Flotation Process Response Surface..... 41
Fig. 4.1 Square Region 44
Fig. 4.2 Sphere Region 45
Fig. 4.3 Restricted Region 46
Fig. 6.1 First-order Model..... 71
Fig. 6.2 Quadratic Model. 73
Fig. 6.3 **Interaction Model for Maize**..... 80
Fig. 6.4 **Quadratic Model for Maize**. 88
Fig. 6.5 **PureQuadratic Model for Maize**..... 96
Fig. 6.6 **Interaction Model for Sorghum/Millet**..... **102**
Fig. 6.7 **Quadratic Model for Sorghum/Millet** **110**
Fig. 6.8 **PureQuadratic Model for Sorghum/Millet**..... **117**

CHAPTER ONE

INTRODUCTION

1.1 BACKGROUND OF THE STUDY

Response surface methodology (RSM) is a collection of mathematical and statistical techniques for empirical model building. By careful design of experiments, the objective is to optimise a response (output variable), which is influenced by several independent variables (input variables). An experiment is a series of tests, called runs, in which changes are made in the input variables in order to identify the reasons for changes in the output response.

Response surface methodology (RSM) consists of a group of techniques used in the empirical study of relationships between one or more measured responses such as yield, colour index and viscosity, on the one hand, and a number of input variables such as time, temperature, pressure, and concentration on the other (Box et al. 1978).

Originally, RSM comprises a group of statistical techniques for empirical model building and model exploitation. By careful design of experiments, it seeks to relate a response or output variable to the levels of a number of predictors or input variable that affect it (Box and Draper, 1987).

According to Khuri and Cornell (1996), response surface methodology is a set of techniques that encompasses:

(i) Setting up a series of experiments (design a set of experiments) that will yield adequate and reliable measurements of the response of interest.

(ii) Determining a mathematical model that best fits the data collected from the design chosen in (i), by conducting appropriate tests of hypothesis concerning the model's parameters.

(iii) Determining the optimal settings of the experimental factors that produce the maximum (or minimum) value of the response.

Khuri and Cornell stated further that; "if discovering the best value, or values, of the response is beyond the available resources of the experiment, then the response surface methods are aimed at obtaining at least a better understanding of the overall system". When the behaviour of the measured response of interest is governed by certain laws which lead to a deterministic relationship between the response and the set of experimental factors chosen, it should then be possible to determine the best conditions (levels) of the factors to optimise a desired output. Quite often, however, because the relationship is either too complex or unknown, an empirical approach is necessary. The strategy employed, outlined in the preceding list, is the basis of RSM, Khuri and Cornell (1996).

What is crystal clear from the foregoing, is that, response surface methodology is a set of techniques for the design of experiments, analysis of data and interpretation of results in situations where a response variable, y, or several response variables are assumed to depend on the levels of continuous factors, $X_1,...,X_k$, to understand, control or optimise the process under study. Adequate approximations to the relationships are often obtained using low-order polynomial models especially the second-order polynomial

$$E(y) = \beta_0+\sum^{k}_{j=1}\beta_j x_j+\sum^{k}_{j=1}\beta_{jj}x^2_j+\sum^{k-1}_{i=1}\sum^{k}_{j=i+1}\beta_{ij}x_i x_j+ \varepsilon \qquad (1.1)$$

And usually the level of the factors are coded, such that, $-1\leq x_i\leq 1$.

Consider a given example (Sutherland, 2001), on an experiment on optimisation of froth flotation process (desired to whiten a wood pulp mixture). Two independent variables, concentration of environmentally safe bleach (X_1) and mixture temperature (X_2) were used. The current operating points of the two independent variables are 4% bleach and 80^0F (which is believed to be well away from the optimum). The allowable variable ranges are 0-20% bleach and 60^0F- 130^0F temperature. The layout of the initial 2^2 factorial design and the subsequent result of the experiment are given below in tables 1.1 and 1.2 respectively.

Variable	Low Level	High Level
(1) % Bleach	2	6
(2) Temperature, ^{0}F	75	85

Table 1.1 Layout of an initial 2^2 factorial design.

% Bleach (X_1)	Temperature, ^{0}F (X_2)	Coded variables		Process response (y)
		x_1	x_2	
2	75	-1	-1	19
6	75	1	-1	31
2	85	-1	1	28
6	85	1	1	44

Table 1.2 Result of the 2^2 factorial design of Froth flotation process.

In the above example one may want to find the levels of bleach (X_1) and temperature (X_2) that maximize the response flotation process (y). The response flotation process is a function of the levels of bleach and temperature, as follows:

$$y = f(x_1, x_2) + \varepsilon \quad (1.2)$$

where ε represents the error or noise observed in the response y. The surface represented by $f(x_1, x_2)$ is called a response surface. The response can be represented graphically, either in the three-dimensional space or as contour plots that help visualize the shape of the response surface. Contours are curves of constant response drawn in the x_i, x_j plane keeping all other variables fixed. Each contour corresponds to a particular height of the response surface.

The general concept in RSM includes response surface models of the type described above and the plan of experiments (designs) where the response has to be evaluated. An important aspect of RSM is the design of experiments (Box and Draper, 1987), usually abbreviated as DoE. These strategies were originally developed for the model fitting of physical experiment, but can also be applied to numerical experiments. The objective of DoE is the selection of the points where the response should be evaluated.

Most of the criteria for optimal design of experiments are associated with the mathematical model of the process. Generally, these mathematical models are polynomials with an unknown structure, so the corresponding experiments are designed only for every particular problem. The choice of the design of experiments can have a large influence on the accuracy of the approximation and the cost of constructing the response surface.

In a traditional DoE, screening experiments are performed in the early stages of the process, when it is likely that many of the design variables initially considered have

little or no effect on the response. The purpose is to identify the design variables that have large effects for further investigation.

A detail description of the design of experiments theory can be found in Cochran and Cox (1957), Box et al. (1978), Box and Draper (1987), Mead (1988), Montgomery (1991), Khuri and Cornell (1996), among others.

As introduced in section 1.1, a particular combination of runs defines an experimental design. The possible settings of each independent variable in the n-dimensional space are called levels.

Most experimental situations call for standard designs that can be constructed with many statistical software packages. Standard designs have assured degrees of precision, orthogonality, and other optimal properties that are important for the exploratory nature of most experiments. In some situations, however, standard designs are not appropriate or are impractical.

When situations such as the above exist, computer-aided designs are a useful option. In some situations, computer-aided designs are the only option an experimenter has. Designs generated from a computer algorithm are referred to as computer-aided designs. Computer-aided designs are experimental designs that are generated based on a particular optimality criterion and are generally 'optimal' only for a specified model. As a result, they are sometimes referred to as optimal designs and generally do not satisfy the desirable properties, such as independence among the estimators that standard classical designs do. The design treatment runs that are generated by the algorithms are chosen from an overall candidate set of possible treatment combinations. The candidate set

consists of all the possible treatment combinations that one wishes to consider in an experiment.

There are various forms of optimality criteria which we shall discuss in chapter five, that are used to select the points for a design. The prominent ones are (i) D-optimality (ii) A-optimality (iii) G-optimality (iv) V-optimality

This dissertation uses D-optimal design criterion to select design points for a multi-factorial experiments which is described in the next sections.

1.2 EXPERIMENTAL PROCEDURE

The experiments are that of I.A.R. – IFDC Fertilizer project (1990) - SAMARU, NIGERIA.

The details descriptions of the experiments are as follows:

Title of Project: Multinutrient interaction trial on maize, sorghum and millet.

Experimental Site: Samaru – Lat. $11^0\ 11^{/}$ N, Long. $7^0\ 38^{/}$ E

Elevation: 704 meters

Nutrients evaluated: Nitrogen (N), Phosphorus (P), Potassium (K), and Sulphur (S)

Other details:

Crop	Maize	Sorghum	Millet
Variety	TZBSR(W)	KSV-8 Farafara	Ex-Borno
Date of planting	6/7/1990	7/7/1990	16/5/1990
Date of harvest	22/10/1990	11/12/1990	28/8/1990

Type of experiment: Experimental station's collaborators

Objectives

1. To determine the response of maize, sorghum and millet to varying rates and combinations of N P K S fertilizers with the view to establishing their requirements by crop in the sub humid tropical savannah.
2. To evaluate the interaction effects of these nutrients on crop yield.
3. To establish the optimum combinations of these nutrients for high yield.

Experimental design: Incomplete factorial combination in a randomised complete block

-viz. 5P × 5N × 3S × 2K.

No. of treatments: 21

Replicates: 3

No. of plots: 63

Plot size: $4.5 \times 6m^2$

Test fertilizer materials:

1. TSP 43% P_2O_5
2. Urea 46% N
3. KCL 60% K_2O
4. Gypsum ($Caso_4.2H_2O$) 17%S

Method of fertilizer application: NPK fertilizers were banded and incorporated. Gypsum was broadcast at planting and incorporated.

DESCRIPTION OF TREATMENTS	
Treatment No.	Treatment combination
1	N_0 P_2 K_1 S_1
2	N_2 P_2 K_1 S_1
3	N_4 P_2 K_1 S_1
4	N_3 P_1 K_1 S_1
5	N_2 P_0 K_1 S_1
6	N_1 P_3 K_1 S_1
7	N_3 P_3 K_1 S_1
8	N_2 P_4 K_1 S_1
9	N_0 P_2 K_1 S_2
10	N_2 P_2 K_1 S_2
11	N_4 P_2 K_1 S_2
12	N_1 P_1 K_1 S_2
13	N_3 P_1 K_1 S_2
14	N_2 P_0 K_1 S_2
15	N_1 P_3 K_1 S_2
16	N_3 P_3 K_1 S_2
17	N_2 P_4 K_1 S_2
18	N_2 P_2 K_0 S_1
19	N_0 P_0 K_0 S_0
20	N_2 P_2 K_1 S_0
21	N_1 P_1 K_1 S_1

Fertilizer rates:

Nitrogen	Maize	Sorghum	Millet
N_0	0 kg N/ha	0 kg N/ha	0 kg N/ha
N_1	30 kg N/ha	20 kg N/ha	20 kg N/ha
N_2	60 kg N/ha	40 kg N/ha	40 kg N/ha
N_3	90 kg N/ha	60 kg N/ha	60 kg N/ha
N_4	120 kg N/ha	80 kg N/ha	80 kg N/ha
phosphorus	Maize	Sorghum	Millet
P_0	0 kg P_20_5/ha	0 kg P_20_5/ha	0 kg P_20_5/ha
P_1	20 kg P_20_5/ha	10 kg P_20_5/ha	10 kg P_20_5/ha
P_2	40 kg P_20_5/ha	20 kg P_20_5/ha	20 kg P_20_5/ha
P_3	60 kg P_20_5/ha	30 kg P_20_5/ha	30 kg P_20_5/ha
P_4	80 kg P_20_5/ha	40 kg P_20_5/ha	40 kg P_20_5/ha
Sulphur	Maize	Sorghum	Millet
S_0	0 kg S/ha	0 kg S/ha	0 kg S/ha
S_1	7.5 kg S/ha	7.5 kg S/ha	7.5 kg S/ha
S_2	15 kg S/ha	15 kg S/ha	15 kg S/ha
Potassium	Maize	Sorghum	Millet
K_0	0 kg K_20/ha	0 kg K_20/ha	0 kg K_20/ha
K_1	60 kg K_20/ha	30 kg K_20/ha	30 kg K_20/ha

Nasal fertilizer treatments: Nil

Plant density: 53,333 stands/ha

Plant spacing: 75 × 25cm

No. of Plants/stand: One

Field preparation: Flat

Parameter estimated: Grain yield

1.3 OBJECTIVES OF THE STUDY

The main aim and objectives of this dissertation are (i) to explore and exploit MATLAB 5.3 to derive D-optimal designs for a multi-factorial experiment under each of three alternative second order response surface models, (ii) to establish D-effeciency and rotatability-effeciency of the optimal designs under each of the three response surface models, and (iii) to determine the optimum Nitrogen, Phosphorus, Potassium and Sulphur (NPKS) fertilizer applications for grain production of maize, sorghum and millet in Savannah zone of Nigeria.

1.4 PURPOSE/SCOPE OF THE STUDY

Response surface methodology is a set of techniques for the design of experiments, analysis of data and interpretation of results in situations where a response variable, y, or several response variables are assumed to depend on the levels of continuous factors, $X_1,...,X_k$, to understand, control or optimise the process under study.

There are several approaches to the realization of RSM objectives, particularly on the criteria of choosing a design. The criteria include the least squares based procedures, the integrated mean square error criterion, the design robustness and the theory of design optimality.

This dissertation focuses mainly on the design optimality theory and most especially the D-optimality criteria. The main aim of the optimality theory is selecting an optimum experimental design which, in most cases is achieved by the use of computer algorithms.

In this research a four factor experiment i.e. effects of fertilizer nutrients (nitrogen, phosphorus, sulphur, potassium) on some crops (maize, sorghum, millet), was used to illustrate how to generate an optimal settings using D-optimality criteria. The percentage of the rotatability of the design was also evaluated.

1.5 SIGNIFICANCE OF THE STUDY

In the above described experiments there are 5 levels of nitrogen (N), 5 levels of phosphorus (P), 3 levels of sulphur (S), and 2 levels of potassium (K). This gives $5\times5\times3\times2 = 150$ treatment combinations. Observe that of the 150 treatment combinations only 21 combinations were used because of limitation of resources and this is only one of the possibilities of 2.248×10^{25} (that is, 150 combinations 21).

Although the experimenters have given these 21 treatment combinations using randomised block incomplete factorial, the criteria used in selecting the combinations cannot be justified. Questions such as why this set of 21 out of the total $2.248 \times 10^{25}$and not others, are they the best, how were they selected, naturally arises. In order to attempt answering these posed questions, we constructed a D-optimum design for the experiments, which gives a feasible and empirical results (or optimal settings for the experiments).

The settings given by the experimenter had been used with a first order model quite often. Hitherto, we have noted that in using the given settings with a general linear model there is high possibility of lack of fit and that, because of the nature of the settings, other models that include the quadratic and interaction terms might be more appropriate.

Therefore the D-optimal design criterion which assumes a prespecified model in selecting optimal or near optimal points was used to obtain the optimal settings.

1.6 LIMITATIONS

The D-optimality criterion used in this dissertation is the most important and widely used in response surface applications (Atkinson and Donev, 1992). It has the advantages of the possibility to use irregular shapes and to include extra design points. There are other optimality criteria like A-optimality, G-optimality, V-optimality, etc. which may also be used in generating designs and we have not compared their performances with the D-optimal designs. Likewise the Pronzato's (2002) procedure for eliminating non desirable points from the required support points could have accelerated the early achievement of the optimal settings. But the detail algorithm wasn't available for our usage as yet.

Also, in generating the designs we only took cognisance of complete randomization process. Blocking response surfaces which is also an emerging research area in RSM was not used for the purpose of this research.

1.7 DEFINITION OF TERMS

(a) Analysis of Variance (ANOVA): A mathematical process for separating the variability of a group of observations into assignable causes and setting up various significant tests.

(b) Balanced Design: A design experiment where all elementary contrasts have equal variances.

(c) Blocking: A schedule for conducting treatment combinations in an experimental study such that any effects on the experimental results due to a known change in raw materials, operators, machines, etc., become concentrated in the levels of the blocking variable. Note: the reason for blocking is to isolate a systematic effect and prevent it from obscuring the main effects. Blocking is achieved by restricting randomization.

(d) Center Points: Points at the center value of all factor ranges.

(e) Coding Factor Levels: Transforming the scale of measurement for a factor so that the high value becomes +1 and the low value becomes -1. After coding all factors in a 2-level full factorial experiment, the design matrix has all orthogonal columns.

Coding is a simple linear transformation of the original measurement scale. If the "high" value is X_h and the "low" value is X_L (in the original scale), then the scaling transformation takes any original X value and converts it to

$(X-a)/b$, where $a = (X_h + X_L)/2$ and $b = (X_h - X_L)/2$.

To go back to the original measurement scale, just take the coded value and multiply it by "b" and add "a" or, X = b(coded value) + a.

(f) Confounding: Is one where some treatment effects (main or interactions) are estimated by the same linear combination of the experimental observations as some blocking effects In this case, the treatment effect and the blocking effect are said to be confounded. Confounding is also used as a general term to indicate that the value of a main effect estimate comes from both the main effect itself and also contamination or bias from higher order interactions.

Note: confounding effects naturally arises when full factorial designs have to be run in blocks and the block size is smaller than the number of different treatment combinations. They also occur whenever a fractional factorial design is chosen instead of a full factorial design.

(g) Design: A set of experimental runs which allows you to fit a particular model and estimate your desired effects.

(h) Design matrix: A matrix description of an experiment that is useful for constructing and analyzing experiments.

(i) Effect: How changing the setting of a factor changes the response. The effect of a single factor is also called main effect.

(j) Error: Unexplained variation in a collection of observations. Note: DOE's typically require understanding of both random error and lack of fit.

(k) Experimental Unit: The entity to which a specific treatment combination is applied. Note: an experimental unit can be individual agricultural plant, plot of land, etc.

(l) Factors: Process input an investigator manipulates to cause a change in the output. Some factors cannot be controlled by the experimenter but may affect the responses. If their effect is significant, these uncontrolled factors should be measured and used in the data analysis. Note: The inputs can be discrete or continuous.

Crossed Factors: Two factors are said to be crossed if every level of one factor occurs with every level of the other factor in the experiment.

Nested Factors: A factor “A” is nested within another factor “B” if the levels or values of “A” are different for every level or value of “B”. Note: Nested factors or effects have a hierarchical relationship.

(m) Fixed effect: An effect associated with an input variable that has a limited number of levels or in which only a limited number of levels are of interest to the experimenter.

(n) Interactions: Occurs when the effect of one factor on a response depends on the levels of another factor(s).

(o) Lack of Fit Error: Error that occurs when the analysis omits one or more important terms or factors from the process model. Or when the model is intrinsically incorrect. Note: Including replication in a DOE allows separation of experimental error into two components: lack of fit and random (pure) error.

(p) Model: Mathematical relationship which relates changes in a given response to changes in one or more factors.

(q) Orthogonality: Two vectors of the same length are orthogonal if the sum of the products of their corresponding elements is 0. Or when variance-covarince matrix of the effects is diagonal. Note: An experimental design is orthogonal if the effects of any factor balance out (sum to zero) across the effects of the other factors.

(r) Random Effect: An effect associated with input variables chosen at random from a population having a large or infinite number of possible values.

(s) Random error: Error that occurs due to natural variation in the process. Note: Random error is typically assumed to be normally distributed with zero mean and a constant variance.

(t) Randomization: A schedule for allocating treatment material and for conducting treatment combination in a DOE such that the conditions in one run neither depend on the conditions of the previous run nor predict the conditions in the subsequent runs. Note: The importance of randomization cannot be over stressed. Randomization is necessary for conclusions drawn from experiment to be correct, unambiguous and defensible.

(u) Replication: Performing the same treatment combination more than once. Note: Replication allows an estimate of the random error independent of any lack of fit error.

(v) Responses: The output(s) of a process. Sometimes called dependent variable(s).

(w) Response Surface Designs: A DOE that fully explores the process window and models the responses.

(x) Rotatability: A design is rotatable if the variance of the predicted response at any point X depends only on the distance of X from the design center point. A design with this property can be rotated around its center point without changing the prediction variance at X. Note: Rotatability is a desirable property for response surface designs.

(y) Scaling Factor Levels: Transforming factor levels so that the high value becomes +1 and the low value becomes -1.

(z) Screening Designs: A DOE that identifies which of many factors have a significant effect on the response. Note: Typically, screening designs have more than five factors.

(aa) Treatment: A treatment is a specific combination of factor levels whose effect is to be compared with other treatments.

(bb) Treatment Combination: The combination of the settings of several factors in a given experimental trial. Also known as a run.

(cc) Variance Components: Partitioning of the overall variation into assignable components.

CHAPTER TWO

LITERATURE REVIEW

2.1 INTRODUCTION

This chapter considers the history and developments in RSM, where several literatures in the area of RSM were reviewed.

2.2 THE EMERGENCE AND DEVELOPMENT OF RESPONSE SURFACE METHODS

The genesis of response surface methodology (RSM) can be traced back to the works of J. Wishart, C.P. Winsor, E.A. Mitscherlich, F. Yates, and others in the early 1930s or even earlier. However it was not until 1951 that RSM was formally developed by G.E.P. Box and K.B. Wilson and other colleagues at Imperial Chemical Industries in England, (Box and Wilson, 1951). Their objective was to explore relationships such as those between the yield of a chemical process and a set of input variables presumed to influence the yield. Since the pioneering work of Box and his co-workers, RSM has been successfully used and applied in many diverse fields such as chemical engineering, industrial development and process improvement, agricultural and biological research, even computer simulation, to mention just a few.

The applications of RSM can be found in Edmondson (1991), Smith et al. (1997), Mountzouris et al. (1999a, 1999b, 2001), Regalado et al. (1994), Rosenthal et al. (2001), Kikafunda et al. 1998, Jauregi et al. (1997), Trinca and Gilmour (1998, 1999, 2000a, 2000b, 2001), Gilmour and Ringrose (1999), Gilmour and Trinca (2003), Gilmour and Mead (2003).

However, there are several procedures that are used in the realization of RSM objectives, especially in the area of criteria for choosing a design. These ranges from the least squares based procedures, the integrated mean square error (IMSE) criterion, the theory of design optimality and the design robustness. In our work we focussed mainly on the theory of design optimality and in particular the D-optimality criterion.

Optimal design theory was developed mainly after World War II. Kiefer (1958, 1959, 1960, 1961, 1962a, 1962b) is attributed to having provided the basic mathematical groundwork for optimal design theory. Presently there are two schools of thought regarding the application of the principles of optimal design theory to the derivation of response surface designs: the "Kiefer school" and the "Box school." In the latter school, bias suspected of being present in the fitted model plays a significant role. In the Kiefer school, however, bias is regarded as insignificant or it does not exist. The main preoccupation in this school is, therefore, with designs that minimize the variance associated with the fitted model, $\hat{y}(x)$.

The aim of the optimality theory is selecting an optimum experimental design which, in most cases, needs to be multifaceted. Therefore the problem of selecting a suitable design is thus a formidable one (Box and Draper, 1987). The optimum designs are usually constructed using computer algorithm and are therefore referred to as computer-aided designs. One form of the computer-aided designs is the D-optimal designs. It possesses the most important design criterion in applications (Atkinson and Donev, 1992). These types of computer-aided designs are particularly useful when classical designs do not apply. Unlike standard classical designs such as factorials and fractional factorials, D-optimal design matrices are usually not orthogonal and effect

estimates are correlated. The D-optimal designs are always an option regardless of the type of model the experimenter wishes to fit (for example, first order, first order plus some interactions, full quadratic, cubic, etc.) or the objective specified for the experiment (for example, screening designs, response surfaces, etc.). The optimality criterion used in generating D-optimal designs is one of maximizing |X'X|, the determinant of the information matrix X'X.

Several researches related to D-optimum designs have been undertaken. Mitchell (1974a, 1974b) in his two papers gave algorithms for the construction of 'D-optimal' experimental designs, Mitchell and Bayne (1978) discussed the D-optimal fractions of three-level factorial designs, Galil and Kiefer (1980) in their paper considered time-and space-saving computer methods, related to Mitchell's DETMAX, for finding D-optimal designs. Cook and Nachtsheim (1980) compared algorithms for constructing exact D-optimal designs. A recent work by DuMouchel and Jones (1994) gave a simple Bayesian modification of D-optimal to reduce dependence on an assumed model. Johnson and Nachtsheim (1983) gave some guidelines for constructing Exact D-optimal designs on convex design spaces. Some of the other works on D-optimal designs include Cook and Nachtsheim (1989), Dykstra (1971), Harville (1974), Johnson et al. (1990), Mitchell and Miller (1970), Snee (1985), Ogolime and Bamiduro (1998), Chigbu (1998), Vance (1986) and Pronzato (2002) who showed in his paper how it is possible, during the search for an optimum design, to remove from X some design points that cannot be support points of the optimum design in order to accelerate the D-optimum design algorithms. Some of the studies on D-optimum designs are the comparison of Lucas (1976) and of Donev and Atkinson (1988) they showed that central composite designs behave well according to the

criteria of D- and G-optimality and also for the average variance criterion, V-optimality. However, the designs are restricted to a few values of N. if a design of a rather different size is required; it will either have to be generated by computer search or looked up in a catalogue. However, for the background theories of optimal experiments see Federov (1972).

The nature of our research problem also calls for generation by a computer search a D-optimal design.

In the next section the various standard experimental designs used in optimality theory are presented.

2.3 STANDARD DESIGNS

2.3.1 Full factorial design

To construct an approximation model that can capture interactions between N design variables, a full factorial approach (Khuri and Cornell, 1996) may be necessary to investigate all possible combinations. A factorial experiment is an experimental strategy in which design variables are varied together instead of one at a time.

The lower and upper bounds of each of K design problem needs to be defined. The allowable range is then discretized to different levels. If each of the variables is defined at only the lower and upper bounds (two levels), the experimental design is called 2^K full factorial. Similarly, if the midpoints are included, the design is called 3^K full factorial. A case of 2^3 is shown in Figure 2.1.

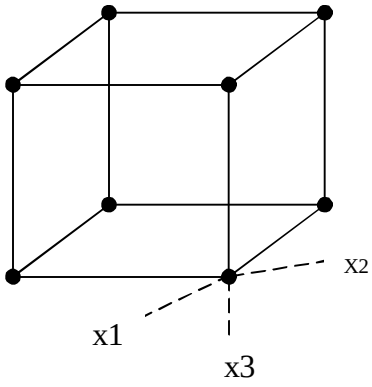


Figure 2.1 A 2^3 full factorial design (8 points)

Factorial designs can be used for fitting second-order models. A second-order model can significantly improve optimisation process when a first-order model suffers lack of fit due to interaction between variables and surface curvature.

A full factorial design is typically for five or fewer variables. If the number of design variables becomes large, a fraction of a full factorial design can be used at the cost of estimating only a few effects of the combinations between variables. This is called fractional factorial and is usually used for screening important design variables. For a 3^K factorial design, a $[1/3]^p$ fraction can be constructed, resulting in 3^{K-p} points. For example, for $p = 1$ in a 3^3 design, the result is a one-third fraction, often called 3^{3-1} design.

The full factorial design used for first-order models is the 2^K factorial designs and possibly its fractional replicates. While the one used for second-order models is the3^K factorial designs and its fractional replicates (Khuri and Cornell, 1996).

However, with more than three x- variables in 3^K series, the experiment becomes too large, and also the coefficients β_{11}, β_{22} of the squared terms are estimated with relatively low precision (Box and Wilson, 1951). Because of the disadvantages (of magnitude and relatively low precision) of the 3^k series, Box and Wilson (1951)

developed new designs specifically for fitting second-order response surfaces. Their earliest designs, called composite designs, were constructed by adding further treatment combinations to those obtained from a 2^k factorial.

2.3.2 Central composite design

A central composite design (CCD) due to Box and Wilson (1951) consists of

1. A complete (or fraction of a) 2^K factorial design, where the factor levels are coded to the usual –1, +1 values. This is called the factorial portion of the design.

2. n_0 centre points ($n_0 \geq 1$) replications.

3. Two axial point on the axis of each design variable (2k) at a distance of α from the design centre. This portion is called the axial portion of the design.

The total number of design points is thus $N = 2^k + 2k + n_0$. The precise values of n_0 and α are chosen depending on certain properties (e.g. rotatability and orthogonality) desired for the design and on the number of factors involved. For instance if it is desired that the CCD should be rotatable then, $\alpha = F^{1/4}$ and $n_0 = 4\sqrt{F} + 4 - 2k$, where F is the number of points in the factorial portion of the design (Khuri and Cornell, 1996). For example, a CCD in k = 2 variables with $n_0 = 1$ and $\alpha = \sqrt{2}$ is of the form

x_1	x_2
-1	-1
1	-1
-1	1
1	1
$\sqrt{2}$	0
$-\sqrt{2}$	0
0	$\sqrt{2}$
0	$-\sqrt{2}$
0	0

The design points are presented graphically in Figure 2.2

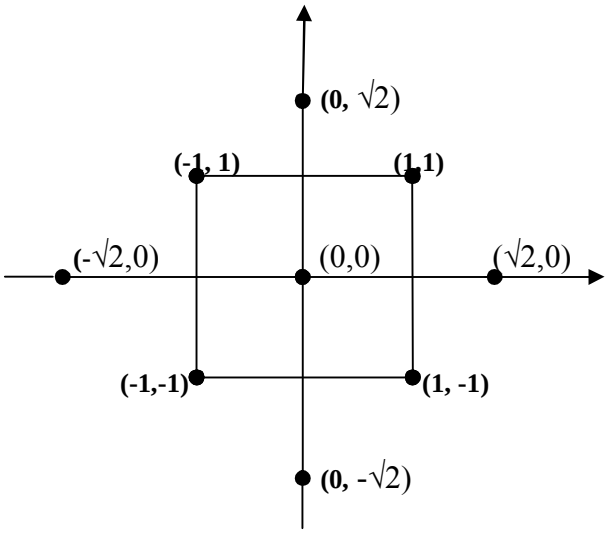


Figure 2.2 Central Composite rotatable design in two x-variables.

In Figure 2.2, the design involves 2^k (2^2) factorial points, 2K (2*2 = 4) axial points and 1 central point.

CCD presents an alternative to 3^k designs in the construction of second-order models because the number of experiments is reduced as compared to a full factorial design.
For instance a 2, 3 and 4 k-variables in a single replicate the CCD experiment requires 9, 15 and 25 units respectively, as compared with 9, 27 and 81 in the 3^k full factorial designs. CCD has been used by Gilmour and Trinca (2003) for Row-Column response surface designs.

The central composite designs satisfy the general requirements of response surface designs (Mead, 1988), which are:

(i) that the parameters of the model to be fitted can be estimated,

(ii) that the number of treatment combinations is not allowed to become too large, and

(iii) the observations are spread fairly evenly over the region within which information about the surface is required.

The last characteristic is very important, but is difficult to appreciate because it involves an assessment of the spread of points in n-dimensional space (Mead, 1988).

However in the case of problems with a large number of design variables, the experiments may be time-consuming even with the use of CCD.

2.3.3 Box-Behnken design

A class of three-level incomplete factorial designs for the estimation of the parameters in a second-order model was developed by Box-Behnken (1960). By definition, a three-level incomplete factorial design is a subset of factorial combinations from the 3^k factorial design. The Box-Behnken designs are formed by combining two-level factorial designs with balanced incomplete block designs (BIBD) in a particular manner. These designs require fewer treatment combinations than a central composite design in cases involving 3 or 4 factors. The Box-Behnken design is rotatable (or nearly so) but it contains regions of poor prediction quality like the CCD. Its "missing corners" may be useful when the experimenter wants to avoid combination of factors at their extreme levels. This property prevents a potential loss of data in those cases (Engineering Statistics Hand book, 2004).

Khuri and Cornell (1996) gave an illustration on the construction of Box-Behnken as follows:

Consider a BIBD involving four treatments and six blocks with each block containing two treatments. Each treatment appears three times in the design, once with

each of the other treatments. If the treatments are denoted by asterisks (*), we obtain the design

Treat.	X_1	X_2	x_3	x_4
1	*	*		
2			*	*
3	*			*
4		*	*	
5		*		*
6	*		*	

We now combine the preceding BIBD with the 2^2 factorial design

$$\begin{array}{cc} x_i & x_j \\ \begin{bmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{bmatrix} & \end{array}$$

in the following manner: The two asterisks in every block are replaced by the two columns of the 2^2 design. A column of zeros is included when no asterisk appears. The design is augmented by the addition of centre points, three being used in this example. The resulting three-level Box-Behnken design in four variables consists of the following 27 points:

x_1	x_2	x_3	x_4
-1	-1	0	0
1	-1	0	0
-1	1	0	0
1	1	0	0
0	0	-1	-1
0	0	1	-1
0	0	-1	1
0	0	1	1
0	0	0	0
-1	0	0	-1
1	0	0	-1
-1	0	0	1
1	0	0	1
0	-1	-1	0
0	1	-1	0
0	-1	1	0
0	1	1	0
0	0	0	0
0	-1	0	-1
0	1	0	-1
0	-1	0	1
0	1	0	1

-1	0	-1	0
1	0	-1	0
-1	0	1	0
1	0	1	0
0	0	0	0

The design obtained is rotatable and blocks orthogonally in three-blocks indicated by the dotted lines. In general, however, Box-Behnken designs are not always rotatable nor are they block orthogonal.

The designs described in section 2.3 above are the designs that commonly feature during response surface optimizations.

However, Box and Draper (1975) list 14 properties of a response surface design, any, all, or some of which might be important, depending on the experimental circumstances. The properties are that, the design should:

1. Generate a satisfactory distribution of information throughout the region of interest.
2. Ensure that the fitted value at x, $\hat{y}(x)$, be as close as possible to the true value at x, $\eta(x)$.
3. Give good detectability of model lack of fit.
4. Allow transformations to be estimated
5. Allow experiments to be performed in blocks.
6. Allow designs of increasing order to be built up sequentially.
7. Provide an internal estimate of the error variance σ^2.

8. Be insensitive to wild observations and to violation of the usual normal theory assumptions.
9. Require a minimum number of experimental points.
10. Provide simple data patterns that allow ready visual appreciation.
11. Ensure simplicity of calculation of the model parameter estimates.
12. Behave well when errors occur in the settings of the predictor variables, the x's.
13. Not require an impractically large number of levels of the predictor variables.
14. Provide a check on the "constancy of variance" assumption.

These requirements are sometimes conflicting, sometimes confluent and in any specific situation, judgement is required to select the design that achieves the best compromise (Box and Draper, 1987).

In addition to the properties listed above, there are times when we shall want the design to possess the property of orthogonality and/or the property of rotatability (Khuri and Cornell, 1996). These two properties now turn out to be almost the most important in response surface designs.

Orthogonality and Rotatability

An orthogonal design is one in which the terms in the fitted model are uncorrelated with one another and thus the parameter estimates are uncorrelated. In this case, the variance of the predicted response at any point x in the experimental region, is expressible as a weighted sum of variances of the parameter estimates in the model. A first-order design, for example, is orthogonal if and only if the corresponding $X'X$ matrix is diagonal.

With a rotatable design, on the other hand, the variance of $\hat{Y}(x)$, which is known to depend on the location of the point x, is a function only of the distance from the point x to the centre of the design. Thus, with a rotatable design, the prediction variance, var[$\hat{Y}(x)$], is the same at all points x that are equidistant from the design centre. Consequently in the space of the input variables, surfaces of constant prediction variance form concentric hyperspheres (circles and spheres in two-dimensional and three-dimensional Euclidean spaces respectively). This constant variance property of the predictor, $\hat{Y}(x)$, is quite appealing when one is faced with determining in which direction to experiment next.

The concept of rotatability was first introduced by Box and Hunter (1957) and has since become an important design criterion. One of the desirable features of rotatability is that the quality of prediction as measured by the magnitude of var[$\hat{Y}(x)$], is invariant to any rotation of the coordinate axes in the space of the input variables.

However, in the literature on RSM, it is often stated, or assumed implicitly, that interest centres on estimating the response at all combinations of levels of the factors within some region of interest (which is referred to as response surface designs). If a model is an adequate representation of the true mean response, then a design chosen for estimating the parameters must support the model to provide adequate prediction of the true response throughout the region of interest.

There are several RSM optimization procedures. In the next chapter we described with an illustration one of the procedures for RSM optimizations i.e. the path of steepest ascent.

CHAPTER THREE

RSM OPTIMIZATION PROCEDURE (PATH OF STEEPEST ASCENT)

3.1 INTRODUCTION

In this chapter we considered one of the RSM optimizations procedures i.e. the Path of Steepest Ascent (PSA). The determination of optimal settings of the experimental factors that produce the maximum (or minimum) value of the response in RSM is achieved using the path of steepest ascent as follows.

3.2 RSM Experimental Optimisation Procedure (PSA)

(i) Plan and run a factorial (or fractional factorial) design near/at a starting point. (x_1^0 , x_2^0 ,….)

(ii) Fit a linear model (excluding interaction or quadratic terms) to the data.

(iii) Determine path of steepest ascent (PSA) – a quick way to move to the optimum that is gradient based.

(iv) Run tests on PSA until response no longer improves.

(v) If curvature of surface (like quadratic or cubic surfaces) is large go to step (vi), else go to step (i).

(vi) Neighbourhood of optimum – design, run, and fit (using least squares) a second order model.

(vii) Based on second order model – pick optimal settings of independent variables.

Path of Steepest Ascent (PSA): When the first experiment has been completed, the region of experimentation is shifted to another set of levels of the x's. This set is to be chosen so that the maximum expected increase in y occurs. If the centre of the first experiment is taken as the origin, the problem is to move from the origin with x-

coordinates (0,0,…0), to the position p, with coordinates (x'_1, x'_2, ….x'_k), so that the response y(x'_1, x'_2, ….x'_k) is maximized.

The change in y clearly depends on the size of the jump that is made from o to the point p, i.e., on whether we change the x's by small or by large amounts. By geometrical analogy, the "distance" r from 0 to p is defined as:

$$r = \sqrt{(x'_1{}^2 + x'_2{}^2 + \ldots. + x'_k{}^2)} \qquad (3.1)$$

We suppose that the experimenter has chosen the value of r.

For a given value of r, i.e., a given size of jump, we determine the values of the x_i that maximize y (x_1, x_2 …x_k). The path of steepest ascent is the path from o to the point p whose coordinates are these maximizing values of x_i.

By calculus, the maximizing values of the x_i are given by the equations

$x_i = \mu\, dy/dx_i$, where dy is the partial derivative of y with respect to x_i taken at the point p, and μ is a multiplier calculated so as to satisfy equation (3.1) above. The actual value of μ is $r / \sqrt{\Sigma(dy/dx_i)^2}$.

In order to apply this method, we must estimate the partial derivatives dy/dx_i from the results of the first experiment. This task is simplified if y can be satisfactorily represented by a linear equation $\hat{y} = y_0 + b_1x_1 + b_2x_2 + \ldots b_kx_k$, Where y_0 is the value of y at origin.

From the linear function it follows that $dy/dx_i = b_i$

Thus the change in x_i in the path of steepest ascent is proportional to b_i, provided that the linear equation holds.

The above procedure is comprehensively given in a flow diagram due to Box et al. (1978).

The RSM experimental procedure has been used by Edmondson (1991), Gilmour and Mead (1995), Smith et al. (1997), Gilmour and Ringrose (1999), Gilmour and Trinca (2003). For a detail illustrations see Bamanga and Asiribo (2005).

3.3 ILLUSTRATION OF RSM PROCEDURE

We now illustrate the above procedure step by step using an example.

Step (i): Plan and run a factorial (or fractional factorial) design near/at a starting point. (x_1^0 , x_2^0 ,….)

Consider the given example on page 3 on an experiment on optimisation of froth flotation process (desired to whiten a wood pulp mixture). Two independent variables, concentration of environmentally safe bleach (X_1) and mixture temperature (X_2) were used. The current operating points of the two independent variables are 4% bleach and 80^0F (which is believed to be well away from the optimum). The allowable variable ranges are 0-20% bleach and 60^0F- 130^0F temperature. The layout of the initial 2^2 factorial design and the subsequent result of the experiment are given below in Tables 4.1 and 4.2 respectively.

Variable	Low Level	High Level
(1) % Bleach	2	6
(2) Temperature, ^{0}F	75	85

Table 3.1 Layout of an initial 2^2 factorial design.

% Bleach (X_1)	Temperature, ^{0}F (X_2)	Coded variables		Process response (y)
		x_1	x_2	
2	75	-1	-1	19
6	75	1	-1	31
2	85	-1	1	28
6	85	1	1	44

Table 3.2 Result of the 2^2 factorial design of Froth flotation process.

In the above example one may wish to find the levels of bleach (X_1) and temperature (X_2) that maximize the response flotation process (y). The response flotation process is a function of the levels of bleach and temperature, as follows:

$$y = f(x_1, x_2) + \varepsilon \qquad (3.2)$$

where ε represents the error or noise observed in the response y. The surface represented by $f(x_1, x_2)$ is called a response surface.

Step (ii): Fit a linear model (excluding interaction or quadratic terms) to the data.

The design planned and ran above (2^2 factorial design) is a member of the first-order designs. Hence, we fit a linear model (no interaction or quadratic terms) to the data, using STATISTICA for windows (1995).

Main effects, interaction and the fitted model

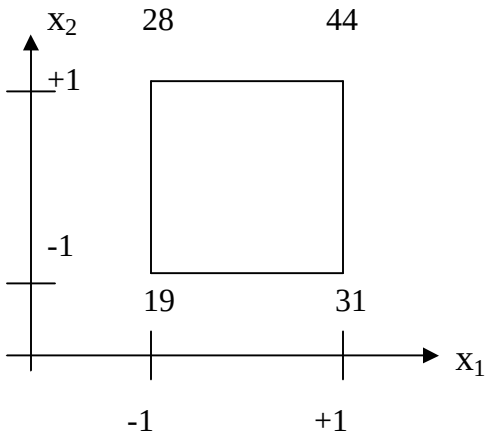


Fig. 3.1 Diagram of results of the 2^2 factorial design of Froth flotation process.

The average = 30.5

The main effects of X_1 = ½{(44-28) + (31-19)} = 14,

X_2 = ½ {(28-19) + (44-31)} =11 and the interaction

X_1X_2 = ½ {16-12} = 2(it is small relative to X_1 and X_2, so the response is linear).

The fitted linear model is: $\hat{y} = 30.5 + 7\,x_1 + 5.5x_2$

From table 1.1, a one unit change in x_1 is a change of 2% in bleach. A one unit change in x_2 is a change of 5 degree in temperature.

The coding rule used for the variables (see Table 3.2) was

$x_1 = \frac{\%\ \text{bleach} - 4}{2}$, bleach % = $2x_1 + 4$.

$x_2 = \frac{\text{Temp} - 80}{5}$, Temp = $5x_2 + 80$.

Step (iii): Determine path of steepest ascent (PSA) – a quick way to move to the optimum that is gradient based.

We want to move from our starting point ($x_1 = 0$, $x_2 = 0$ or %bleach = 4, Temp = 80) in the direction that will increase the response the fastest. Thus, we want to move in a direction normal to the contours which is achieved through the path of steepest ascent. This is the line passing through point ($x_1 = 0$, $x_2 = 0$) that is perpendicular to the contours. That is:

. Define contour passing through (0,0) $\hat{y} = 30.5 + 7\,x_1 + 5.5x_2 = 30.5$

. relation between x_1 and x_2 for this contour $7\,x_1 + 5.5x_2 = 0$ or $x_2 = -7\,x_1 / 5.5$

. Line normal to this contour (slope of PSA = $\frac{-1}{\text{contour slope}}$)

. $x_2 = 5.5x_1 / 7$

. Hence, for a one unit change in x_1, x_2 must change by 5.5/7.0 units to remain on the PSA. A 7 unit change in x_1 implies a 5.5 unit change in x_2.

Let's define some points (candidate tests) on the path of steepest ascent (PSA) as follows:

Candidate Test	x_1	$X_2 = 5.5x_1 / 7$	bleach % $= 2x_1 + 4$	Temp $= 5x_2 + 80$	Y
1	0	0	4	80	
2	0.5	0.39	5	82	
3	1.0	0.79	6	84	43
4	1.5	1.18	7	86	49
5	2.0	1.57	8	88	52
6	2.5	1.96	9	90	59
7	3.0	2.36	10	92	66
8	3.5	2.75	11	94	75
9	4.0	3.14	12	96	81
10	**4.5**	**3.54**	**13**	**98**	**86**
11	5.0	3.93	14	100	80
12	5.5	4.32	15	102	69
13	6.0	4.71	16	104	

Table 3.3 Test plan 1.

Since it appears that the response surface is fairly linear (with the interaction X_1X_2 small) in the region covered by the tests, no reason to examine/conduct test 1 or 2 in Table 3.3.

Step (iv): Run tests on PSA until response no longer improves.

We run 1st test on or beyond boundary defined by x_1, $x_2 = \pm 1$. Continue running tests on the PSA until response no longer increases. Highest response occurs at (Bleach = 13%, Temp = 98^0). We run new factorial at this point as shown in Table 3.4.

Table 3.4 Result of the second 2^2 factorial design of Froth flotation process.

% Bleach (X_1)	Temperature, ^{0}F (X_2)	Coded variables		Process response (y)
		X_1	X_2	
12	92	-1	-1	75
14	92	1	-1	88
12	102	-1	1	77
14	102	1	1	76

Main effects, interaction and the fitted model

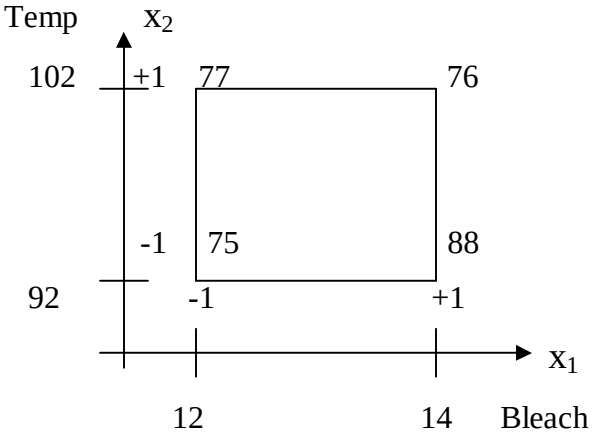


Fig. 3.2 Diagram of Results of the second 2^2 factorial design of Froth flotation process.

The average = 79

The main effects of X_1 = ½{(76-77) + (88-75)} = 6,

X_2 = ½ {(77-75) + (76-88)} = -5 and the interaction

X_1X_2 = ½ {-1-13} = -7(it is fairly large).

The fitted linear model is: $\hat{y} = 79 + 3x_1 - 2.5x_2$ describes response surface with a plane.

At $x_1 = 0$, $x_2 = 0$, $\hat{y} = 79$

The combinations of (x_1,x_2) that give $\hat{y} = 79$ are specified by:

$3x_1 - 2.5x_2 = 0$ or $x_2 = 3x_1/2.5$ which implies the relationship along the contour slope of PSA = $\frac{-2.5}{3}$ $x_1 = -0.833\ x_1$ or $x_1 = -1.2\ x_2$

Step (v): If curvature of surface (like quadratic or cubic surfaces) is large go to step (vi), else go to step (i).

Let's follow the PSA but take steps in the x_1 direction since X_1 bigger than X_2.

Candidate Test	x_1	$x_2 = -0.833x_1$	bleach % = $13+x_1$	Temp = $97+5x_2$	Y
1	0	0	13	97	
2	0.5	-0.4165	13.5	94.9	
3	1.0	-0.833	14	92.8	88
4	1.25	-1.04125	14.25	91.8	90
5	**1.5**	**-1.2495**	**14.50**	**90.8**	**92**
6	1.75	-1.4578	14.75	89.7	89
7	2.00	-1.666	15.00	88.7	84
8	2.25	-1.87425	15.25	87.6	
9	2.50	-2.0825	15.50	86.6	
10	2.75	-2.29075	15.75	85.5	
11	3.00	-2.50	16.00	84.5	

Table 3.5 Test plan 2.

From Table 3.5, highest response at Bleach 14.50%, Temperature 90.8^0 implies 92% Whiteness.

Note that we weren't able to move as far along the path before we "fell off".

Step (vi): Neighbourhood of optimum – design, run, and fit (using least squares) a second order model.

We now believe we are fairly close to the optimum, so we must characterize the response surface with more than a plane, perhaps a model of the form:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon \qquad (3.3)$$

and the fitted model $y = b_0 + b_1 x_1 + b_2 x_2 + b_{12} x_1 x_2 + b_{11} x_1^2 + b_{22} x_2^2 + \varepsilon$

To estimate the β's in this model, we need more than a 2- level factorial design. A Central Composite Design (CCD) is more efficient than a 3- level factorial design (Box and Wilson, 1951).

A plan of the central composite design is shown in fig. 3.3 for a two factorial experiment.

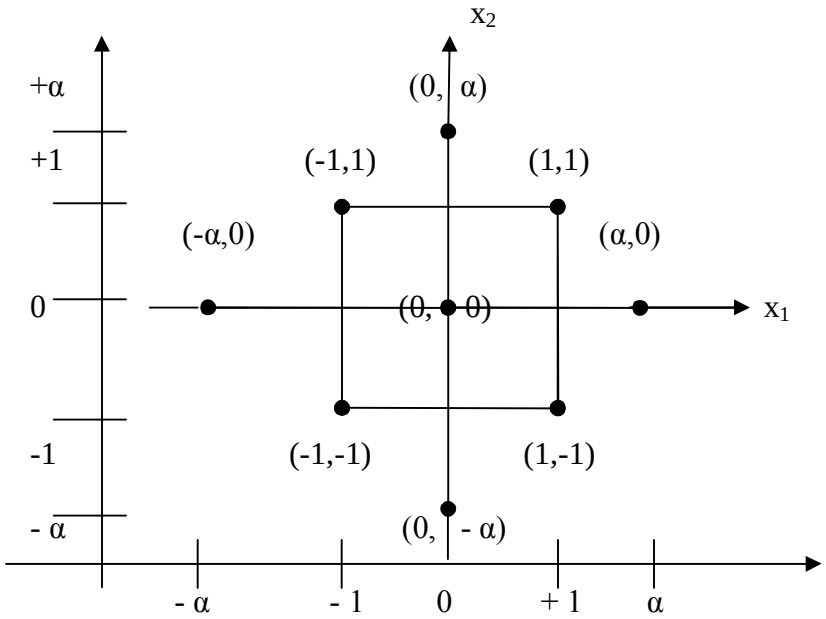


Fig. 3.3 Diagram of Central Composite Design.

In general, a central composite design (CCD) consists of 2^k points that form the base design, 2k star points, and several centre points. A star point, often denoted as α is generally defined as $\alpha = F^{1/4}$ where $F= 2^k$. Thus for our example, the total number of runs/tests is given as 9 where $\alpha = \sqrt{2}$. Table 3.6 gives the resulting test plan.

Test	X_1	X_2	Bleach (%)	Temp (deg)	y
1	-1	-1	13.5	86	87
2	+1	-1	15.5	86	85
3	-1	+1	13.5	96	89
4	+1	+1	15.5	96	83
5	-√2	0	13.1	91	86
6	+√2	0	15.9	91	82
7	0	-√2	14.5	84	98
8	0	+√2	14.5	98	87
9	0	0	14.5	91	92

Tab1e 3.6. Test plan 3.

To fit the model in equation (3.6), we use the unit square matrix approach.

Define the information matrix as

$$x = \begin{bmatrix} 1 & -1 & -1 & +1 & +1 & +1 \\ 1 & +1 & -1 & -1 & +1 & +1 \\ 1 & -1 & +1 & -1 & +1 & +1 \\ 1 & +1 & +1 & +1 & +1 & +1 \\ 1 & -\sqrt{2} & 0 & 0 & 2 & 0 \\ 1 & +\sqrt{2} & 0 & 0 & 2 & 0 \\ 1 & 0 & -\sqrt{2} & 0 & 0 & 2 \\ 1 & 0 & +\sqrt{2} & 0 & 0 & 2 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$Y = \begin{bmatrix} 87 \\ 85 \\ 89 \\ 83 \\ 86 \\ 82 \\ 98 \\ 87 \\ 92 \end{bmatrix}$$

then,

$$(x^T x) = \begin{bmatrix} 9 & 0 & 0 & 0 & 8 & 8 \\ 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 \\ 8 & 0 & 0 & 0 & 12 & 4 \\ 8 & 0 & 0 & 0 & 4 & 12 \end{bmatrix}$$

$$(x^T x)^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & -0.5 & -0.5 \\ 0 & 0.125 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.125 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.25 & 0 & 0 \\ -0.5 & 0 & 0 & 0 & 0.344 & 0.219 \\ -0.5 & 0 & 0 & 0 & 0.219 & 0.344 \end{bmatrix}$$

$$(x^T y) = \begin{bmatrix} 789 \\ -13.657 \\ -15.556 \\ -4 \\ 680 \\ 714 \end{bmatrix}$$

and the least square estimates are given as

$$b = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_{12} \\ b_{11} \\ b_{22} \end{bmatrix} = (x^T x)^{-1} x^T y = \begin{bmatrix} 92 \\ -1.707 \\ -1.945 \\ -1.000 \\ -4.563 \\ -0.313 \end{bmatrix}$$

The fitted model is now,

$$\hat{y} = 92 - 1.707x_1 - 1.945x_2 - 1.000x_1x_2 - 4.563\, x_1^2 - 0.313\, x_2^2$$

and is graphically shown below.

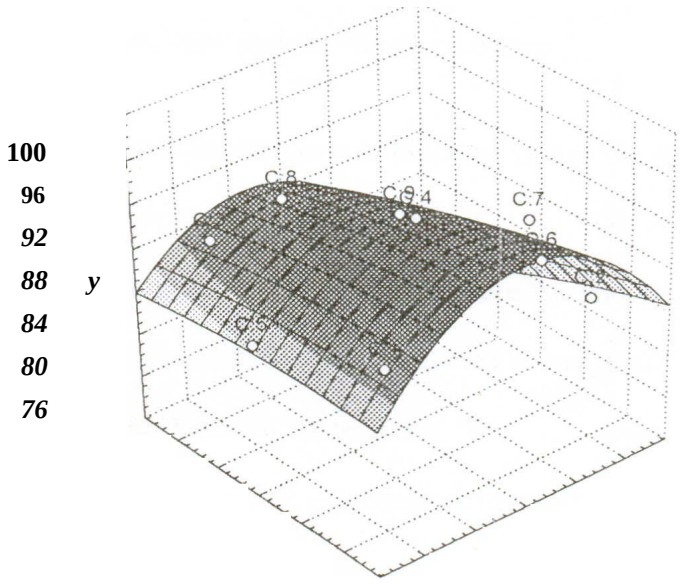


Fig. 3.4 The three-dimensional predicted froth flotation process response surface as a function of % bleach and temperature (X1and X2).

Step (vi): Based on second order model – pick optimal settings of independent variables.

The fitted model, $\hat{y} = 92 - 1.707x_1 - 1.945x_2 - 1.000x_1x_2 - 4.563\ x_1^2 - 0.313\ x_2^2$, has a maximum value of 92 over design region at $x_1 = 0$ and $x_2 = 0$.

From Table 6, that is, test plan 3, the value $\hat{y} = 92$ coincides with the bleach = 14.5% and temperature = 91^0, which are the recommended maximum (optimal) settings.

This recommendation can also be confirmed if we critically observe the table of predicted and residual values below.

s/n	1	2	3	4	5	6	7	8	9
Design Points	(-1,-1)	(1,-1)	(-1,1)	(1,1)	(-√2,0)	(√2,0)	(0,-√2)	(0, √2)	(0,0)
Predicted Values	89.78	88.36	87.89	82.47	85.29	80.46	94.13	88.63	92
Residual Values	-2.78	-3.36	1.11	0.53	0.71	1.54	3.87	-1.63	-0.00

Table 3.7 Predicted and residual values.

We note that observation 9, with predicted value of 92, has 0 residual. We therefore recommend the design point (0,0) associated to the ninth observation as the optimal setting.

The illustrations in this chapter showed how we can generate the optimal settings of experiments using path of steepest ascent. In the optimisation procedure, we started with a first-order model and the process led us to a second-order model as the best fit model. The second-order model was plotted in fig. 3.4 while the predicted and residual values are given in table 3.7.

The results for this type of experiments which tests adequacy of a model at any given stage can be analyzed using available statistical softwares e.g. SAS (1999), Stat Soft (1995), etc

In the next chapter we considered situations when a researcher has to generate designs by computer algorithms. Unlike the procedures described above, in a computer search for designs, a model is prespecified before optimal settings are generated and the spread of the settings (points) studied.

CHAPTER FOUR

COMPUTER-AIDED DESIGNS METHODOLOGY

4.1 INTRODUCTON

In this chapter we present the concept of design regions and the conditions necessitating the use of computer-aided designs. The details concerning D-optimal designs, starting from its least squares, properties and sequential algorithms were all discussed. The models to be employed and the measure of rotatability were stated.

4.2 DESIGN REGIONS

The common structure to all experiments is the allocation of treatments, or factor combinations to experimental units. Thus, a desirable design of experiments should provide a distribution of points throughout the region of interest, that is, to provide as much information as possible on the problem. The unit (or region of interest), for example, might be a plot of land receiving a unique treatment combination. As is the tradition in RSM, it is convenient for most applications to scale the quantitative factors (variables) which vary between a minimum and a maximum value ($x_{i,min} \leq x_i \leq x_{i,max}$; i = 1,2,…,k). The unscaled factor (variable) X_1, X_2,…....., X_k are replaced by standardized, or coded, variables, which are often, but not invariably, scaled to lie between -1 and 1.

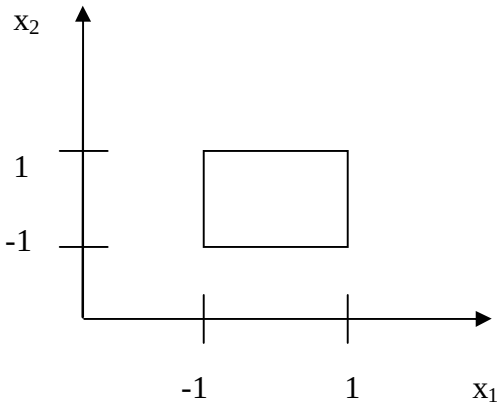


fig. 4.1 Square Region

For k = 2 the experimental region is a square shown in fig. 4.1 above. The cubic design region (see fig. 2.1) is the most frequently encountered for quantitative variables.

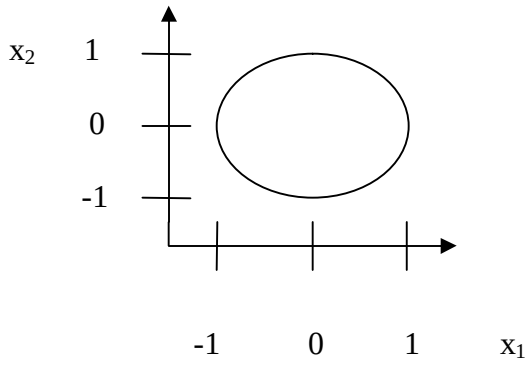


fig. 4.2 Sphere Region

However, the nature of the experiment may sometimes cause more complicated specification of the factor intervals and of the design region. For example, the region will be spherical if it is defined by the equation $\Sigma x_i^2 \leq R^2$ where the radius of the sphere is R. This design region for k = 2 is shown in fig. 4.2. Such a region suggests equal interest in departures in any direction from the centre of the sphere, which might be current experimental or operational conditions.

The experimental regions may also be more complicated than those shown in figures 4.1 and 4.2, often because of imposition of extra constraints. An example of this kind can be found in organic chemistry, where reactions have the ability to produce tar, rather than the desired product, when run for a long time at a higher temperature. Such areas of the experimental region are best avoided, leaving a region of the shape shown in the fig. 4.3.

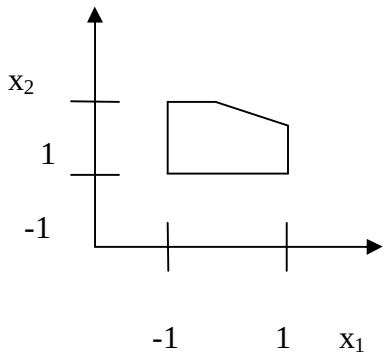


fig. 4.3 Restricted Region

This type of region which we shall discuss in the next section is known as restricted design region. Whatever the shape of the design region, which we call Ω, the principles of experimental design remain the same. The algorithms of optimum design lead to a search over Ω for a design minimizing a function which often depends on the variances of the parameter estimates. The structure of Ω partially determines whether a standard design can be used or whether, and what kind of, a search is needed for the optimum design.

4.3 RESTRICTED DESIGN REGION (NON-STANDARD DESIGN)

A description of a variety of non-standard design problems is given by Snee (1985). His major contribution is in the usefulness of the computer in the design and conduct of a wide variety of experiments. One area of application is the construction of D-optimum designs for irregular experimental regions. He gave several examples of such regions and discussed desirable properties of designs, but did not evaluate the D-optimum designs. Examples of such non-standard regions are summarised below.

1. Polymer density: A central composite design over a circular design region was used for a study in which the factors were annealing time and annealing temperature. However, the highest temperature was so great that the polymer

melted. The circular design was therefore made non-standard by the introduction of an upper bound on one of the factors.

2. Product stability: If two variables of interest are product age and the amount of time the product has spent in the customer's warehouse, the design region is triangular.
3. Fertilizer trials: High levels of two or more fertilizers can produce conditions under which plants die, perhaps because the concentration of ions in the soil becomes so high that osmosis fails to provide the plant with water. Imposition of the constraint $x_1 + x_2 < c$ avoids simultaneous high values of both factors. The design is a square with one corner removed, as in Fig.4.3.
4. Ortho-xylene oxidation: In this extension of the ideas in example 3, the three-factor region is constrained by two non-parallel hyper planes (Juusola et al. 1972).
5. Synthetic fibre manufacture: In an experiment on the physical properties of a synthetic fibre it was found that, because of physical constraints on the system, it was not possible to run all the points of a full $3^4 \times 4$ factorial in the process variables. Kennard and Stone (1969) selected a subset of the points of the full factorial.

In constructing optimum designs for non-standard regions, such as the ones listed above, there are two general ways to proceed. One is to take a 'standard' design and to try to adapt it to the non-standard region. The second is to use the algorithms for exact (or continuous) optimum designs to find the best design for the specific region.

Atkinson and Donev (1992) favoured the second possibility which involves little more work than finding the optimum design for a standard region. For exact designs the

main complication may arise in finding the set of candidate points. In example 5 above, the candidate set was taken as the points of a five factor factorial from which infeasible combinations were eliminated. This is an easy way of finding a set of feasible design points. However, particularly if the constraints can be expressed analytically, it will often be desirable to add candidate points which lie on the constraints. Otherwise too sparse a candidate may result. In the next section we considered the optimum designs.

4.4 COMPUTER-AIDED/ OPTIMUM DESIGNS

A major advantage of a general theory such as that of optimum experimental design is the provision of methods for the solution of non-standard problems.

Most experimental situations call for standard designs that can be constructed with many statistical software packages. Standard designs have assured degrees of precision, orthogonality, and other optimal properties that are important for the exploratory nature of most experiments. In some situations, however, standard designs are not appropriate or practicable. These may include situations where

1. The required blocking structure or blocking size of the experimental situation does not fit into a standard blocked design
2. Not all combinations of the factor settings are feasible, or for some other reason the region of experimentation is constrained or irregularly shaped.
3. A classical design needs to be 'repaired'. This can happen due to improper planning with the original design treatment combinations containing forbidden or unreachable combinations that were not considered before the design was generated.

4. A nonlinear model is appropriate.
5. A quadratic or response surface design is required in the presence of qualitative factors.
6. The factors in the experiment include both components of a mixture and other process variables.
7. There are multiple sources of variation leading to nested or hierarchical data structures and restrictions on what can be randomized.
8. A standard fractional factorial design requires too many treatment combinations for the given amount of time and/or resources.

When situations such as the above exist, computer-aided designs are a useful option and in some situations, computer-aided designs are the only option an experimenter has.

Designs generated from a computer algorithm are referred to as computer-aided designs. Computer-aided designs are experimental designs that are generated based on a particular optimality criterion and are generally 'optimal' only for a specified model. As a result, they are sometimes referred to as optimal designs and generally do not satisfy the desirable properties such as independence among the estimators that standard classical designs do. The design treatment runs that are generated by the algorithms are chosen from an overall candidate set of possible treatment combinations, that one wishes to consider in an experiment.

There are various forms of optimality criteria that are used to select the points for a design. These include

(i) D-optimality: One popular criterion is *D-optimality*, which seeks to maximize |X'X|, the determinant of the *information matrix* X'X of the design. This criterion results

in minimizing the generalized variance of the parameter estimates based on a pre-specified model.

(ii) A-optimality: Another criterion is *A-optimality*, which seeks to minimize the trace of the inverse of the information matrix. This criterion results in minimizing the average variance of the parameter estimates based on a pre-specified model.

(iii)G-optimality: A third criterion is *G-optimality*, which seeks to minimize the maximum prediction variance, i.e., minimize max. $[d=x'(X'X)^{-1}x]$, over a specified set of design points.

(iv)V-optimality: A fourth criterion is *V-optimality*, which seeks to minimize the average prediction variance over a specified set of design points.

Since the optimality criterion of most computer-aided designs is based on some function of the information matrix, the 'optimality' of a given design is model dependent. That is, the experimenter must specify a model for the design and the final number of design points desired before the 'optimal' design can be generated. The design generated by the computer algorithm is 'optimal' only for that model.

The optimality criteria selected for use in our work is the D-optimality criteria because it has the advantages of (i) the possibility to use irregular shapes and (ii) the possibility to include extra design points.

4.5 THE D-OPTIMAL DESIGNS

D-optimal designs are one form of design provided by a computer algorithm. Its objective is to select P design points from a larger set of candidate points. It is the most important design criterion in applications (Atkinson and Donev, 1992) and enables a

more efficient construction of a quadratic model (Myers and Montgomery, 1995). These types of computer-aided designs are particularly useful when classical designs do not apply. Unlike standard classical designs such as factorials and fractional factorials, D-optimal design matrices are usually not orthogonal and effect estimates are correlated.

The D-optimal designs are always an option regardless of the type of model the experimenter wishes to fit (for example, first order, first order plus some interactions, full quadratic, cubic, etc.) or the objective specified for the experiment (for example, screening, response surface, etc.). D-optimal designs are straight optimizations based on a chosen optimality criterion and the model that will be fit. The optimality criterion used in generating D-optimal designs is one of maximizing |X'X|, the determinant of the information matrix X'X. This optimality criterion results in minimizing the generalized variance of the parameter estimates for a pre-specified model. As a result, the 'optimality' of a given D-optimal design is model dependent.

The reasons for using D-optimal designs instead of standard classical designs generally fall into two categories:

1. Standard factorial or fractional factorial designs require too many runs for the amount of resources or time allowed for the experiment.

2. The design space is constrained (the process space contains factor settings that are not feasible or are impossible to run).

Generally, D-optimality is one of the most used criteria in computer-generated design of experiments. Several applications are described in Lucas (1976), Box and Draper (1987), Donev and Atkinson (1988), Khuri and Cornell (1996).

4.6 THE LEAST SQUARES OF D-OPTIMAL DESIGNS

For most of the response surfaces, the functions for the approximations are polynomials because of simplicity, though the functions are not limited to the polynomials. For the cases of quadratic polynomials, the response surface is described as follows:

$$y_u = \beta_0 + \sum^{k}_{j=1}\beta_j x_{uj} + \sum^{k}_{j=1}\beta_{jj} x^2_{uj} + \sum^{k-1}_{i=1}\sum^{k}_{j=i+1}\beta_{ij} x_{ui} x_{uj} + \varepsilon_u$$

$$u = 1, 2, \ldots, N \quad (4.1)$$

where k is the number of variables.

In the case that the number of experiments is N, the response surface can be expressed as follows using matrix expression.

$$E(Y) = F\beta \quad (4.2)$$

Where, in general, Y is the N×1 vector of responses, β is a vector of p unknown parameters, and F is the N×p extended design matrix.

E.g. for a quadratic regression, if the model is $E(Y_i) = \beta_0 + \beta_1 x_i + \beta_2 x^2_i$, i = 1,2,3,4

With

$$X = \begin{bmatrix} -1 \\ -1/3 \\ 1/3 \\ 1 \end{bmatrix} \text{ then, } \quad F = \begin{bmatrix} 1 & -1 & 1 \\ 1 & -1/3 & 1/9 \\ 1 & 1/3 & 1/9 \\ 1 & 1 & 1 \end{bmatrix}$$

where the final column gives the value of x^2_i .

For model (4.2) the sum of squares to be minimized is

$$S(\beta) = (y - F\beta)^T (y - F\beta). \qquad (4.3)$$

The least squares estimates of β, found by differentiation of (4.3), satisfy the p least squares, or normal equations

$$F^T F \text{ ь} = F^T y. \qquad (4.4)$$

The p×p matrix $F^T F$ is the information matrix for β. The larger $F^T F$, the greater is the information in the experiment.

By solving (4.4) the least squares estimate of the parameters are found to be

$$\text{ь} = (F^T F)^{-1} F^T y. \qquad (4.5)$$

if the model is not of full rank, $F^T F$ cannot be uniquely inverted, and only a set of linear combinations of the parameters can be estimated, perhaps a subset of β.

The variance-covariance matrix of the least squares estimates is

$$\text{Var}(\text{ь}) = \sigma^2 (F^T F)^{-1}. \qquad (4.6)$$

The variance of ь_j is proportional to the jth diagonal element of $(F^T F)^{-1}$: the covariance of ь_j and ь_k is proportional to the (j,k)th off-diagonal element. If interest is in the comparison of experimental designs, the value σ^2 is not relevant, since the value is the same for all proposed designs for a specific experiment.

Test of hypothesis about the individual parameters β_j can use the t test, with the variance of ь_j from (4.6) in the denominator. For test about several parameters, the F test is used. The 100(1 - α) percent confidence region for all p elements of β is of the form

$$(\beta - \text{ь})^T F^T F (\beta - \text{ь}) \leq p s^2 F_{p, v, \alpha} \qquad (4.7)$$

where s^2 is an estimate of σ^2 on v degrees of freedom and $F_{p, v, \alpha}$ is the α percent point of the F distribution on p and v degrees of freedom.

In the p-dimensional space of the parameters, (4.7) defines an ellipsoid, the boundary of which is the contour of constant residual sum of squares

$$S(\beta) - S(\text{ь}) = ps^2 F_{p, v, \alpha}$$

The volume of the ellipsoid is inversely proportional to the square root of the determinant $|F^TF|$. For a single slope parameter in simple regression, the variance, is minimized if $\Sigma(x_i - x)^2$ is large. From (4.5) $|(F^TF)^{-1}| = 1/|F^TF|$ is called the generalized variance. Designs which maximize $|F^TF|$ are called D-optimum (for determinant).

The predicted value of the response, for simple regression is

$$\hat{y}(x) = f^T(x)\ \text{ь} \qquad (4.8)$$

where ь is a vector, with variance

$$\text{var}\{\hat{y}(x)\} = \sigma^2 f^T(x)(F^TF)^{-1}f(x). \qquad (4.9)$$

4.7 PROPERTIES OF D-OPTIMUM DESIGNS

If $M(\xi)$ is an information matrix of a design ξ and $|M(\xi)|$ its determinant. Atkinson and Donev(1992) gave 8 general properties of D-optimum designs.

1. The D-optimum design ξ^* maximizes $|M(\xi)|$ or, equivalently, minimizes $|M^{-1}(\xi)|$.

2. The design-efficiency, D_{eff}, of an arbitrary design ξ is defined as

$$D_{eff} = [\,|M(\xi)| / |M(\xi^*)|\,]^{1/p}$$

taking the ratio of the determinants in (1) to the (1/p)th power results in an efficiency measure which is proportional to design size irrespective of the dimension of the model. So two replicates of a design measure for which $D_{eff} = 0.5$ would be as efficient as one replicate of the optimum measure.

3. A generalized G-optimum design over the region R is one for which

$$\max_{x \in R} w(x)d(x,\xi^*) = \min_{\xi} \max_{x \in R} w(x)d(x,\xi).$$

usually R is taken as the design region Ω and $w(x) = 1$, when the equivalence of D- and G-optimum design results. Then, with

$$\hat{d}(\xi) = \max_{x \in R} d(x,\xi),$$

the G-efficiency of a design ξ is given by

$$G_{eff} = \frac{\hat{d}(\xi^*)}{\hat{d}(\xi)} = \frac{p}{\hat{d}(\xi)}.$$

4. The D-optimum design need not be unique. If ξ^*_1 and ξ^*_2 are D-optimum designs, the design

$$\xi^* = c\xi^*_1 + (1 - c)\xi^*_2 \qquad (0 \le c \le 1)$$

is also D-optimum.

5. The D-optimality criterion is model dependent. However, the design is invariant to non-degenerate linear transformation of the model. Thus, a design D-optimum for the model $\eta = \beta^T f(x)$ is also D-optimum for the model $\eta = \gamma^T g(x)$, if $g(x) = Af(x)$ and $|A| \neq 0$. Here β and γ are both $p \times 1$ vectors of unknown parameters.

6. The number of support points of the design is n. Hence there exists a D-optimum ξ^*, with $p \le n \le p(p+1)/2$, although from property 4 above, there may also be optimum designs with the same information matrix but with n greater than this limit.

7. The determinant of the information matrices of the D-optimum continuous design ξ^* and the D-optimum N-trial exact design ξ^*_N satisfy

$$1 \le \frac{|M(\xi^*)|}{|M(\xi^*_N)|} \le \frac{N^p}{N(N-1)\ldots(N+1-P)}.$$

8. If the design ξ^* is D-optimum with the number of support points $n = p$, then

ξ_i=1/p, (i =1,…,n). This design will clearly be D-optimum exact design for N = p. For these designs

$$Cov(\hat{Y}_i, \hat{Y}_j) \propto d(x_i,x_j) = f^T(x_i)\, M^{-1}(\xi^*)\, f(x_j) = 0$$

(i.j = 1,2,…,n; i≠ j).

This result, which also holds for non-optimum ξ with ξ_i = 1/p and n = p, is of particular use in the construction of mixture designs with blocking.

4.8 ALGORITHM FOR THE CONSRUCTION OF D-OPTIMUM DESIGNS

4.8.1 EXCHANGE ALGORITHMS

The initial design of size N can be constructed sequentially from a starting design of size N_0, either by the addition of points if $N_0 < N$, or by the deletion of points if $N_0 > N$. improvement of the design is made by an exchange in which points in the design are replaced by those selected from the candidate list, with the number of points N remaining fixed. The common structure is that the algorithms add a point x_L to the design, delete a point x_k from it, or replace a point x_k from the design with a point x_L from the list of candidate points. For D-optimal algorithms, the choice of the points x_k and x_L depends on the determinant of the information matrix. However, the formulae which provide updated information at each iteration are as follows.

Let n ($n \geq 0$) be the number of iterations already performed. To combine the sequential and interchange steps in a single formula we require constants c_k and c_L such that

(1) $c_L = (N + 1)^{-1}$, $c_k = 0$ if a point x_L is added to the design;

(2) $c_k = (N + 1)^{-1}$, $c_L = 0$ if a point x_k is deleted;

(3) $c_k = c_L = (N + 1)^{-1}$, if the design point x_L is exchanged with the point x_k.

Let the vector of model terms which form the rows of F at these points be $f^T_k = f^T(x_k)$ and $f^T_L = f^T(x_L)$. For D-optimal algorithms the following formula gives the relation between the information matrices and their determinants at the nth and (n+1)th iterations:

$$M(\xi_{n+1}) = (1 - c_L)/ (1 - c_k)\, M(\xi_n) + 1 / (1 - c_k)\, (c_L f_L f^T_L - c_k f_k f^T_k) \qquad (5.12)$$

$$|M(\xi_{n+1})| = [\{1 + c_L/(1 + c_L)\, d(x_L,\xi_n)\}\ \{1 + c_k/(1 - c_k)\, d(x_k,\xi_n)\}$$
$$+ c_k c_L/(1 + c_L)^2\, d^2(x_k,x_L,\ \xi_n)]\, ((1 - c_L)/ (1 - c_k))^p\, |M(\xi_n)| \qquad (5.13)$$

where $d^2(x_k,x_L,\xi_n) = f^T_L\, M^{-1}(\xi_n) f_k$

4.8.2 SEQUENTIAL ALGORITHMS

An exact design for N trials can be found either by the sequential addition of trials to a smaller design, or by the sequential deletion of trials from a larger design. The formulae for exchange algorithms apply for either addition or deletion.

1. Forward procedure Given a starting design with N_0 trials the N-trial exact design ($N > N_0$) is found by application of the algorithm illustrated above, i.e. each trial is added sequentially at the point where the variance of the predicted response is greatest :

   $$d(x_L,\xi_i) = \max d(x,\xi_i) = (N_0 \le i \le N) \qquad (5.10)$$

   Continuation of this process leads, as $N \to \infty$, to the D-optimum continuous design ξ^*.

2. Backward procedure This starts from a design with $N_0 \gg p$ and proceeds by sequential deletion of points with low variance. At each iteration we delete the design point x_k at which the variance of the predicted response is minimum:

   $$d(x_k,\xi_i) = \min d(x,\xi_i) = (N \le i \le N_0). \qquad (5.11)$$

We note that the decrease in the value of the determinant of the information matrix at each iteration is the minimum possible. Often the list of candidate points is taken as the starting design for this procedure. However, if N is so large that the N-trial design might contain some replication, the starting design could contain two or more trials at each candidate point.

Atkinson and Donev (1992) gave an algorithm of the first-order which sequentially adds a trial at the point where $d(x,\xi_N)$ is a maximum. The purpose is to find the optimum design measure ξ^*. The algorithm is as follows.

Let the determinant of the information matrix after N trials be

$$\Delta_N = | F^TF|,$$

Then addition of one further trial at x yields the determinant

$$\Delta_{N+1} = | F^TF + f(x)\, f^Tf(x) |. \text{ But,}$$

$$\Delta_{N+1} = | F^TF |\{1+ \ f^T(x)\ (F^TF\ )^{-1}f(x)\ \}.$$

Therefore

$$\Delta_{N+1} = \ \Delta_N \{\ 1 + d(x,\xi_N)/N\}.$$

So that the addition to the design of a trial where $d(x,\xi_N)$ is a maximum will result in the largest possible increase in Δ_N.

4.9 MODELS

The experiment considered in this thesis is a multifactor with levels of the factors ranging between two and five. Clearly the first order model can not be used because most of their levels are above two. Therefore, the following models that have the

capacity to explain the relationship among the factor-levels would be employed as prespecified models while searching for the optimal settings.

(i) Interaction: This includes constant, linear, and cross product terms and is denoted by

$$y_u = \beta_0 + \sum^{k}_{j=1}\beta_j x_{uj} + \sum^{k-1}_{i=1}\sum^{k}_{j=i+1}\beta_{ij}x_{ui}x_{uj} + \varepsilon_u,$$

$$u = 1, 2, \ldots, N.$$

(ii) Quadratic: This includes interactions plus squared terms and is denoted by

$$y_u = \beta_0 + \sum^{k}_{j=1}\beta_j x_{uj} + \sum^{k}_{j=1}\beta_{jj}x^2_{uj} + \sum^{k-1}_{i=1}\sum^{k}_{j=i+1}\beta_{ij}x_{ui}x_{uj} + \varepsilon_u,$$

$$u = 1,2,\ldots,N$$

(iii) PureQuadratic: This includes constant, linear and squared terms and is denoted by

$$y_u = \beta_0 + \sum^{k}_{j=1}\beta_j x_{uj} + \sum^{k}_{j=1}\beta_{jj}x^2_{uj} + \varepsilon_u, \quad u = 1,2,\ldots, N$$

The appropriate model to be selected will be based on the spread of points each model is able to provide and by the use of measure of rotatability.

4.10 MEASURE OF ROTATABILITY

Recall that in chapter two, rotatability was defined as a design property in which the prediction variance, var[$\hat{Y}(x)$], is a function of only the distance from the point **x** to the centre of the design. This is a desirable invariance property. The constant prediction variance is particularly appealing also when searching for the optimum response on concentric spheres.

There may be situations, however, in which rotatability is sacrificed for the sake of more important design properties, such as orthogonal blocking, uniform precision, or bias reduction. In this case, it would be desirable to preserve some degree of rotatability

wherever possible. Previously, near rotatability was assessed by a visual examination of the contour plots of the prediction variance to determine whether they are close to being circular. Although this method is reasonable when the number of input variables is two, it certainly is infeasible in higher dimensions than two.

The measure of rotatability initially introduced by Khuri (1988) enables us to quantify the degree of rotatability of any given design. The measure is given by

$$\Phi_N(D) = \frac{100}{\|u^*(M)\|^2} \sum_{i=2}^{d} \frac{[u^{*\prime}(M)\omega_{2i}]^2}{\|\omega_{2i}\|^2}, \qquad 0 \leq \Phi_N(D) \leq 100.$$

where D is a design of order d with its design moment given by $M = 1/N\ (X'X)$, N is the number of experimental runs, u(M) is the transformation of v(M), the vector consisting of the elements of M which are located above its diagonal as well as those along the diagonal, ω_δ ($\delta = 0, 2, \ldots, 2d$) are vectors whose elements are in one-to-one correspondence with the elements of v(M) and $\|\omega_{2i}\|$ is the Euclidean norm of ω_{2i}.

The measure $\Phi_N(D)$ represents the percent rotatability that is inherent in D. It is essentially similar to the coefficient of determination used in regression, which measures the percent of total variation in a data set that is attributed to the fitted model. If D is rotatable, $\Phi_N(D) = 100$. Thus a large value of $\Phi_N(D)$ indicates that D is near rotatable.
For a detail derivation and application of the measure of rotatability see Khuri and Cornell (1996).

In the next chapter we considered the software that we used for the development and implementation of D-optimal designs algorithms.

CHAPTER FIVE

MATLAB SOFTWARE

5.1 INTRODUCTON

In this chapter we considered the MATLAB software which was used in implementing our algorithm for the determination of D-optimal designs.

MATLAB is an acronym for Matrix Laboratory; a powerful fourth generation programming language. It is a high performance language for technical computing it integrates computation, visualization, and programming in an easy-to-use environment where problems and solutions are expressed in familiar mathematical notation. Typical uses include:

(i) Math and computation

(ii) Algorithm development

(iii) Modelling, simulation, and prototyping

(iv) Data analysis, exploration, and visualization

(v) Scientific and engineering graphics

(vi) Application development, including graphical user interface building.

MATLAB is an interactive system and a programming language whose basic data element is an array that does not require dimensioning. This allows solving of many technical computing problems especially those with matrix and vector formulations in a fraction of time it would take to write a program in a scalar non-interactive language such as C or FORTRAN.

MATLAB is a user-friendly programming language more advanced and much easier to use than BASIC, PASCAL or C. It has features such as Toolboxes, Simulink, and State flow.

Toolboxes are collections of routines written in the MATLAB language that solve problems for specific applications (you can create your own toolboxes).

Simulink is a program for simulating dynamic systems. As an extension to MATLAB, Simulink add many features specific to dynamic systems while retaining all of MATLAB'S general purpose functionality.

Stateflow is a graphical tool for designing complex control and supervisory logic systems.

5.2 THE D-OPTIMUM DESIGNS

From a statistical point of view, a D-optimal design leads to response surface models for which the maximum variance of the predicted responses is minimized. This means that the points of the experiment will minimize the error in the estimated coefficients of the response model. That is, the experimenter must specify a model for the design before MATLAB can generate the specific treatment combinations.

Given the total number of runs for an experiment and a specified model, the MATLAB algorithm chooses the optimal set of design runs from a *candidate set* of possible design treatment runs. This candidate set of treatment runs usually consists of all possible combinations of various factor levels that one wishes to use in the experiment. In other words, the candidate set is a collection of treatment combinations from which the D-optimal algorithm chooses the treatment combinations to include in the design. The

MATLAB algorithm generally uses a stepping and exchanging process to select the set of treatment runs.

5.3 MATLAB ALGORITHM FOR D-OPTIMUM DESIGNS

We determine our D-optimal designs using the algorithms in MATLAB M-files using the following steps:

(i) Module 1: Transform Variables

(ii) Module 2: Generate Treatment Combinations

(iii) Module 3: Search for the D-optimal Designs, the optimal settings is the one with the maximum determinant.

These modules are given in details in the following subsections that is, 5.3.1 through 5.3.3.

5.3.1 Transforming Variables

First the original values of the variables are coded using the following program (to lie between -1 and +1). The program file is named transform.Mfile.

```
%transforming original values to lie between -1 & +1
X1=input('what are the original values of X1')
x1=(2.*X1-(min(X1)+ max(X1)))/range(X1);
X2=input('what are the original values of X2')
x2=(2.*X2-(min(X2)+ max(X2)))/range(X2);
X3=input('what are the original values of X3')
x3=(2.*X3-(min(X3)+ max(X3)))/range(X3);
X4=input('what are the original values of X4')
x4=(2.*X4-(min(X4)+ max(X4)))/range(X4);
```

5.3.2 Generating Treatment combinations

Here the transformed variables are used to generate the treatment combinations.
The treatment combinations are generated in a matrix **z** using the following MATLAB program which we called tcomb.Mfile.

```
%the determination of total treatment combinations for a four factor experiments with 5 x 5 x 3 x 2 levels
Transform
N=5;
P=5;
```

```
S=3;
K=2;
X=4;
Z=N*P*S*K;
n=x1’;
p=x2’;
s=x3’;
k=x4’;
for i=1

r1=[n(i),p(1),s(1),k(1);n(i),p(1),s(1),k(2);n(i),p(1),s(2),k(1);

n(i),p(1),s(2),k(2);n(i),p(1),s(3),k(1);n(i),p(1),s(3),k(2);

n(i),p(2),s(1),k(1);n(i),p(2),s(1),k(2);n(i),p(2),s(2),k(1);

n(i),p(2),s(2),k(2);n(i),p(2),s(3),k(1);n(i),p(2),s(3),k(2);

n(i),p(3),s(1),k(1);n(i),p(3),s(1),k(2);n(i),p(3),s(2),k(1);

n(i),p(3),s(2),k(2);n(i),p(3),s(3),k(1);n(i),p(3),s(3),k(2);

n(i),p(4),s(1),k(1);n(i),p(4),s(1),k(2);n(i),p(4),s(2),k(1);

n(i),p(4),s(2),k(2);n(i),p(4),s(3),k(1);n(i),p(4),s(3),k(2);

n(i),p(5),s(1),k(1);n(i),p(5),s(1),k(2);n(i),p(5),s(2),k(1);

n(i),p(5),s(2),k(2);n(i),p(5),s(3),k(1);n(i),p(5),s(3),k(2)];
end
for i=2

r2=[n(i),p(1),s(1),k(1);n(i),p(1),s(1),k(2);n(i),p(1),s(2),k(1);

n(i),p(1),s(2),k(2);n(i),p(1),s(3),k(1);n(i),p(1),s(3),k(2);

n(i),p(2),s(1),k(1);n(i),p(2),s(1),k(2);n(i),p(2),s(2),k(1);

n(i),p(2),s(2),k(2);n(i),p(2),s(3),k(1);n(i),p(2),s(3),k(2);

n(i),p(3),s(1),k(1);n(i),p(3),s(1),k(2);n(i),p(3),s(2),k(1);

n(i),p(3),s(2),k(2);n(i),p(3),s(3),k(1);n(i),p(3),s(3),k(2);

n(i),p(4),s(1),k(1);n(i),p(4),s(1),k(2);n(i),p(4),s(2),k(1);

n(i),p(4),s(2),k(2);n(i),p(4),s(3),k(1);n(i),p(4),s(3),k(2);

n(i),p(5),s(1),k(1);n(i),p(5),s(1),k(2);n(i),p(5),s(2),k(1);

n(i),p(5),s(2),k(2);n(i),p(5),s(3),k(1);n(i),p(5),s(3),k(2)];
end
```

```
for i=3
 r3=[n(i),p(1),s(1),k(1);n(i),p(1),s(1),k(2);n(i),p(1),s(2),k(1);
n(i),p(1),s(2),k(2);n(i),p(1),s(3),k(1);n(i),p(1),s(3),k(2);
n(i),p(2),s(1),k(1);n(i),p(2),s(1),k(2);n(i),p(2),s(2),k(1);
n(i),p(2),s(2),k(2);n(i),p(2),s(3),k(1);n(i),p(2),s(3),k(2);
n(i),p(3),s(1),k(1);n(i),p(3),s(1),k(2);n(i),p(3),s(2),k(1);
n(i),p(3),s(2),k(2);n(i),p(3),s(3),k(1);n(i),p(3),s(3),k(2);
n(i),p(4),s(1),k(1);n(i),p(4),s(1),k(2);n(i),p(4),s(2),k(1);
n(i),p(4),s(2),k(2);n(i),p(4),s(3),k(1);n(i),p(4),s(3),k(2);
n(i),p(5),s(1),k(1);n(i),p(5),s(1),k(2);n(i),p(5),s(2),k(1);
n(i),p(5),s(2),k(2);n(i),p(5),s(3),k(1);n(i),p(5),s(3),k(2)];
end
for i=4
r4=[n(i),p(1),s(1),k(1);n(i),p(1),s(1),k(2);n(i),p(1),s(2),k(1);
n(i),p(1),s(2),k(2);n(i),p(1),s(3),k(1);n(i),p(1),s(3),k(2);
n(i),p(2),s(1),k(1);n(i),p(2),s(1),k(2);n(i),p(2),s(2),k(1);
n(i),p(2),s(2),k(2);n(i),p(2),s(3),k(1);n(i),p(2),s(3),k(2);
n(i),p(3),s(1),k(1);n(i),p(3),s(1),k(2);n(i),p(3),s(2),k(1);
n(i),p(3),s(2),k(2);n(i),p(3),s(3),k(1);n(i),p(3),s(3),k(2);
n(i),p(4),s(1),k(1);n(i),p(4),s(1),k(2);n(i),p(4),s(2),k(1);
n(i),p(4),s(2),k(2);n(i),p(4),s(3),k(1);n(i),p(4),s(3),k(2);
n(i),p(5),s(1),k(1);n(i),p(5),s(1),k(2);n(i),p(5),s(2),k(1);
n(i),p(5),s(2),k(2);n(i),p(5),s(3),k(1);n(i),p(5),s(3),k(2)];
end
for i=5

r5=[n(i),p(1),s(1),k(1);n(i),p(1),s(1),k(2);n(i),p(1),s(2),k(1);
n(i),p(1),s(2),k(2);n(i),p(1),s(3),k(1);n(i),p(1),s(3),k(2);
n(i),p(2),s(1),k(1);n(i),p(2),s(1),k(2);n(i),p(2),s(2),k(1);
```

```
n(i),p(2),s(2),k(2);n(i),p(2),s(3),k(1);n(i),p(2),s(3),k(2);

n(i),p(3),s(1),k(1);n(i),p(3),s(1),k(2);n(i),p(3),s(2),k(1);

n(i),p(3),s(2),k(2);n(i),p(3),s(3),k(1);n(i),p(3),s(3),k(2);

n(i),p(4),s(1),k(1);n(i),p(4),s(1),k(2);n(i),p(4),s(2),k(1);

n(i),p(4),s(2),k(2);n(i),p(4),s(3),k(1);n(i),p(4),s(3),k(2);

n(i),p(5),s(1),k(1);n(i),p(5),s(1),k(2);n(i),p(5),s(2),k(1);

n(i),p(5),s(2),k(2);n(i),p(5),s(3),k(1);n(i),p(5),s(3),k(2)];
end
z=[r1;r2;r3;r4;r5];
```

5.3.3 Searching for the D-optimal Designs

The search for the D-optimal designs is conducted on the treatment combinations (z) generated in 5.3.2 using the Matlab (1999) modified program.

A MATLAB M-file (rowexch.Mfile) gave the algorithm for determining d-optimum design for a uniformly generated random numbers which we modified (and named rowexch1.Mfile) to suit the generation of our D-optimal designs as follows:

rowexch1.Mfile

```
function [settings, X] = rowexch1(nfactors,nruns,model)

tcomb;
settings = z;

if nargin < 3
  model = 'linear';
end

X = x2fx(settings,model);
[Q,R]=qr(X,0);
logdetX = 2*sum(log(abs(diag(R))));

info = inv(X'*X);

maxiter = 10;
iter = 0;
madeswitch = 1;
```

```
% Create Iteration Counter Figure.
screen = get(0,'ScreenSize');
f   =   figure('Units','Pixels','Position',[25   screen(4)-150   300
60],...
    'Color',[0.5 0.5 0.5]);
ax = gca;
set(ax,'Visible','off');
t=text(0,0.7,'Row exchange iteration counter.');
set(t,'FontName','Geneva','FontSize',12);

while madeswitch > 0 & iter < maxiter
   madeswitch = 0;
   iter = iter + 1;

   % Update iteration counter.
   s=sprintf('Iteration %4i',iter);
   set(f,'CurrentAxes',ax);
   h=text(0,0.2,s);
   set(h,'FontName','Geneva','FontSize',12);
   drawnow;

   for row = 1:nruns
      fx = x2fx(settings(row,:),model);
      xi = settings(row,:);
      if                strcmp(model,'quadratic')                |
strcmp(model,'purequadratic') | ...
         strcmp(model,'q') | strcmp(model,'p')
         xnew = fullfact(3*ones(nfactors,1)) - 2;
         fxold = fx(ones(3.^nfactors,1),:);
      elseif strcmp(model,'linear') | strcmp(model,'interaction')
...
         | strcmp(model,'l') | strcmp(model,'i')
         xnew = 2*(fullfact(2*ones(nfactors,1)) - 1.5);
         fxold = fx(ones(2.^nfactors,1),:);
      else
         xnew = (fullfact(5*ones(nfactors,1)) - 3)/2;
         fxold = fx(ones(5.^nfactors,1),:);
      end
      fxnew = x2fx(xnew,model);

      E = fxold/R;
      F = fxnew/R;
      dxold = sum((E.*E)')';
      dxnew = sum((F.*F)')';
      dxno  = sum((E.*F)')';

      d = (1 + dxnew).*(1 - dxold) + dxno.^2;

      % Find the maximum change in the determinant.
     [d,idx] = max(d);

      % Switch rows if the maximum change is greater than 1.
```

```
      if d > 1,
         madeswitch = 1;
         logdetX = log(d) + logdetX;
         settings(row,:) = xnew(idx,:);
         X(row,:) = fxnew(idx,:);
         [Q,R] = qr(X,0);
      end
   end
delete(h);
end
close(f);
```

Note:

(i) The command **[settings, X] = rowexch1(nfactors,nruns,model)** is used to determine the optimal final settings(**settings**), the information matrix (**X**). **rowexch1(nfactors,nruns,model)** is the rowexchange algorithm file with number of factors in the experiment (**nfactors**), number of runs(**nruns**)and the prespecified model to be used (**model**). Hence **[settings, X] = rowexch1(4,21,'i'), [settings, X] =rowexch1(4,21,'q')and [settings, X] = rowexch1(4,21,'p')** signifies generating D-optimal design and its information matrix, using rowexchange algorithm for an experiment with 4 factors and 21 number of runs desired. i, q and p represents the prespecified models interaction, quadratic and purequadratic respectively.

(ii) The commands, h = plot3(settings(:,1), settings(:,2), settings(:,3), '.') and set(h,'markersize',25) are used in plotting the points for optimal settings of without control.

In the next chapter we implemented our program and generatd the D-optimal designs for our experiment.

CHAPTER SIX

CONSTRUCTION OF D-OPTIMUM DESIGNS

6.1 INTRODUCTON

In this chapter we implemented the programs given in chapter five with the aim of generating the D-optimum designs.

Observe that our experiment has 5 levels of nitrogen (N), 5 levels of phosphorus (P), 3 levels of sulphur (S), and 2 levels of potassium (K) giving $5\times5\times3\times2 = 150$ treatment combinations. A maximum of the best 21 treatment combinations is required.

The first levels of all the factors are zero levels which are regarded as controls. Without the controls the treatment combinations would be $4\times4\times2\times1= 32$. We shall be generating our designs based on with and without controls.

The construction of a D-optimum design for the experiment would be for runs or support points or treatment combinations based on property (6) of the D-optimal designs, which states that, n the number of support point should be $p \leq n \leq p(p+1)/2$, where p is the number of parameter estimates. The procedure for searching for the designs (as described in chapter five), using our program in MATLAB is as follows.

(i) We first transform (code) the levels of the factors to lie between -1 and 1.

(ii) We generate the 150 or 32 treatment combinations as the case may be.

(iii) Select the best D-optimal designs based on our models.

Since the generation of D-optimal designs depends on a prespecified model, the models that would be used are those described in chapter 4 section 9. They are:

(i) Interaction - includes constant, linear, and cross product terms.

(ii) Quadratic - interactions plus squared terms.

(iii) PureQuadratic - includes constant, linear and squared terms.

6.2 An illustration with a 2^2 factorial experiment

Because of the magnitude of our experiment, a sizeable amount of computer space and time would be consumed while generating the designs. We present first lucidly, illustrations of the workability of our program using standard examples of a 2^2 and 3^2 factorial experiments. In this section we start with the example given in page3 which happens to be a 2^2 factorial experiment. The layout of the experiment is

Bleach(X1)	2	6	2	6
Temperature(X2)	75	75	85	85

On running our program using the above data the following results were obtained

```
[settings,x]=rowexch1(2,4,'l')

z =
    -1    -1
     1    -1
    -1     1
     1     1
```

Where z is the treatment combinations after tranformation.

6.2.1 FINAL SETTINGS

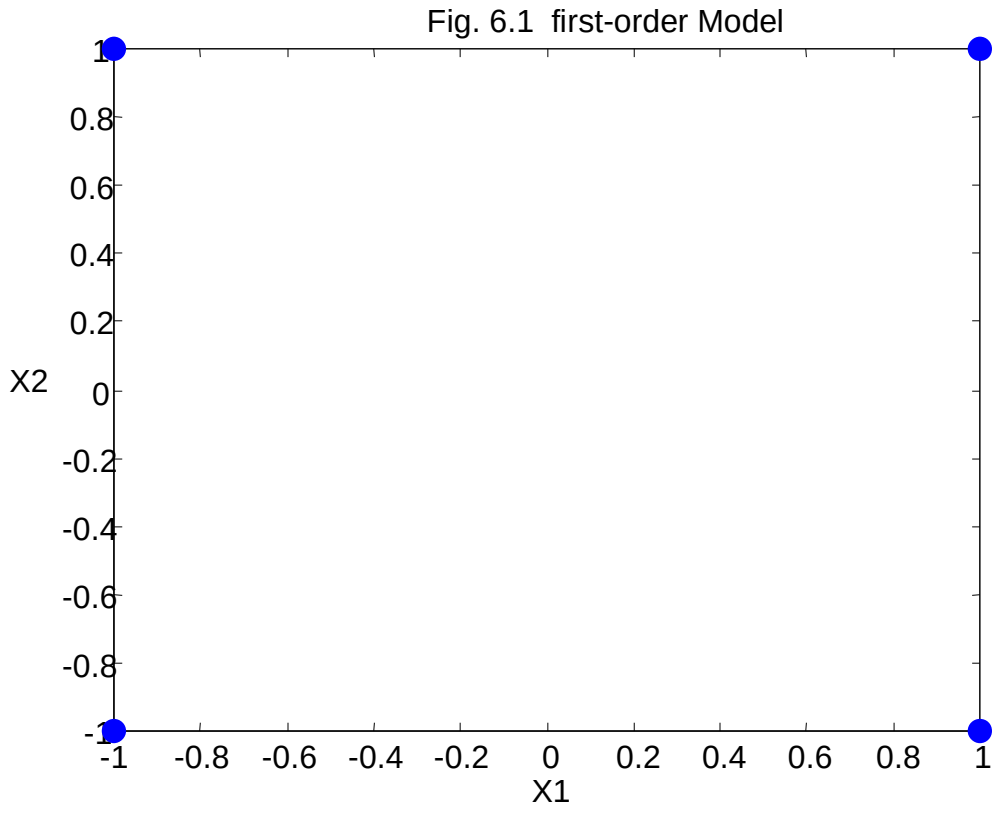
The final settings for the 2^2 experiment, its information matrix x, and graph in fig. 6.1, are as follows:

```
settings =
    -1    -1
     1    -1
    -1     1
     1     1

x =
     1    -1    -1
     1     1    -1
     1    -1     1
     1     1     1
```

See appendix A for the details of the process of generating the settings and information matrix for the 2^2 experiment.

The figure below show the plot of the final settings and it can be seen clearly that the points fell on the corners or spreads like a square; this is an indication of a fit of first-order model.



In the next section we considered an illustration using 3^2 factorial experiment.

6.3 An illustration with a 3^2 factorial experiment

Here we use the example of the Box-Wilson (1951) celebrated Central Composite Design which is a second order design and in the category of 3^2 factorial experiments where quadratic models are used. The coded data are;

```
r =
   -1.0000   -1.0000
    1.0000   -1.0000
   -1.4142         0
         0    1.4142
         0   -1.4142
```

```
         0         0
   -1.0000    1.0000
    1.0000    1.0000
    1.4142         0
```

On running our program on the coded data we obtained the following results.

```
[settings,x]=rowexch1(2,9,'q')

z =

   -1.0000   -1.0000
    1.0000   -1.0000
   -1.4142         0
         0    1.4142
         0   -1.4142
         0         0
   -1.0000    1.0000
    1.0000    1.0000
    1.4142         0
```

Where z is the treatment combinations after tranformation which is the same with the coded data.

6.3.1 FINAL SETTINGS

The final settings for the 3^2 experiment, its information matrix x, and graph in fig. 6.2, are as follows:

```
settings =

   -1.0000   -1.0000
    1.0000   -1.0000
   -1.4142         0
         0    1.4142
         0   -1.4142
         0         0
   -1.0000    1.0000
    1.0000    1.0000
    1.4142         0


x =

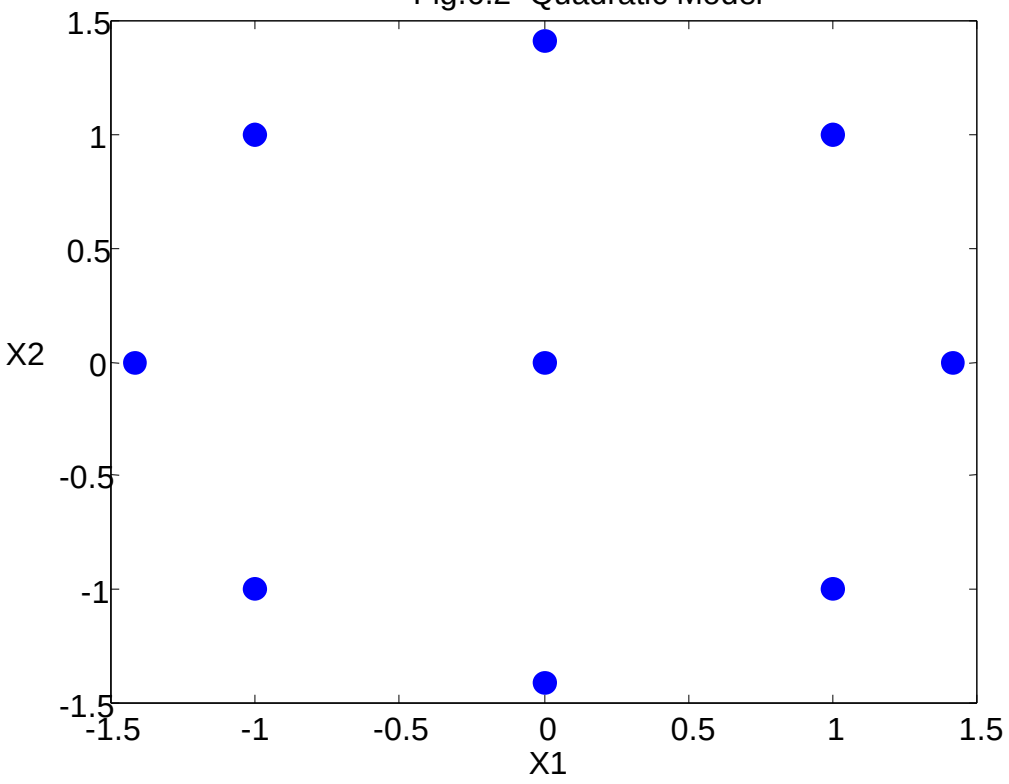
    1.0000   -1.0000   -1.0000    1.0000    1.0000    1.0000
    1.0000    1.0000   -1.0000   -1.0000    1.0000    1.0000
    1.0000   -1.4142         0         0    2.0000         0
    1.0000         0    1.4142         0         0    2.0000
    1.0000         0   -1.4142         0         0    2.0000
    1.0000         0         0         0         0         0
    1.0000   -1.0000    1.0000   -1.0000    1.0000    1.0000
```

```
    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
    1.0000    1.4142         0         0    2.0000         0
```

See appendix B for the details of the process of generating the settings and information matrix for the 3^2 experiment.

The figure below show the plot of the final settings and it can be seen clearly that the points are spread spherically in shape; this is an indication of a fit of quadratic or second-order model.

Fig.6.2 Quadratic Model



We now generate the D-optimal designs for our four factor experiment.

6.4 Generation of D-optimal Designs for Maize

The designs would be searched based on interactions, quadratic and pure-quadratic models.

First we generate the 150 treatment combinations as follows:

The original values of X1 = [0 30 60 90 120] for Nitrogen.

The original values of X2 = [0 20 40 60 80] for Phosphorus.

The original values of X3 = [0 7.5 15] for Sulphur.

The original values of X4 = [0 60] for Potassium.

When the levels are coded the four factors become respectively,

```
x1 = [ -1.0000    -0.5000    0    0.5000    1.0000]
x2 = [ -1.0000    -0.5000    0    0.5000    1.0000]
x3 = [ -1.0000     0        1.0000]
x4 = [ -1.0000     1.0000]

The computer generated treatment combinations are given by
z =
   -1.0000   -1.0000   -1.0000   -1.0000
   -1.0000   -1.0000   -1.0000    1.0000
   -1.0000   -1.0000         0   -1.0000
   -1.0000   -1.0000         0    1.0000
   -1.0000   -1.0000    1.0000   -1.0000
   -1.0000   -1.0000    1.0000    1.0000
   -1.0000   -0.5000   -1.0000   -1.0000
   -1.0000   -0.5000   -1.0000    1.0000
   -1.0000   -0.5000         0   -1.0000
   -1.0000   -0.5000         0    1.0000
   -1.0000   -0.5000    1.0000   -1.0000
   -1.0000   -0.5000    1.0000    1.0000
   -1.0000         0   -1.0000   -1.0000
   -1.0000         0   -1.0000    1.0000
   -1.0000         0         0   -1.0000
   -1.0000         0         0    1.0000
   -1.0000         0    1.0000   -1.0000
   -1.0000         0    1.0000    1.0000
   -1.0000    0.5000   -1.0000   -1.0000
   -1.0000    0.5000   -1.0000    1.0000
   -1.0000    0.5000         0   -1.0000
   -1.0000    0.5000         0    1.0000
   -1.0000    0.5000    1.0000   -1.0000
   -1.0000    0.5000    1.0000    1.0000
   -1.0000    1.0000   -1.0000   -1.0000
   -1.0000    1.0000   -1.0000    1.0000
   -1.0000    1.0000         0   -1.0000
```

-1.0000	1.0000	0	1.0000
-1.0000	1.0000	1.0000	-1.0000
-1.0000	1.0000	1.0000	1.0000
-0.5000	-1.0000	-1.0000	-1.0000
-0.5000	-1.0000	-1.0000	1.0000
-0.5000	-1.0000	0	-1.0000
-0.5000	-1.0000	0	1.0000
-0.5000	-1.0000	1.0000	-1.0000
-0.5000	-1.0000	1.0000	1.0000
-0.5000	-0.5000	-1.0000	-1.0000
-0.5000	-0.5000	-1.0000	1.0000
-0.5000	-0.5000	0	-1.0000
-0.5000	-0.5000	0	1.0000
-0.5000	-0.5000	1.0000	-1.0000
-0.5000	-0.5000	1.0000	1.0000
-0.5000	0	-1.0000	-1.0000
-0.5000	0	-1.0000	1.0000
-0.5000	0	0	-1.0000
-0.5000	0	0	1.0000
-0.5000	0	1.0000	-1.0000
-0.5000	0	1.0000	1.0000
-0.5000	0.5000	-1.0000	-1.0000
-0.5000	0.5000	-1.0000	1.0000
-0.5000	0.5000	0	-1.0000
-0.5000	0.5000	0	1.0000
-0.5000	0.5000	1.0000	-1.0000
-0.5000	0.5000	1.0000	1.0000
-0.5000	1.0000	-1.0000	-1.0000
-0.5000	1.0000	-1.0000	1.0000
-0.5000	1.0000	0	-1.0000
-0.5000	1.0000	0	1.0000
-0.5000	1.0000	1.0000	-1.0000
-0.5000	1.0000	1.0000	1.0000
0	-1.0000	-1.0000	-1.0000
0	-1.0000	-1.0000	1.0000
0	-1.0000	0	-1.0000
0	-1.0000	0	1.0000
0	-1.0000	1.0000	-1.0000
0	-1.0000	1.0000	1.0000
0	-0.5000	-1.0000	-1.0000
0	-0.5000	-1.0000	1.0000
0	-0.5000	0	-1.0000
0	-0.5000	0	1.0000
0	-0.5000	1.0000	-1.0000
0	-0.5000	1.0000	1.0000
0	0	-1.0000	-1.0000
0	0	-1.0000	1.0000
0	0	0	-1.0000
0	0	0	1.0000
0	0	1.0000	-1.0000
0	0	1.0000	1.0000
0	0.5000	-1.0000	-1.0000

```
     0    0.5000   -1.0000    1.0000
     0    0.5000         0   -1.0000
     0    0.5000         0    1.0000
     0    0.5000    1.0000   -1.0000
     0    0.5000    1.0000    1.0000
     0    1.0000   -1.0000   -1.0000
     0    1.0000   -1.0000    1.0000
     0    1.0000         0   -1.0000
     0    1.0000         0    1.0000
     0    1.0000    1.0000   -1.0000
     0    1.0000    1.0000    1.0000
0.5000   -1.0000   -1.0000   -1.0000
0.5000   -1.0000   -1.0000    1.0000
0.5000   -1.0000         0   -1.0000
0.5000   -1.0000         0    1.0000
0.5000   -1.0000    1.0000   -1.0000
0.5000   -1.0000    1.0000    1.0000
0.5000   -0.5000   -1.0000   -1.0000
0.5000   -0.5000   -1.0000    1.0000
0.5000   -0.5000         0   -1.0000
0.5000   -0.5000         0    1.0000
0.5000   -0.5000    1.0000   -1.0000
0.5000   -0.5000    1.0000    1.0000
0.5000         0   -1.0000   -1.0000
0.5000         0   -1.0000    1.0000
0.5000         0         0   -1.0000
0.5000         0         0    1.0000
0.5000         0    1.0000   -1.0000
0.5000         0    1.0000    1.0000
0.5000    0.5000   -1.0000   -1.0000
0.5000    0.5000   -1.0000    1.0000
0.5000    0.5000         0   -1.0000
0.5000    0.5000         0    1.0000
0.5000    0.5000    1.0000   -1.0000
0.5000    0.5000    1.0000    1.0000
0.5000    1.0000   -1.0000   -1.0000
0.5000    1.0000   -1.0000    1.0000
0.5000    1.0000         0   -1.0000
0.5000    1.0000         0    1.0000
0.5000    1.0000    1.0000   -1.0000
0.5000    1.0000    1.0000    1.0000
1.0000   -1.0000   -1.0000   -1.0000
1.0000   -1.0000   -1.0000    1.0000
1.0000   -1.0000         0   -1.0000
1.0000   -1.0000         0    1.0000
1.0000   -1.0000    1.0000   -1.0000
1.0000   -1.0000    1.0000    1.0000
1.0000   -0.5000   -1.0000   -1.0000
1.0000   -0.5000   -1.0000    1.0000
1.0000   -0.5000         0   -1.0000
1.0000   -0.5000         0    1.0000
1.0000   -0.5000    1.0000   -1.0000
```

```
    1.0000   -0.5000    1.0000    1.0000
    1.0000         0   -1.0000   -1.0000
    1.0000         0   -1.0000    1.0000
    1.0000         0         0   -1.0000
    1.0000         0         0    1.0000
    1.0000         0    1.0000   -1.0000
    1.0000         0    1.0000    1.0000
    1.0000    0.5000   -1.0000   -1.0000
    1.0000    0.5000   -1.0000    1.0000
    1.0000    0.5000         0   -1.0000
    1.0000    0.5000         0    1.0000
    1.0000    0.5000    1.0000   -1.0000
    1.0000    0.5000    1.0000    1.0000
    1.0000    1.0000   -1.0000   -1.0000
    1.0000    1.0000   -1.0000    1.0000
    1.0000    1.0000         0   -1.0000
    1.0000    1.0000         0    1.0000
    1.0000    1.0000    1.0000   -1.0000
    1.0000    1.0000    1.0000    1.0000
```

After generating the treatment combinations, we now search for the D-optimal designs using the models mentioned earlier.

6.4.1 Interaction model for Maize

```
[settings,x]=rowexch1(4,21,'i')
```

For the interaction model the searched D-optimal designs (settings), information matrix (x), and settings converted to original values (ox), for, with and without control are given as follows:

With control

```
settings =
   [-1    -1    -1    -1
    -1    -1    -1     1
    -1    -1    -1    -1
    -1    -1     1     1
    -1    -1     1    -1
    -1    -1     1     1
    -1    -1    -1     1
    -1    -1     1    -1
    -1     1    -1    -1
    -1    -1    -1    -1
    -1     1     1    -1
    -1    -1     1     1
     1    -1    -1    -1
    -1     1    -1     1
    -1    -1    -1     1
    -1    -1     1    -1]
```

```
x =
     1    -1    -1    -1    -1     1     1     1     1     1     1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1
     1    -1    -1    -1    -1     1     1     1     1     1     1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1
     1    -1     1    -1    -1    -1     1     1    -1    -1     1
     1    -1    -1    -1    -1     1     1     1     1     1     1
     1    -1     1     1    -1    -1    -1     1     1    -1    -1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1
     1     1    -1    -1    -1    -1    -1    -1     1     1     1
     1    -1     1    -1     1    -1     1    -1    -1     1    -1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1


ox =
     0     0     0     0
     0     0     0    60
     0     0     0     0
     0     0    15    60
     0     0    15     0
     0     0    15    60
     0     0     0    60
     0     0    15     0
     0    80     0     0
     0     0     0     0
     0    80    15     0
     0     0    15    60
   120     0     0     0
     0    80     0    60
     0     0     0    60
     0     0    15     0
```

Without control

```
[settings,x]=rowexch1(3,21,'i')
settings =
    -1    -1    -1
    -1    -1     1
    -1    -1    -1
    -1    -1     1
    -1     1    -1
    -1     1     1
    -1     1    -1
    -1     1     1
```

```
x =
     1    -1    -1    -1     1     1     1
     1    -1    -1     1     1    -1    -1
     1    -1    -1    -1     1     1     1
     1    -1    -1     1     1    -1    -1
     1    -1     1    -1    -1     1    -1
     1    -1     1     1    -1    -1     1
     1    -1     1    -1    -1     1    -1
     1    -1     1     1    -1    -1     1

ox =
   30.0000   20.0000    7.5000
   30.0000   20.0000   15.0000
   30.0000   20.0000    7.5000
   30.0000   20.0000   15.0000
   30.0000   80.0000    7.5000
   30.0000   80.0000   15.0000
   30.0000   80.0000    7.5000
   30.0000   80.0000   15.0000
```

In order study the spread of the optimal settings, we now plot a three-dimensional graph of the optimal settings for without control, since it is not feasible for us to plot a four dimensional graph of the optimal settings for with control using MATLAB 5.3.

Fig.6.3 Interaction Model for Maize

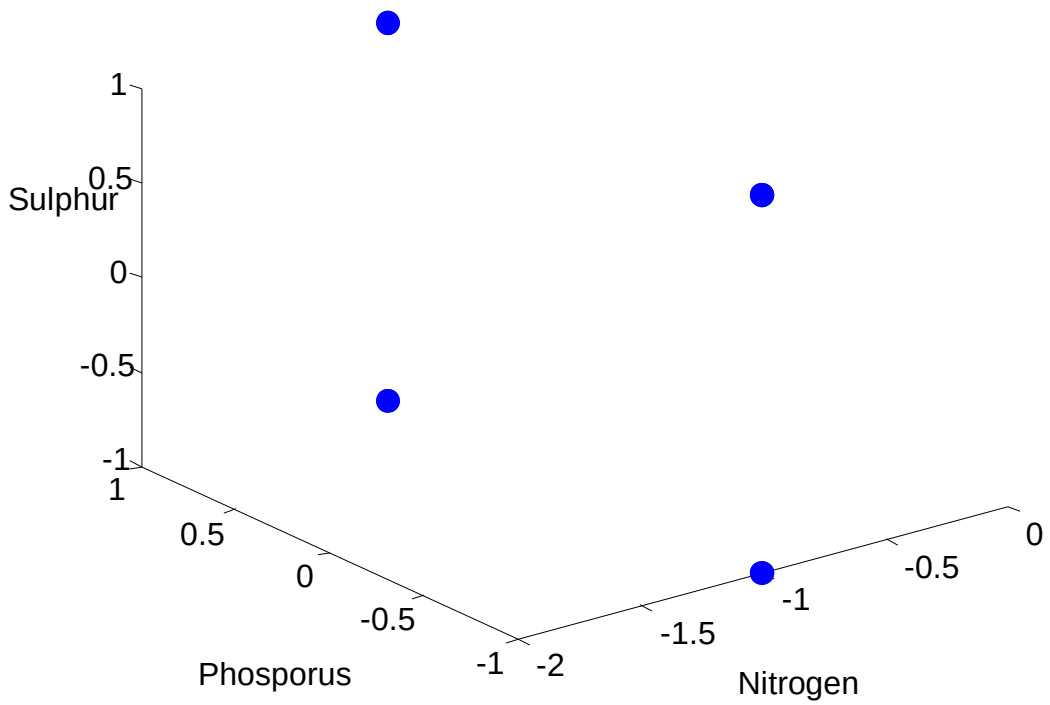


Figure 6.3 show the plot of the final settings of an interaction model for without control. Only four support points were generated by the model.

Remark 1: The interaction model generated 8 optimal design points for with control and 4 optimal design points for without control, although some points are replicated.

6.4.2 Quadratic model for Maize

For the quadratic model the searched D-optimal designs (settings), information matrix (x), and settings converted to original values (ox), for with and without control are given as follows:

With control

```
[settings,x]=rowexch1(4,21,'q')
settings =
     1     1     0     1
     1     0     1     1
    -1     1     1     0
     1     1    -1     0
```

```
-1     0     1    -1
 0     0     0     0
-1    -1    -1     0
 1    -1    -1     0
 1    -1     1     0
-1    -1    -1    -1
-1    -1     1    -1
-1    -1     1     1
-1    -1    -1     1
 1     1     1    -1
-1    -1     1     0
-1    -1    -1    -1
-1    -1     1    -1
-1    -1     1     1
-1     1    -1     0
-1    -1    -1     1
 1    -1    -1     0
-1     1    -1     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
-1     1     1    -1
-1     1     1     1
-1    -1    -1    -1
-1    -1    -1     1
-1     1     1     1
-1     0     0     0
-1    -1     1    -1
-1    -1     1     1
-1     1     1    -1
 1    -1     1     0
 1     1    -1     0
-1     1    -1    -1
-1    -1    -1     1
-1    -1     1    -1
-1    -1    -1    -1
-1     1    -1     1
-1     0     0     0
-1    -1     1     1
 1    -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     1     0
-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     1     1     0
    -1    -1    -1    -1
    -1     1     1    -1
    -1    -1    -1     1
     0     1     0     0
    -1     1     1     1
    -1    -1     1     1
    -1    -1     1    -1
     0    -1    -1     0
    -1     0    -1     0
    -1     1    -1    -1
     1    -1     1    -1
    -1     1     0     1
     1    -1    -1     1
    -1    -1     0    -1
     1    -1     1     1
     1    -1    -1    -1
     1     1     0     0
     0    -1     1     0
    -1    -1     0     1
    -1     0    -1     1
     1     1    -1     1

x =
  Columns 1 through 12
     1     1     1     0     1     1     0     1     0     1     0     1
     1     1     0     1     1     0     1     1     0     0     1     1
     1    -1     1     1     0    -1    -1     0     1     0     0     1
     1     1     1    -1     0     1    -1     0    -1     0     0     1
     1    -1     0     1    -1     0    -1     1     0     0    -1     1
     1     0     0     0     0     0     0     0     0     0     0     0
     1    -1    -1    -1     0     1     1     0     1     0     0     1
     1     1    -1    -1     0    -1    -1     0     1     0     0     1
     1     1    -1     1     0    -1     1     0    -1     0     0     1
     1    -1    -1    -1    -1     1     1     1     1     1     1     1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1     1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1     1
     1    -1    -1    -1     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     1    -1     0    -1     0     0     1
     1    -1    -1    -1    -1     1     1     1     1     1     1     1
     1    -1    -1     1    -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    -1     1     0    -1     0     0     1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1     1
     1     1    -1    -1     0    -1    -1     0     1     0     0     1
     1    -1     1    -1     1    -1     1    -1    -1     1    -1     1
     1    -1     1     1    -1    -1    -1     1     1    -1    -1     1
     1    -1     1     1     1    -1    -1    -1     1     1     1     1
     1    -1     1    -1    -1    -1     1     1    -1    -1     1     1
     1    -1     1    -1     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     1     1     0     1     0     0     1
     1    -1     1     1    -1    -1    -1     1     1    -1    -1     1
```

```
    1    -1     1     1     1    -1    -1    -1     1     1     1     1
    1    -1    -1    -1    -1     1     1     1     1     1     1     1
    1    -1    -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     1
    1    -1    -1     1    -1     1    -1     1    -1     1    -1     1
    1    -1    -1     1     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    -1     1     0    -1     0     0     1
    1     1     1    -1     0     1    -1     0    -1     0     0     1
    1    -1     1    -1    -1    -1     1     1    -1    -1     1     1
    1    -1    -1    -1     1     1     1    -1     1    -1    -1     1
    1    -1    -1     1    -1     1    -1     1    -1     1    -1     1
    1    -1    -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     1
    1    -1    -1     1     1     1    -1    -1    -1    -1     1     1
    1     1    -1     1     1    -1     1     1    -1    -1     1     1
    1     1    -1    -1    -1    -1    -1    -1     1     1     1     1
    1    -1     1     1    -1    -1    -1     1     1    -1    -1     1
    1     1     1    -1     1     1    -1     1    -1     1    -1     1
    1     1     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     1     0     0    -1     0     0     0     0     1
    1    -1     1     1     1    -1    -1    -1     1     1     1     1
    1    -1     1    -1    -1    -1     1     1    -1    -1     1     1
    1     1     1    -1    -1     1    -1    -1    -1    -1     1     1
    1     1    -1     1    -1    -1     1    -1    -1     1    -1     1
    1     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     1     1     0     0     0     0     1     0     0     0
    1    -1    -1    -1    -1     1     1     1     1     1     1     1
    1    -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     1     0     0     0     0     0     0     0     0     0
    1    -1     1     1     1    -1    -1    -1     1     1     1     1
    1    -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    -1    -1     0     0     0     0     1     0     0     0
    1    -1     0    -1     0     0     1     0     0     0     0     1
    1    -1     1    -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     1    -1     0    -1     0     1     0     1
    1     1    -1    -1     1    -1    -1     1     1    -1    -1     1
    1    -1    -1     0    -1     1     0     1     0     1     0     1
    1     1    -1     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     1     0     0     0     0     0     1
    1     0    -1     1     0     0     0     0    -1     0     0     0
    1    -1    -1     0     1     1     0    -1     0    -1     0     1
    1    -1     0    -1     1     0     1    -1     0     0    -1     1
    1     1     1    -1     1     1    -1     1    -1     1    -1     1

Columns 13 through 15

    1     0     1
    0     1     1
    1     1     0
    1     1     0
    0     1     1
    0     0     0
    1     1     0
```

1	1	0
1	1	0
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
1	1	0
1	1	1
1	1	1
1	1	1
1	1	0
1	1	1
1	1	0
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
1	1	0
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
0	0	0
1	1	1
1	1	1
1	1	1
1	1	0
1	1	0
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
0	0	0
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
0	1	0
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1
1	1	0
1	1	1
1	1	1
1	1	1
1	0	0

```
     1     1     1
     1     1     1
     1     1     1
     1     1     0
     0     1     0
     1     1     1
     1     1     1
     1     0     1
     1     1     1
     1     0     1
     1     1     1
     1     1     1
     1     0     0
     1     1     0
     1     0     1
     0     1     1
     1     1     1

ox =
  120.0000   80.0000    7.5000   60.0000
  120.0000   40.0000   15.0000   60.0000
         0   80.0000   15.0000   30.0000
  120.0000   80.0000         0   30.0000
         0   40.0000   15.0000         0
   60.0000   40.0000    7.5000   30.0000
         0         0         0   30.0000
  120.0000         0         0   30.0000
  120.0000         0   15.0000   30.0000
         0         0         0         0
         0         0   15.0000         0
         0         0   15.0000   60.0000
         0         0         0   60.0000
  120.0000   80.0000   15.0000         0
         0         0   15.0000   30.0000
         0         0         0         0
         0         0   15.0000         0
         0         0   15.0000   60.0000
         0   80.0000         0   30.0000
         0         0         0   60.0000
  120.0000         0         0   30.0000
         0   80.0000         0   60.0000
         0   80.0000   15.0000         0
         0   80.0000   15.0000   60.0000
         0   80.0000         0         0
         0   80.0000         0   60.0000
         0   80.0000         0         0
  120.0000   80.0000   15.0000   30.0000
         0   80.0000   15.0000         0
         0   80.0000   15.0000   60.0000
         0         0         0         0
         0         0         0   60.0000
         0   80.0000   15.0000   60.0000
         0   40.0000    7.5000   30.0000
         0         0   15.0000         0
         0         0   15.0000   60.0000
         0   80.0000   15.0000         0
  120.0000         0   15.0000   30.0000
```

```
  120.0000   80.0000         0   30.0000
         0   80.0000         0         0
         0         0         0   60.0000
         0         0   15.0000         0
         0         0         0         0
         0   80.0000         0   60.0000
         0   40.0000    7.5000   30.0000
         0         0   15.0000   60.0000
  120.0000         0   15.0000   60.0000
  120.0000         0         0         0
         0   80.0000   15.0000         0
  120.0000   80.0000         0   60.0000
  120.0000   80.0000   15.0000         0
         0   80.0000         0   60.0000
         0   40.0000   15.0000   30.0000
         0   80.0000   15.0000   60.0000
         0   80.0000         0         0
  120.0000   80.0000         0         0
  120.0000         0   15.0000         0
  120.0000         0         0   60.0000
  120.0000   80.0000   15.0000   60.0000
   60.0000   80.0000   15.0000   30.0000
         0         0         0         0
         0   80.0000   15.0000         0
         0         0         0   60.0000
   60.0000   80.0000    7.5000   30.0000
         0   80.0000   15.0000   60.0000
         0         0   15.0000   60.0000
         0         0   15.0000         0
   60.0000         0         0   30.0000
         0   40.0000         0   30.0000
         0   80.0000         0         0
  120.0000         0   15.0000         0
         0   80.0000    7.5000   60.0000
  120.0000         0         0   60.0000
         0         0    7.5000         0
  120.0000         0   15.0000   60.0000
  120.0000         0         0         0
  120.0000   80.0000    7.5000   30.0000
   60.0000         0   15.0000   30.0000
         0         0    7.5000   60.0000
         0   40.0000         0   60.0000
  120.0000   80.0000         0   60.0000
```

Without control

```
[settings,x]=rowexch1(3,21,'q')
settings =
     0     0     0
    -1    -1     0
     1    -1     0
    -1    -1     1
    -1    -1    -1
    -1     1     0
    -1     1    -1
    -1     1     1
     1     1     0
```

```
    -1    -1    -1
    -1    -1     1
    -1     0     0
    -1     1    -1
    -1     1     1
     0    -1     0
     1    -1     1
     1    -1    -1
     0    -1    -1
    -1     0    -1
     0    -1     1
     1     1     1
     0     0     1
     0     1    -1
     0     1     1
     1    -1    -1
     1    -1     1
     1     1    -1

x =
     1     0     0     0     0     0     0     0     0     0
     1    -1    -1     0     1     0     0     1     1     0
     1     1    -1     0    -1     0     0     1     1     0
     1    -1    -1     1     1    -1    -1     1     1     1
     1    -1    -1    -1     1     1     1     1     1     1
     1    -1     1     0    -1     0     0     1     1     0
     1    -1     1    -1    -1     1    -1     1     1     1
     1    -1     1     1    -1    -1     1     1     1     1
     1     1     1     0     1     0     0     1     1     0
     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     0     0
     1    -1     1    -1    -1     1    -1     1     1     1
     1    -1     1     1    -1    -1     1     1     1     1
     1     0    -1     0     0     0     0     0     1     0
     1     1    -1     1    -1     1    -1     1     1     1
     1     1    -1    -1    -1    -1     1     1     1     1
     1     0    -1    -1     0     0     1     0     1     1
     1    -1     0    -1     0     1     0     1     0     1
     1     0    -1     1     0     0    -1     0     1     1
     1     1     1     1     1     1     1     1     1     1
     1     0     0     1     0     0     0     0     0     1
     1     0     1    -1     0     0    -1     0     1     1
     1     0     1     1     0     0     1     0     1     1
     1     1    -1    -1    -1    -1     1     1     1     1
     1     1    -1     1    -1     1    -1     1     1     1
     1     1     1    -1     1    -1    -1     1     1     1

ox =
   75.0000   50.0000   11.2500
   30.0000   20.0000   11.2500
  120.0000   20.0000   11.2500
   30.0000   20.0000   15.0000
   30.0000   20.0000    7.5000
   30.0000   80.0000   11.2500
   30.0000   80.0000    7.5000
```

30.0000	80.0000	15.0000
120.0000	80.0000	11.2500
30.0000	20.0000	7.5000
30.0000	20.0000	15.0000
30.0000	50.0000	11.2500
30.0000	80.0000	7.5000
30.0000	80.0000	15.0000
75.0000	20.0000	11.2500
120.0000	20.0000	15.0000
120.0000	20.0000	7.5000
75.0000	20.0000	7.5000
30.0000	50.0000	7.5000
75.0000	20.0000	15.0000
120.0000	80.0000	15.0000
75.0000	50.0000	15.0000
75.0000	80.0000	7.5000
75.0000	80.0000	15.0000
120.0000	20.0000	7.5000
120.0000	20.0000	15.0000
120.0000	80.0000	7.5000

To study the spread of the optimal settings, we now plot a three-dimensional graph of the optimal settings for without control.

Fig.6.4 Quadratic Model for Maize

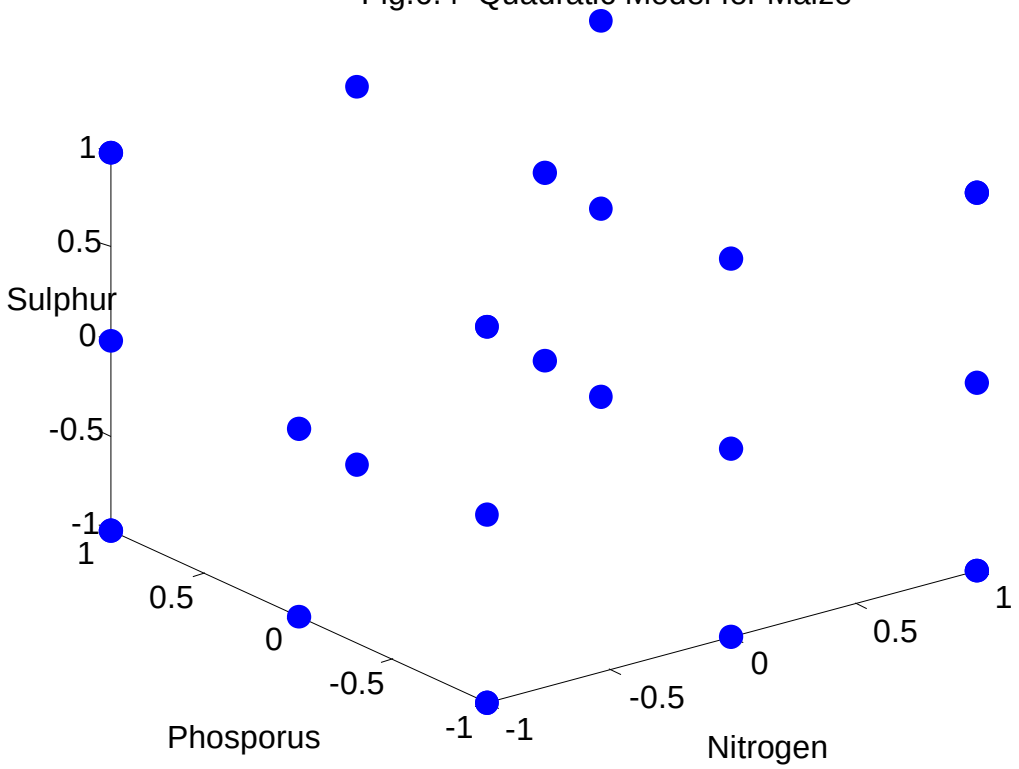


Figure 6.4 show the plot of the final settings of a quadratic model for without control. Twenty one fairly spread optimal design points were generated by the model.

Remark 2: The quadratic model generated 42 optimal design points for with control and 21 optimal design points for without control, although some points are replicated.

6.4.3 Pure-quadratic model for Maize

For the pure-quadratic model the searched D-optimal designs (settings), information matrix (x), and settings converted to original values (ox), for, with and without control are given as follows:

With control

```
[settings,x]=rowexch1(4,21,'p')
settings =
    -1    -1    -1     1
     1     1    -1    -1
     1     1     1     0
    -1    -1     0     0
     0     0     1     0
     1     1    -1     0
    -1    -1     1     0
     0     1     0     0
     1     0    -1     0
    -1    -1     0     0
     0     1     0     0
    -1    -1    -1     0
     1     0     0     0
    -1     1    -1     0
    -1     0    -1     0
     1    -1     1     0
    -1     0     1     0
     0     1     0     0
    -1     0    -1     0
     0     1     1     0
    -1     0     0     0
     0    -1    -1     0
    -1    -1     1    -1
     1    -1     0     0
    -1     1    -1    -1
    -1     1    -1     1
    -1     1     0    -1
    -1     1     0     1
    -1     1     1    -1
    -1     1     1     1
```

```
    -1     0     1     0
    -1    -1    -1     1
    -1    -1     0    -1
     0    -1    -1     0
    -1    -1     0     1
     0     1     1     0
    -1    -1     1     1
     0    -1     1     0
    -1     0    -1     0
     1     1     1     0
    -1    -1     1    -1
    -1     0     0     0
    -1     1    -1    -1
     1     1     0     0
     0    -1    -1     0
    -1    -1     0     1
    -1     0     1     0
     1     1    -1     0
    -1     0    -1    -1
    -1     0    -1     1
     1    -1     1     0
    -1     0     0    -1
    -1     1     1     1
     1    -1    -1     0
    -1     1    -1    -1
    -1     0     1     0
    -1    -1     0    -1
    -1     1     0     1
     0     1     0     0
    -1     1     1     1
     1    -1     0     0
    -1    -1    -1     1
     0    -1    -1     0
    -1     0     1     0
    -1    -1     1    -1
     0    -1     0     0
     1     1    -1     0
    -1     1     0    -1
     1     1     1     0
    -1     0     0     0
     0    -1     1    -1
     0    -1     0     0
    -1    -1    -1     1
     0    -1    -1    -1
     1     1    -1     0
    -1     1    -1    -1
     0     0    -1     0
     0    -1     1     1
    -1     0     0     1
     0     0    -1     0
     1    -1     1     0

x =
     1    -1    -1    -1     1     1     1     1     1
     1     1     1    -1    -1     1     1     1     1
     1     1     1     1     0     1     1     1     0
     1    -1    -1     0     0     1     1     0     0
```

ci

```
1     0     0     1     0     0     0     1     0
1     1     1    -1     0     1     1     1     0
1    -1    -1     1     0     1     1     1     0
1     0     1     0     0     0     1     0     0
1     1     0    -1     0     1     0     1     0
1    -1    -1     0     0     1     1     0     0
1     0     1     0     0     0     1     0     0
1    -1    -1    -1     0     1     1     1     0
1     1     0     0     0     1     0     0     0
1    -1     1    -1     0     1     1     1     0
1    -1     0    -1     0     1     0     1     0
1     1    -1     1     0     1     1     1     0
1    -1     0     1     0     1     0     1     0
1     0     1     0     0     0     1     0     0
1    -1     0    -1     0     1     0     1     0
1     0     1     1     0     0     1     1     0
1    -1     0     0     0     1     0     0     0
1     0    -1    -1     0     0     1     1     0
1    -1    -1     1    -1     1     1     1     1
1     1    -1     0     0     1     1     0     0
1    -1     1    -1    -1     1     1     1     1
1    -1     1    -1     1     1     1     1     1
1    -1     1     0    -1     1     1     0     1
1    -1     1     0     1     1     1     0     1
1    -1     1     1    -1     1     1     1     1
1    -1     1     1     1     1     1     1     1
1    -1     0     1     0     1     0     1     0
1    -1    -1    -1     1     1     1     1     1
1    -1    -1     0    -1     1     1     0     1
1     0    -1    -1     0     0     1     1     0
1    -1    -1     0     1     1     1     0     1
1     0     1     1     0     0     1     1     0
1    -1    -1     1     1     1     1     1     1
1     0    -1     1     0     0     1     1     0
1    -1     0    -1     0     1     0     1     0
1     1     1     1     0     1     1     1     0
1    -1    -1     1    -1     1     1     1     1
1    -1     0     0     0     1     0     0     0
1    -1     1    -1    -1     1     1     1     1
1     1     1     0     0     1     1     0     0
1     0    -1    -1     0     0     1     1     0
1    -1    -1     0     1     1     1     0     1
1    -1     0     1     0     1     0     1     0
1     1     1    -1     0     1     1     1     0
1    -1     0    -1    -1     1     0     1     1
1    -1     0    -1     1     1     0     1     1
1     1    -1     1     0     1     1     1     0
1    -1     0     0    -1     1     0     0     1
1    -1     1     1     1     1     1     1     1
1     1    -1    -1     0     1     1     1     0
1    -1     1    -1    -1     1     1     1     1
1    -1     0     1     0     1     0     1     0
1    -1    -1     0    -1     1     1     0     1
1    -1     1     0     1     1     1     0     1
1     0     1     0     0     0     1     0     0
1    -1     1     1     1     1     1     1     1
1     1    -1     0     0     1     1     0     0
```

```
     1    -1    -1    -1     1     1     1     1     1
     1     0    -1    -1     0     0     1     1     0
     1    -1     0     1     0     1     0     1     0
     1    -1    -1     1    -1     1     1     1     1
     1     0    -1     0     0     0     1     0     0
     1     1     1    -1     0     1     1     1     0
     1    -1     1     0    -1     1     1     0     1
     1     1     1     1     0     1     1     1     0
     1    -1     0     0     0     1     0     0     0
     1     0    -1     1    -1     0     1     1     1
     1     0    -1     0     0     0     1     0     0
     1    -1    -1    -1     1     1     1     1     1
     1     0    -1    -1    -1     0     1     1     1
     1     1     1    -1     0     1     1     1     0
     1    -1     1    -1    -1     1     1     1     1
     1     0     0    -1     0     0     0     1     0
     1     0    -1     1     1     0     1     1     1
     1    -1     0     0     1     1     0     0     1
     1     0     0    -1     0     0     0     1     0
     1     1    -1     1     0     1     1     1     0
```

```
ox =
         0         0         0   60.0000
  120.0000   80.0000         0         0
  120.0000   80.0000   15.0000   30.0000
         0         0    7.5000   30.0000
   60.0000   40.0000   15.0000   30.0000
  120.0000   80.0000         0   30.0000
         0         0   15.0000   30.0000
   60.0000   80.0000    7.5000   30.0000
  120.0000   40.0000         0   30.0000
         0         0    7.5000   30.0000
   60.0000   80.0000    7.5000   30.0000
         0         0         0   30.0000
  120.0000   40.0000    7.5000   30.0000
         0   80.0000         0   30.0000
         0   40.0000         0   30.0000
  120.0000         0   15.0000   30.0000
         0   40.0000   15.0000   30.0000
   60.0000   80.0000    7.5000   30.0000
         0   40.0000         0   30.0000
   60.0000   80.0000   15.0000   30.0000
         0   40.0000    7.5000   30.0000
   60.0000         0         0   30.0000
         0         0   15.0000         0
  120.0000         0    7.5000   30.0000
         0   80.0000         0         0
         0   80.0000         0   60.0000
         0   80.0000    7.5000         0
         0   80.0000    7.5000   60.0000
         0   80.0000   15.0000         0
         0   80.0000   15.0000   60.0000
         0   40.0000   15.0000   30.0000
         0         0         0   60.0000
         0         0    7.5000         0
   60.0000         0         0   30.0000
```

```
         0         0    7.5000   60.0000
   60.0000   80.0000   15.0000   30.0000
         0         0   15.0000   60.0000
   60.0000         0   15.0000   30.0000
         0   40.0000         0   30.0000
  120.0000   80.0000   15.0000   30.0000
         0         0   15.0000         0
         0   40.0000    7.5000   30.0000
         0   80.0000         0         0
  120.0000   80.0000    7.5000   30.0000
   60.0000         0         0   30.0000
         0         0    7.5000   60.0000
         0   40.0000   15.0000   30.0000
  120.0000   80.0000         0   30.0000
         0   40.0000         0         0
         0   40.0000         0   60.0000
  120.0000         0   15.0000   30.0000
         0   40.0000    7.5000         0
         0   80.0000   15.0000   60.0000
  120.0000         0         0   30.0000
         0   80.0000         0         0
         0   40.0000   15.0000   30.0000
         0         0    7.5000         0
         0   80.0000    7.5000   60.0000
   60.0000   80.0000    7.5000   30.0000
         0   80.0000   15.0000   60.0000
  120.0000         0    7.5000   30.0000
         0         0         0   60.0000
   60.0000         0         0   30.0000
         0   40.0000   15.0000   30.0000
         0         0   15.0000         0
   60.0000         0    7.5000   30.0000
  120.0000   80.0000         0   30.0000
         0   80.0000    7.5000         0
  120.0000   80.0000   15.0000   30.0000
         0   40.0000    7.5000   30.0000
   60.0000         0   15.0000         0
   60.0000         0    7.5000   30.0000
         0         0         0   60.0000
   60.0000         0         0         0
  120.0000   80.0000         0   30.0000
         0   80.0000         0         0
   60.0000   40.0000         0   30.0000
   60.0000         0   15.0000   60.0000
         0   40.0000    7.5000   60.0000
   60.0000   40.0000         0   30.0000
  120.0000         0   15.0000   30.0000
```

Without control

```
[settings,x]=rowexch1(3,21,'p')
settings =
     0    -1    -1
    -1    -1     0
     1     1     0
    -1    -1     0
```

```
     0     1     0
    -1     0     0
    -1     1    -1
    -1     1     1
    -1     0     1
    -1    -1    -1
     0    -1     0
     1     1     0
    -1     0    -1
     1     0     0
    -1    -1     1
     1    -1     0
     0    -1    -1
     0    -1     1
    -1     1     1
     0     0     0
     0     0    -1
     0     0     1
     0     1    -1
     0     1     1
     1    -1    -1
     1    -1     1
    -1     1     0

x =
     1     0    -1    -1     0     1     1
     1    -1    -1     0     1     1     0
     1     1     1     0     1     1     0
     1    -1    -1     0     1     1     0
     1     0     1     0     0     1     0
     1    -1     0     0     1     0     0
     1    -1     1    -1     1     1     1
     1    -1     1     1     1     1     1
     1    -1     0     1     1     0     1
     1    -1    -1    -1     1     1     1
     1     0    -1     0     0     1     0
     1     1     1     0     1     1     0
     1    -1     0    -1     1     0     1
     1     1     0     0     1     0     0
     1    -1    -1     1     1     1     1
     1     1    -1     0     1     1     0
     1     0    -1    -1     0     1     1
     1     0    -1     1     0     1     1
     1    -1     1     1     1     1     1
     1     0     0     0     0     0     0
     1     0     0    -1     0     0     1
     1     0     0     1     0     0     1
     1     0     1    -1     0     1     1
     1     0     1     1     0     1     1
     1     1    -1    -1     1     1     1
     1     1    -1     1     1     1     1
     1    -1     1     0     1     1     0
```

```
ox =

   75.0000   20.0000    7.5000
   30.0000   20.0000   11.2500
  120.0000   80.0000   11.2500
   30.0000   20.0000   11.2500
   75.0000   80.0000   11.2500
   30.0000   50.0000   11.2500
   30.0000   80.0000    7.5000
   30.0000   80.0000   15.0000
   30.0000   50.0000   15.0000
   30.0000   20.0000    7.5000
   75.0000   20.0000   11.2500
  120.0000   80.0000   11.2500
   30.0000   50.0000    7.5000
  120.0000   50.0000   11.2500
   30.0000   20.0000   15.0000
  120.0000   20.0000   11.2500
   75.0000   20.0000    7.5000
   75.0000   20.0000   15.0000
   30.0000   80.0000   15.0000
   75.0000   50.0000   11.2500
   75.0000   50.0000    7.5000
   75.0000   50.0000   15.0000
   75.0000   80.0000    7.5000
   75.0000   80.0000   15.0000
  120.0000   20.0000    7.5000
  120.0000   20.0000   15.0000
   30.0000   80.0000   11.2500
```

To study the spread of the optimal settings, we now plot a three-dimensional graph of the optimal settings for without control.

Fig.6.5 PureQuadratic Model for Maize

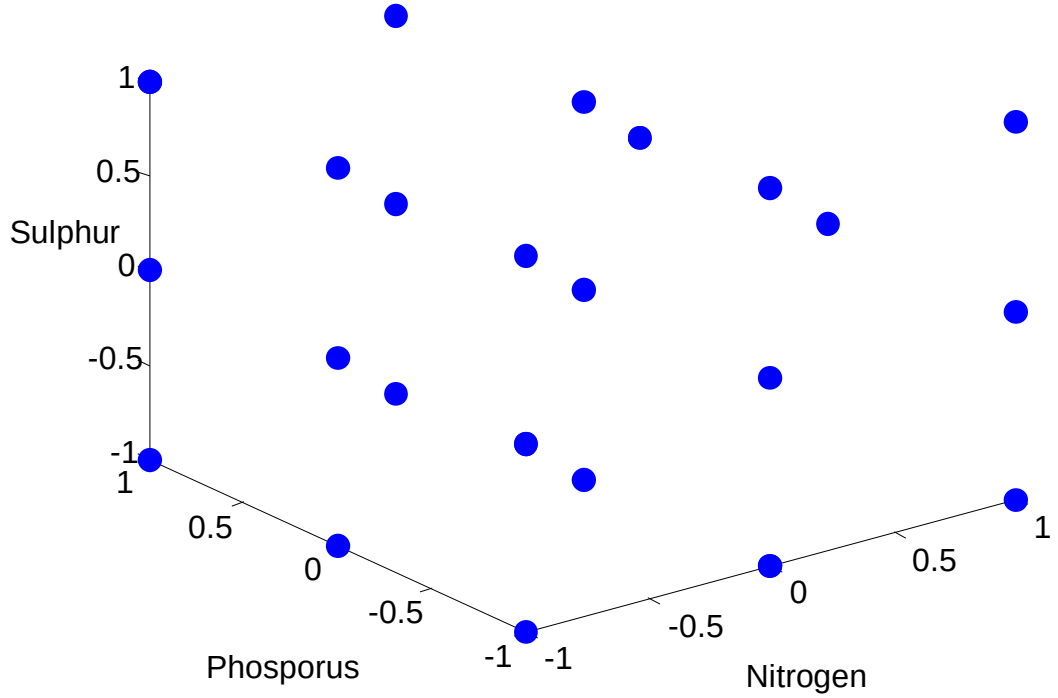


Figure 6.5 show the plot of the final settings of the pure-quadratic model for without control. Twenty three fairly spread optimal design points were generated by the model.

Remark 3: The pure-quadratic model generated 43 optimal design points for with control and 23 optimal design points for without control, although some points are replicated.

6.5 Generation of D-optimal Designs for Sorghum & Millet

Here we search for the D-optimal designs using the three models described earlier for both Sorghum and Millet because they have the same factor levels.

First we generate the 150 treatment combinations as follows:

The original values of X1 = [0 20 40 60 80] for Nitrogen.

The original values of X2 = [0 10 20 30 40] for Phosphorus.

The original values of X3 = [0 7.5 15] for Sulphur.

The original values of X4 = [0 30] for Potassium.

When the levels are coded the four factors become respectively,

```
x1 = [ -1.0000    -0.5000    0    0.5000    1.0000]
x2 = [ -1.0000    -0.5000    0    0.5000    1.0000]
x3 = [ -1.0000     0        1.0000]
x4 = [ -1.0000     1.0000]
```

The computer generated treatment combinations are given by

```
z =
   -1.0000   -1.0000   -1.0000   -1.0000
   -1.0000   -1.0000   -1.0000    1.0000
   -1.0000   -1.0000         0   -1.0000
   -1.0000   -1.0000         0    1.0000
   -1.0000   -1.0000    1.0000   -1.0000
   -1.0000   -1.0000    1.0000    1.0000
   -1.0000   -0.5000   -1.0000   -1.0000
   -1.0000   -0.5000   -1.0000    1.0000
   -1.0000   -0.5000         0   -1.0000
   -1.0000   -0.5000         0    1.0000
   -1.0000   -0.5000    1.0000   -1.0000
   -1.0000   -0.5000    1.0000    1.0000
   -1.0000         0   -1.0000   -1.0000
   -1.0000         0   -1.0000    1.0000
   -1.0000         0         0   -1.0000
   -1.0000         0         0    1.0000
   -1.0000         0    1.0000   -1.0000
   -1.0000         0    1.0000    1.0000
   -1.0000    0.5000   -1.0000   -1.0000
   -1.0000    0.5000   -1.0000    1.0000
   -1.0000    0.5000         0   -1.0000
   -1.0000    0.5000         0    1.0000
   -1.0000    0.5000    1.0000   -1.0000
   -1.0000    0.5000    1.0000    1.0000
   -1.0000    1.0000   -1.0000   -1.0000
   -1.0000    1.0000   -1.0000    1.0000
   -1.0000    1.0000         0   -1.0000
   -1.0000    1.0000         0    1.0000
   -1.0000    1.0000    1.0000   -1.0000
   -1.0000    1.0000    1.0000    1.0000
   -0.5000   -1.0000   -1.0000   -1.0000
   -0.5000   -1.0000   -1.0000    1.0000
   -0.5000   -1.0000         0   -1.0000
   -0.5000   -1.0000         0    1.0000
   -0.5000   -1.0000    1.0000   -1.0000
   -0.5000   -1.0000    1.0000    1.0000
   -0.5000   -0.5000   -1.0000   -1.0000
   -0.5000   -0.5000   -1.0000    1.0000
   -0.5000   -0.5000         0   -1.0000
   -0.5000   -0.5000         0    1.0000
```

-0.5000	-0.5000	1.0000	-1.0000
-0.5000	-0.5000	1.0000	1.0000
-0.5000	0	-1.0000	-1.0000
-0.5000	0	-1.0000	1.0000
-0.5000	0	0	-1.0000
-0.5000	0	0	1.0000
-0.5000	0	1.0000	-1.0000
-0.5000	0	1.0000	1.0000
-0.5000	0.5000	-1.0000	-1.0000
-0.5000	0.5000	-1.0000	1.0000
-0.5000	0.5000	0	-1.0000
-0.5000	0.5000	0	1.0000
-0.5000	0.5000	1.0000	-1.0000
-0.5000	0.5000	1.0000	1.0000
-0.5000	1.0000	-1.0000	-1.0000
-0.5000	1.0000	-1.0000	1.0000
-0.5000	1.0000	0	-1.0000
-0.5000	1.0000	0	1.0000
-0.5000	1.0000	1.0000	-1.0000
-0.5000	1.0000	1.0000	1.0000
0	-1.0000	-1.0000	-1.0000
0	-1.0000	-1.0000	1.0000
0	-1.0000	0	-1.0000
0	-1.0000	0	1.0000
0	-1.0000	1.0000	-1.0000
0	-1.0000	1.0000	1.0000
0	-0.5000	-1.0000	-1.0000
0	-0.5000	-1.0000	1.0000
0	-0.5000	0	-1.0000
0	-0.5000	0	1.0000
0	-0.5000	1.0000	-1.0000
0	-0.5000	1.0000	1.0000
0	0	-1.0000	-1.0000
0	0	-1.0000	1.0000
0	0	0	-1.0000
0	0	0	1.0000
0	0	1.0000	-1.0000
0	0	1.0000	1.0000
0	0.5000	-1.0000	-1.0000
0	0.5000	-1.0000	1.0000
0	0.5000	0	-1.0000
0	0.5000	0	1.0000
0	0.5000	1.0000	-1.0000
0	0.5000	1.0000	1.0000
0	1.0000	-1.0000	-1.0000
0	1.0000	-1.0000	1.0000
0	1.0000	0	-1.0000
0	1.0000	0	1.0000
0	1.0000	1.0000	-1.0000
0	1.0000	1.0000	1.0000
0.5000	-1.0000	-1.0000	-1.0000
0.5000	-1.0000	-1.0000	1.0000
0.5000	-1.0000	0	-1.0000
0.5000	-1.0000	0	1.0000
0.5000	-1.0000	1.0000	-1.0000
0.5000	-1.0000	1.0000	1.0000
0.5000	-0.5000	-1.0000	-1.0000

```
0.5000   -0.5000   -1.0000    1.0000
0.5000   -0.5000         0   -1.0000
0.5000   -0.5000         0    1.0000
0.5000   -0.5000    1.0000   -1.0000
0.5000   -0.5000    1.0000    1.0000
0.5000         0   -1.0000   -1.0000
0.5000         0   -1.0000    1.0000
0.5000         0         0   -1.0000
0.5000         0         0    1.0000
0.5000         0    1.0000   -1.0000
0.5000         0    1.0000    1.0000
0.5000    0.5000   -1.0000   -1.0000
0.5000    0.5000   -1.0000    1.0000
0.5000    0.5000         0   -1.0000
0.5000    0.5000         0    1.0000
0.5000    0.5000    1.0000   -1.0000
0.5000    0.5000    1.0000    1.0000
0.5000    1.0000   -1.0000   -1.0000
0.5000    1.0000   -1.0000    1.0000
0.5000    1.0000         0   -1.0000
0.5000    1.0000         0    1.0000
0.5000    1.0000    1.0000   -1.0000
0.5000    1.0000    1.0000    1.0000
1.0000   -1.0000   -1.0000   -1.0000
1.0000   -1.0000   -1.0000    1.0000
1.0000   -1.0000         0   -1.0000
1.0000   -1.0000         0    1.0000
1.0000   -1.0000    1.0000   -1.0000
1.0000   -1.0000    1.0000    1.0000
1.0000   -0.5000   -1.0000   -1.0000
1.0000   -0.5000   -1.0000    1.0000
1.0000   -0.5000         0   -1.0000
1.0000   -0.5000         0    1.0000
1.0000   -0.5000    1.0000   -1.0000
1.0000   -0.5000    1.0000    1.0000
1.0000         0   -1.0000   -1.0000
1.0000         0   -1.0000    1.0000
1.0000         0         0   -1.0000
1.0000         0         0    1.0000
1.0000         0    1.0000   -1.0000
1.0000         0    1.0000    1.0000
1.0000    0.5000   -1.0000   -1.0000
1.0000    0.5000   -1.0000    1.0000
1.0000    0.5000         0   -1.0000
1.0000    0.5000         0    1.0000
1.0000    0.5000    1.0000   -1.0000
1.0000    0.5000    1.0000    1.0000
1.0000    1.0000   -1.0000   -1.0000
1.0000    1.0000   -1.0000    1.0000
1.0000    1.0000         0   -1.0000
1.0000    1.0000         0    1.0000
1.0000    1.0000    1.0000   -1.0000
1.0000    1.0000    1.0000    1.0000
```

After generating the treatment combinations, we now search for the D-optimal designs using the models mentioned earlier.

6.5.1 Interaction model for Sorghum and Millet

For the interaction model the searched D-optimal designs (settings), information matrix (x), and settings converted to original values (ox), for, with and without control are given as follows:

With control

```
[settings,x]=rowexch1(4,21,'i')
settings =
    -1    -1    -1    -1
    -1    -1    -1     1
    -1    -1    -1    -1
    -1    -1     1     1
    -1    -1     1    -1
    -1    -1     1     1
    -1    -1    -1     1
    -1    -1     1    -1
    -1     1    -1    -1
    -1    -1    -1    -1
    -1     1     1    -1
    -1    -1     1     1
     1    -1    -1    -1
    -1     1    -1     1
    -1    -1    -1     1
    -1    -1     1    -1


x =
     1    -1    -1    -1    -1     1     1     1     1     1     1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1
     1    -1    -1    -1    -1     1     1     1     1     1     1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1
     1    -1     1    -1    -1    -1     1     1    -1    -1     1
     1    -1    -1    -1    -1     1     1     1     1     1     1
     1    -1     1     1    -1    -1    -1     1     1    -1    -1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1
     1     1    -1    -1    -1    -1    -1    -1     1     1     1
     1    -1     1    -1     1    -1     1    -1    -1     1    -1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1


ox =
     0     0     0     0
     0     0     0    30
     0     0     0     0
     0     0    15    30
     0     0    15     0
     0     0    15    30
     0     0     0    30
```

```
     0     0    15     0
     0    40     0     0
     0     0     0     0
     0    40    15     0
     0     0    15    30
    80     0     0     0
     0    40     0    30
     0     0     0    30
     0     0    15     0
```

Without control

```
[settings,x]=rowexch1(3,21,'i')
settings =
    -1    -1    -1
    -1    -1     1
    -1    -1    -1
    -1    -1     1
    -1     1    -1
    -1     1     1
    -1     1    -1
    -1     1     1

x =

     1    -1    -1    -1     1     1     1
     1    -1    -1     1     1    -1    -1
     1    -1    -1    -1     1     1     1
     1    -1    -1     1     1    -1    -1
     1    -1     1    -1    -1     1    -1
     1    -1     1     1    -1    -1     1
     1    -1     1    -1    -1     1    -1
     1    -1     1     1    -1    -1     1

ox =
   20.0000   10.0000    7.5000
   20.0000   10.0000   15.0000
   20.0000   10.0000    7.5000
   20.0000   10.0000   15.0000
   20.0000   40.0000    7.5000
   20.0000   40.0000   15.0000
   20.0000   40.0000    7.5000
   20.0000   40.0000   15.0000
```

In order to study the spread of the optimal settings, we now plot a three-dimensional graph of the optimal settings for without control, since it is not feasible for us to plot a four dimensional graph of the optimal settings for with control using MATLAB 5.3.

Fig.6.6 Interaction Model for Sorghum/Millet

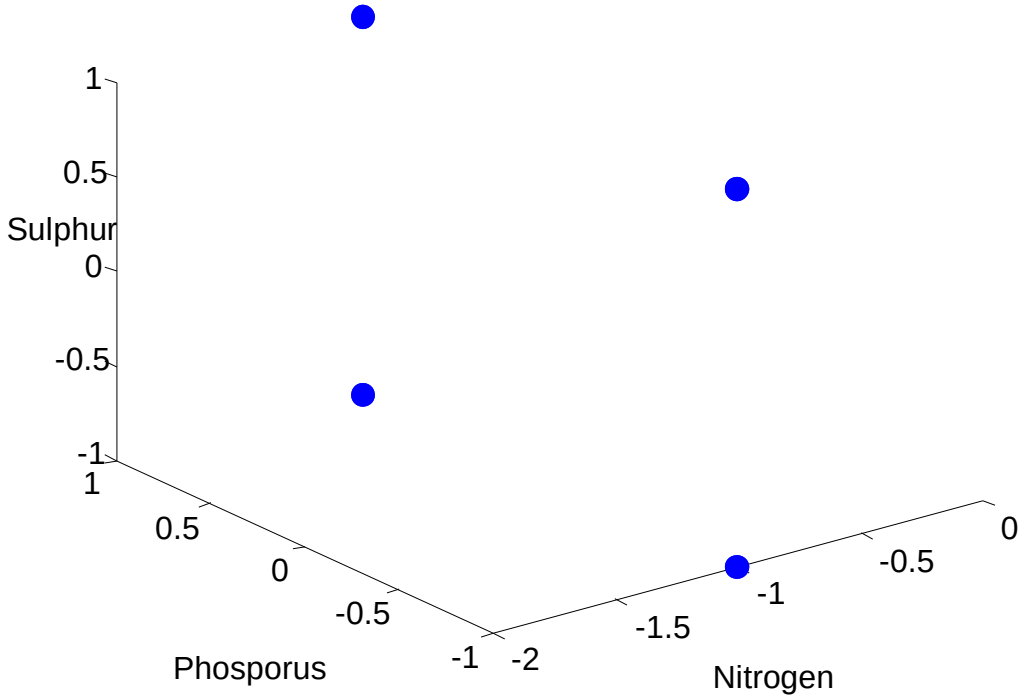


Figure 6.3 show the plot of the final settings of an interaction model for without control. Only four support points were generated by the model.

Remark 4: The interaction model generated 8 optimal design points for with control and 4 optimal design points for without control, although some points are replicated.

6.5.2 Quadratic model for Sorghum & Millet

For the quadratic model the searched D-optimal designs (settings), information matrix (x), and settings converted to original values (ox), for with and without control are given as follows:

With control

```
[settings,x]=rowexch1(4,21,'q')
settings =
     1     1     0     1
     1     0     1     1
    -1     1     1     0
     1     1    -1     0
    -1     0     1    -1
     0     0     0     0
    -1    -1    -1     0
     1    -1    -1     0
     1    -1     1     0
```

```
-1    -1    -1    -1
-1    -1     1    -1
-1    -1     1     1
-1    -1    -1     1
 1     1     1    -1
-1    -1     1     0
-1    -1    -1    -1
-1    -1     1    -1
-1    -1     1     1
-1     1    -1     0
-1    -1    -1     1
 1    -1    -1     0
-1     1    -1     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
-1     1     1    -1
-1     1     1     1
-1    -1    -1    -1
-1    -1    -1     1
-1     1     1     1
-1     0     0     0
-1    -1     1    -1
-1    -1     1     1
-1     1     1    -1
 1    -1     1     0
 1     1    -1     0
-1     1    -1    -1
-1    -1    -1     1
-1    -1     1    -1
-1    -1    -1    -1
-1     1    -1     1
-1     0     0     0
-1    -1     1     1
 1    -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     1     0
-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     1     1     0
-1    -1    -1    -1
-1     1     1    -1
-1    -1    -1     1
 0     1     0     0
-1     1     1     1
-1    -1     1     1
```

```
    -1    -1     1    -1
     0    -1    -1     0
    -1     0    -1     0
    -1     1    -1    -1
     1    -1     1    -1
    -1     1     0     1
     1    -1    -1     1
    -1    -1     0    -1
     1    -1     1     1
     1    -1    -1    -1
     1     1     0     0
     0    -1     1     0
    -1    -1     0     1
    -1     0    -1     1
     1     1    -1     1
```

```
x =

  Columns 1 through 12
     1     1     1     0     1     1     0     1     0     1     0     1
     1     1     0     1     1     0     1     1     0     0     1     1
     1    -1     1     1     0    -1    -1     0     1     0     0     1
     1     1     1    -1     0     1    -1     0    -1     0     0     1
     1    -1     0     1    -1     0    -1     1     0     0    -1     1
     1     0     0     0     0     0     0     0     0     0     0     0
     1    -1    -1    -1     0     1     1     0     1     0     0     1
     1     1    -1    -1     0    -1    -1     0     1     0     0     1
     1     1    -1     1     0    -1     1     0    -1     0     0     1
     1    -1    -1    -1    -1     1     1     1     1     1     1     1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1     1
     1    -1    -1     1     1     1    -1    -1    -1    -1     1     1
     1    -1    -1    -1     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     1    -1     0    -1     0     0     1
     1    -1    -1    -1    -1     1     1     1     1     1     1     1
     1    -1    -1     1    -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    -1     1     0    -1     0     0     1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1     1
     1     1    -1    -1     0    -1    -1     0     1     0     0     1
     1    -1     1    -1     1    -1     1    -1    -1     1    -1     1
     1    -1     1     1    -1    -1    -1     1     1    -1    -1     1
     1    -1     1     1     1    -1    -1    -1     1     1     1     1
     1    -1     1    -1    -1    -1     1     1    -1    -1     1     1
     1    -1     1    -1     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     1     1     0     1     0     0     1
     1    -1     1     1    -1    -1    -1     1     1    -1    -1     1
     1    -1     1     1     1    -1    -1    -1     1     1     1     1
     1    -1    -1    -1    -1     1     1     1     1     1     1     1
     1    -1    -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     1
     1    -1    -1     1    -1     1    -1     1    -1     1    -1     1
     1    -1    -1     1     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    -1     1     0    -1     0     0     1
     1     1     1    -1     0     1    -1     0    -1     0     0     1
     1    -1     1    -1    -1    -1     1     1    -1    -1     1     1
     1    -1    -1    -1     1     1     1    -1     1    -1    -1     1
```

```
   1    -1    -1     1    -1     1    -1     1    -1     1    -1     1
   1    -1    -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     1
   1    -1    -1     1     1     1    -1    -1    -1    -1     1     1
   1     1    -1     1     1    -1     1     1    -1    -1     1     1
   1     1    -1    -1    -1    -1    -1    -1     1     1     1     1
   1    -1     1     1    -1    -1    -1     1     1    -1    -1     1
   1     1     1    -1     1     1    -1     1    -1     1    -1     1
   1     1     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     1     0     0    -1     0     0     0     0     1
   1    -1     1     1     1    -1    -1    -1     1     1     1     1
   1    -1     1    -1    -1    -1     1     1    -1    -1     1     1
   1     1     1    -1    -1     1    -1    -1    -1    -1     1     1
   1     1    -1     1    -1    -1     1    -1    -1     1    -1     1
   1     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     1     1     0     0     0     0     1     0     0     0
   1    -1    -1    -1    -1     1     1     1     1     1     1     1
   1    -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     1     0     0     0     0     0     0     0     0     0
   1    -1     1     1     1    -1    -1    -1     1     1     1     1
   1    -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    -1    -1     0     0     0     0     1     0     0     0
   1    -1     0    -1     0     0     1     0     0     0     0     1
   1    -1     1    -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     1    -1     0    -1     0     1     0     1
   1     1    -1    -1     1    -1    -1     1     1    -1    -1     1
   1    -1    -1     0    -1     1     0     1     0     1     0     1
   1     1    -1     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     1     0     0     0     0     0     1
   1     0    -1     1     0     0     0     0    -1     0     0     0
   1    -1    -1     0     1     1     0    -1     0    -1     0     1
   1    -1     0    -1     1     0     1    -1     0     0    -1     1
   1     1     1    -1     1     1    -1     1    -1     1    -1     1

Columns 13 through 15
   1     0     1
   0     1     1
   1     1     0
   1     1     0
   0     1     1
   0     0     0
   1     1     0
   1     1     0
   1     1     0
   1     1     1
   1     1     1
   1     1     1
   1     1     1
   1     1     0
   1     1     1
   1     1     1
   1     1     1
   1     1     0
```

```
1     1     1
1     1     0
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
1     1     0
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
0     0     0
1     1     1
1     1     1
1     1     1
1     1     0
1     1     0
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
0     0     0
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
0     1     0
1     1     1
1     1     1
1     1     1
1     1     1
1     1     1
1     1     0
1     1     1
1     1     1
1     1     1
1     0     0
1     1     1
1     1     1
1     1     1
1     1     0
0     1     0
1     1     1
1     1     1
1     0     1
1     1     1
1     0     1
1     1     1
1     1     1
```

```
     1     0     0
     1     1     0
     1     0     1
     0     1     1
     1     1     1

ox =
   80.0000   40.0000    7.5000   30.0000
   80.0000   20.0000   15.0000   30.0000
         0   40.0000   15.0000   15.0000
   80.0000   40.0000         0   15.0000
         0   20.0000   15.0000         0
   40.0000   20.0000    7.5000   15.0000
         0         0         0   15.0000
   80.0000         0         0   15.0000
   80.0000         0   15.0000   15.0000
         0         0         0         0
         0         0   15.0000         0
         0         0   15.0000   30.0000
         0         0         0   30.0000
   80.0000   40.0000   15.0000         0
         0         0   15.0000   15.0000
         0         0         0         0
         0         0   15.0000         0
         0         0   15.0000   30.0000
         0   40.0000         0   15.0000
         0         0         0   30.0000
   80.0000         0         0   15.0000
         0   40.0000         0   30.0000
         0   40.0000   15.0000         0
         0   40.0000   15.0000   30.0000
         0   40.0000         0         0
         0   40.0000         0   30.0000
         0   40.0000         0         0
   80.0000   40.0000   15.0000   15.0000
         0   40.0000   15.0000         0
         0   40.0000   15.0000   30.0000
         0         0         0         0
         0         0         0   30.0000
         0   40.0000   15.0000   30.0000
         0   20.0000    7.5000   15.0000
         0         0   15.0000         0
         0         0   15.0000   30.0000
         0   40.0000   15.0000         0
   80.0000         0   15.0000   15.0000
   80.0000   40.0000         0   15.0000
         0   40.0000         0         0
         0         0         0   30.0000
         0         0   15.0000         0
         0         0         0         0
         0   40.0000         0   30.0000
         0   20.0000    7.5000   15.0000
         0         0   15.0000   30.0000
   80.0000         0   15.0000   30.0000
   80.0000         0         0         0
         0   40.0000   15.0000         0
   80.0000   40.0000         0   30.0000
```

```
   80.0000   40.0000   15.0000         0
         0   40.0000         0   30.0000
         0   20.0000   15.0000   15.0000
         0   40.0000   15.0000   30.0000
         0   40.0000         0         0
   80.0000   40.0000         0         0
   80.0000         0   15.0000         0
   80.0000         0         0   30.0000
   80.0000   40.0000   15.0000   30.0000
   40.0000   40.0000   15.0000   15.0000
         0         0         0         0
         0   40.0000   15.0000         0
         0         0         0   30.0000
   40.0000   40.0000    7.5000   15.0000
         0   40.0000   15.0000   30.0000
         0         0   15.0000   30.0000
         0         0   15.0000         0
   40.0000         0         0   15.0000
         0   20.0000         0   15.0000
         0   40.0000         0         0
   80.0000         0   15.0000         0
         0   40.0000    7.5000   30.0000
   80.0000         0         0   30.0000
         0         0    7.5000         0
   80.0000         0   15.0000   30.0000
   80.0000         0         0         0
   80.0000   40.0000    7.5000   15.0000
   40.0000         0   15.0000   15.0000
         0         0    7.5000   30.0000
         0   20.0000         0   30.0000
   80.0000   40.0000         0   30.0000
```

Without control

```
[settings,x]=rowexch1(3,21,'q')
settings =
     0     0     0
    -1    -1     0
     1    -1     0
    -1    -1     1
    -1    -1    -1
    -1     1     0
    -1     1    -1
    -1     1     1
     1     1     0
    -1    -1    -1
    -1    -1     1
    -1     0     0
    -1     1    -1
    -1     1     1
     0    -1     0
     1    -1     1
     1    -1    -1
     0    -1    -1
    -1     0    -1
     0    -1     1
```

```
     1     1     1
     0     0     1
     0     1    -1
     0     1     1
     1    -1    -1
     1    -1     1
     1     1    -1

x =
     1     0     0     0     0     0     0     0     0     0
     1    -1    -1     0     1     0     0     1     1     0
     1     1    -1     0    -1     0     0     1     1     0
     1    -1    -1     1     1    -1    -1     1     1     1
     1    -1    -1    -1     1     1     1     1     1     1
     1    -1     1     0    -1     0     0     1     1     0
     1    -1     1    -1    -1     1    -1     1     1     1
     1    -1     1     1    -1    -1     1     1     1     1
     1     1     1     0     1     0     0     1     1     0
     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     0     0
     1    -1     1    -1    -1     1    -1     1     1     1
     1    -1     1     1    -1    -1     1     1     1     1
     1     0    -1     0     0     0     0     0     1     0
     1     1    -1     1    -1     1    -1     1     1     1
     1     1    -1    -1    -1    -1     1     1     1     1
     1     0    -1    -1     0     0     1     0     1     1
     1    -1     0    -1     0     1     0     1     0     1
     1     0    -1     1     0     0    -1     0     1     1
     1     1     1     1     1     1     1     1     1     1
     1     0     0     1     0     0     0     0     0     1
     1     0     1    -1     0     0    -1     0     1     1
     1     0     1     1     0     0     1     0     1     1
     1     1    -1    -1    -1    -1     1     1     1     1
     1     1    -1     1    -1     1    -1     1     1     1
     1     1     1    -1     1    -1    -1     1     1     1

ox =
   50.0000   25.0000   11.2500
   20.0000   10.0000   11.2500
   80.0000   10.0000   11.2500
   20.0000   10.0000   15.0000
   20.0000   10.0000    7.5000
   20.0000   40.0000   11.2500
   20.0000   40.0000    7.5000
   20.0000   40.0000   15.0000
   80.0000   40.0000   11.2500
   20.0000   10.0000    7.5000
   20.0000   10.0000   15.0000
   20.0000   25.0000   11.2500
   20.0000   40.0000    7.5000
   20.0000   40.0000   15.0000
   50.0000   10.0000   11.2500
   80.0000   10.0000   15.0000
   80.0000   10.0000    7.5000
   50.0000   10.0000    7.5000
   20.0000   25.0000    7.5000
```

50.0000	10.0000	15.0000
80.0000	40.0000	15.0000
50.0000	25.0000	15.0000
50.0000	40.0000	7.5000
50.0000	40.0000	15.0000
80.0000	10.0000	7.5000
80.0000	10.0000	15.0000
80.0000	40.0000	7.5000

To study the spread of the optimal settings, we now plot a three-dimensional graph of the optimal settings for without control.

Fig. 6.7 Quadratic Model for Sorghum/Millet

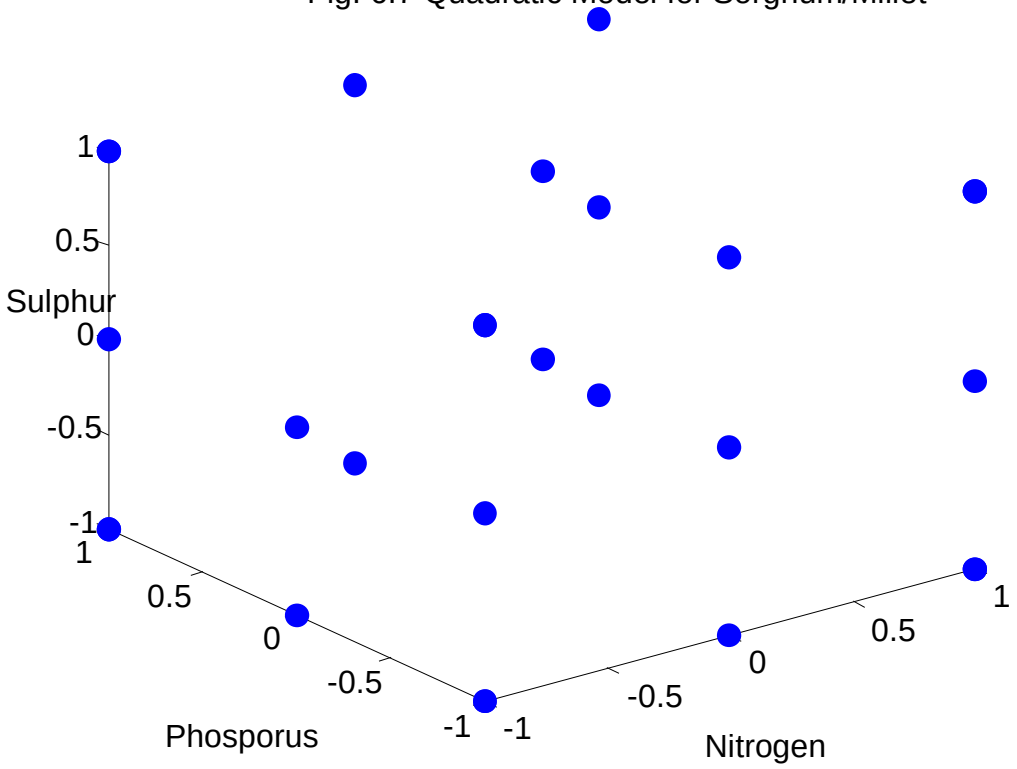


Figure 6.7 show the plot of the final settings of a quadratic model for without control. Twenty one fairly spread optimal design points were generated by the model.

Remark 7: The quadratic model generated 42 optimal design points for with control and 21 optimal design points for without control, although some points are replicated.

6.5.3 Pure-quadratic model for Sorghum & Millet

For the pure-quadratic model the searched D-optimal designs (settings), information matrix (x), and settings converted to original values (ox), for, with and without control are given as follows:

With control

```
[settings,x]=rowexch1(4,21,'p')
settings =
    -1    -1    -1     1
     1     1    -1    -1
     1     1     1     0
    -1    -1     0     0
     0     0     1     0
     1     1    -1     0
    -1    -1     1     0
     0     1     0     0
     1     0    -1     0
    -1    -1     0     0
     0     1     0     0
    -1    -1    -1     0
     1     0     0     0
    -1     1    -1     0
    -1     0    -1     0
     1    -1     1     0
    -1     0     1     0
     0     1     0     0
    -1     0    -1     0
     0     1     1     0
    -1     0     0     0
     0    -1    -1     0
    -1    -1     1    -1
     1    -1     0     0
    -1     1    -1    -1
    -1     1    -1     1
    -1     1     0    -1
    -1     1     0     1
    -1     1     1    -1
    -1     1     1     1
    -1     0     1     0
    -1    -1    -1     1
    -1    -1     0    -1
     0    -1    -1     0
    -1    -1     0     1
     0     1     1     0
    -1    -1     1     1
     0    -1     1     0
    -1     0    -1     0
     1     1     1     0
    -1    -1     1    -1
    -1     0     0     0
    -1     1    -1    -1
     1     1     0     0
     0    -1    -1     0
    -1    -1     0     1
```

```
    -1     0     1     0
     1     1    -1     0
    -1     0    -1    -1
    -1     0    -1     1
     1    -1     1     0
    -1     0     0    -1
    -1     1     1     1
     1    -1    -1     0
    -1     1    -1    -1
    -1     0     1     0
    -1    -1     0    -1
    -1     1     0     1
     0     1     0     0
    -1     1     1     1
     1    -1     0     0
    -1    -1    -1     1
     0    -1    -1     0
    -1     0     1     0
    -1    -1     1    -1
     0    -1     0     0
     1     1    -1     0
    -1     1     0    -1
     1     1     1     0
    -1     0     0     0
     0    -1     1    -1
     0    -1     0     0
    -1    -1    -1     1
     0    -1    -1    -1
     1     1    -1     0
    -1     1    -1    -1
     0     0    -1     0
     0    -1     1     1
    -1     0     0     1
     0     0    -1     0
     1    -1     1     0

x =
     1    -1    -1    -1     1     1     1     1     1
     1     1     1    -1    -1     1     1     1     1
     1     1     1     1     0     1     1     1     0
     1    -1    -1     0     0     1     1     0     0
     1     0     0     1     0     0     0     1     0
     1     1     1    -1     0     1     1     1     0
     1    -1    -1     1     0     1     1     1     0
     1     0     1     0     0     0     1     0     0
     1     1     0    -1     0     1     0     1     0
     1    -1    -1     0     0     1     1     0     0
     1     0     1     0     0     0     1     0     0
     1    -1    -1    -1     0     1     1     1     0
     1     1     0     0     0     1     0     0     0
     1    -1     1    -1     0     1     1     1     0
     1    -1     0    -1     0     1     0     1     0
     1     1    -1     1     0     1     1     1     0
     1    -1     0     1     0     1     0     1     0
     1     0     1     0     0     0     1     0     0
     1    -1     0    -1     0     1     0     1     0
     1     0     1     1     0     0     1     1     0
```

1	-1	0	0	0	1	0	0	0
1	0	-1	-1	0	0	1	1	0
1	-1	-1	1	-1	1	1	1	1
1	1	-1	0	0	1	1	0	0
1	-1	1	-1	-1	1	1	1	1
1	-1	1	-1	1	1	1	1	1
1	-1	1	0	-1	1	1	0	1
1	-1	1	0	1	1	1	0	1
1	-1	1	1	-1	1	1	1	1
1	-1	1	1	1	1	1	1	1
1	-1	0	1	0	1	0	1	0
1	-1	-1	-1	1	1	1	1	1
1	-1	-1	0	-1	1	1	0	1
1	0	-1	-1	0	0	1	1	0
1	-1	-1	0	1	1	1	0	1
1	0	1	1	0	0	1	1	0
1	-1	-1	1	1	1	1	1	1
1	0	-1	1	0	0	1	1	0
1	-1	0	-1	0	1	0	1	0
1	1	1	1	0	1	1	1	0
1	-1	-1	1	-1	1	1	1	1
1	-1	0	0	0	1	0	0	0
1	-1	1	-1	-1	1	1	1	1
1	1	1	0	0	1	1	0	0
1	0	-1	-1	0	0	1	1	0
1	-1	-1	0	1	1	1	0	1
1	-1	0	1	0	1	0	1	0
1	1	1	-1	0	1	1	1	0
1	-1	0	-1	-1	1	0	1	1
1	-1	0	-1	1	1	0	1	1
1	1	-1	1	0	1	1	1	0
1	-1	0	0	-1	1	0	0	1
1	-1	1	1	1	1	1	1	1
1	1	-1	-1	0	1	1	1	0
1	-1	1	-1	-1	1	1	1	1
1	-1	0	1	0	1	0	1	0
1	-1	-1	0	-1	1	1	0	1
1	-1	1	0	1	1	1	0	1
1	0	1	0	0	0	1	0	0
1	-1	1	1	1	1	1	1	1
1	1	-1	0	0	1	1	0	0
1	-1	-1	-1	1	1	1	1	1
1	0	-1	-1	0	0	1	1	0
1	-1	0	1	0	1	0	1	0
1	-1	-1	1	-1	1	1	1	1
1	0	-1	0	0	0	1	0	0
1	1	1	-1	0	1	1	1	0
1	-1	1	0	-1	1	1	0	1
1	1	1	1	0	1	1	1	0
1	-1	0	0	0	1	0	0	0
1	0	-1	1	-1	0	1	1	1
1	0	-1	0	0	0	1	0	0
1	-1	-1	-1	1	1	1	1	1
1	0	-1	-1	-1	0	1	1	1
1	1	1	-1	0	1	1	1	0
1	-1	1	-1	-1	1	1	1	1
1	0	0	-1	0	0	0	1	0

```
     1     0    -1     1     1     0     1     1     1
     1    -1     0     0     1     1     0     0     1
     1     0     0    -1     0     0     0     1     0
     1     1    -1     1     0     1     1     1     0
     1     0    -1     0     1     0     1     0     1

ox =
         0         0         0   30.0000
   80.0000   40.0000         0         0
   80.0000   40.0000   15.0000   15.0000
         0         0    7.5000   15.0000
   40.0000   20.0000   15.0000   15.0000
   80.0000   40.0000         0   15.0000
         0         0   15.0000   15.0000
   40.0000   40.0000    7.5000   15.0000
   80.0000   20.0000         0   15.0000
         0         0    7.5000   15.0000
   40.0000   40.0000    7.5000   15.0000
         0         0         0   15.0000
   80.0000   20.0000    7.5000   15.0000
         0   40.0000         0   15.0000
         0   20.0000         0   15.0000
   80.0000         0   15.0000   15.0000
         0   20.0000   15.0000   15.0000
   40.0000   40.0000    7.5000   15.0000
         0   20.0000         0   15.0000
   40.0000   40.0000   15.0000   15.0000
         0   20.0000    7.5000   15.0000
   40.0000         0         0   15.0000
         0         0   15.0000         0
   80.0000         0    7.5000   15.0000
         0   40.0000         0         0
         0   40.0000         0   30.0000
         0   40.0000    7.5000         0
         0   40.0000    7.5000   30.0000
         0   40.0000   15.0000         0
         0   40.0000   15.0000   30.0000
         0   20.0000   15.0000   15.0000
         0         0         0   30.0000
         0         0    7.5000         0
   40.0000         0         0   15.0000
         0         0    7.5000   30.0000
   40.0000   40.0000   15.0000   15.0000
         0         0   15.0000   30.0000
   40.0000         0   15.0000   15.0000
         0   20.0000         0   15.0000
   80.0000   40.0000   15.0000   15.0000
         0         0   15.0000         0
         0   20.0000    7.5000   15.0000
         0   40.0000         0         0
   80.0000   40.0000    7.5000   15.0000
   40.0000         0         0   15.0000
         0         0    7.5000   30.0000
         0   20.0000   15.0000   15.0000
   80.0000   40.0000         0   15.0000
         0   20.0000         0         0
         0   20.0000         0   30.0000
```

```
   80.0000         0   15.0000   15.0000
         0   20.0000    7.5000         0
         0   40.0000   15.0000   30.0000
   80.0000         0         0   15.0000
         0   40.0000         0         0
         0   20.0000   15.0000   15.0000
         0         0    7.5000         0
         0   40.0000    7.5000   30.0000
   40.0000   40.0000    7.5000   15.0000
         0   40.0000   15.0000   30.0000
   80.0000         0    7.5000   15.0000
         0         0         0   30.0000
   40.0000         0         0   15.0000
         0   20.0000   15.0000   15.0000
         0         0   15.0000         0
   40.0000         0    7.5000   15.0000
   80.0000   40.0000         0   15.0000
         0   40.0000    7.5000         0
   80.0000   40.0000   15.0000   15.0000
         0   20.0000    7.5000   15.0000
   40.0000         0   15.0000         0
   40.0000         0    7.5000   15.0000
         0         0         0   30.0000
   40.0000         0         0         0
   80.0000   40.0000         0   15.0000
         0   40.0000         0         0
   40.0000   20.0000         0   15.0000
   40.0000         0   15.0000   30.0000
         0   20.0000    7.5000   30.0000
   40.0000   20.0000         0   15.0000
   80.0000         0   15.0000   15.0000
```

Without control

```
[settings,x]=rowexch1(3,21,'p')
settings =
     0    -1    -1
    -1    -1     0
     1     1     0
    -1    -1     0
     0     1     0
    -1     0     0
    -1     1    -1
    -1     1     1
    -1     0     1
    -1    -1    -1
     0    -1     0
     1     1     0
    -1     0    -1
     1     0     0
    -1    -1     1
     1    -1     0
     0    -1    -1
     0    -1     1
    -1     1     1
     0     0     0
     0     0    -1
```

```
     0     0     1
     0     1    -1
     0     1     1
     1    -1    -1
     1    -1     1
    -1     1     0


x =
     1     0    -1    -1     0     1     1
     1    -1    -1     0     1     1     0
     1     1     1     0     1     1     0
     1    -1    -1     0     1     1     0
     1     0     1     0     0     1     0
     1    -1     0     0     1     0     0
     1    -1     1    -1     1     1     1
     1    -1     1     1     1     1     1
     1    -1     0     1     1     0     1
     1    -1    -1    -1     1     1     1
     1     0    -1     0     0     1     0
     1     1     1     0     1     1     0
     1    -1     0    -1     1     0     1
     1     1     0     0     1     0     0
     1    -1    -1     1     1     1     1
     1     1    -1     0     1     1     0
     1     0    -1    -1     0     1     1
     1     0    -1     1     0     1     1
     1    -1     1     1     1     1     1
     1     0     0     0     0     0     0
     1     0     0    -1     0     0     1
     1     0     0     1     0     0     1
     1     0     1    -1     0     1     1
     1     0     1     1     0     1     1
     1     1    -1    -1     1     1     1
     1     1    -1     1     1     1     1
     1    -1     1     0     1     1     0

ox =
   50.0000   10.0000    7.5000
   20.0000   10.0000   11.2500
   80.0000   40.0000   11.2500
   20.0000   10.0000   11.2500
   50.0000   40.0000   11.2500
   20.0000   25.0000   11.2500
   20.0000   40.0000    7.5000
   20.0000   40.0000   15.0000
   20.0000   25.0000   15.0000
   20.0000   10.0000    7.5000
   50.0000   10.0000   11.2500
   80.0000   40.0000   11.2500
   20.0000   25.0000    7.5000
   80.0000   25.0000   11.2500
   20.0000   10.0000   15.0000
   80.0000   10.0000   11.2500
   50.0000   10.0000    7.5000
   50.0000   10.0000   15.0000
   20.0000   40.0000   15.0000
```

50.0000	25.0000	11.2500
50.0000	25.0000	7.5000
50.0000	25.0000	15.0000
50.0000	40.0000	7.5000
50.0000	40.0000	15.0000
80.0000	10.0000	7.5000
80.0000	10.0000	15.0000
20.0000	40.0000	11.2500

To study the spread of the optimal settings, we now plot a three-dimensional graph of the optimal settings for without control.

Fig.6.8. PureQuadratic Model for Sorghum/Millet

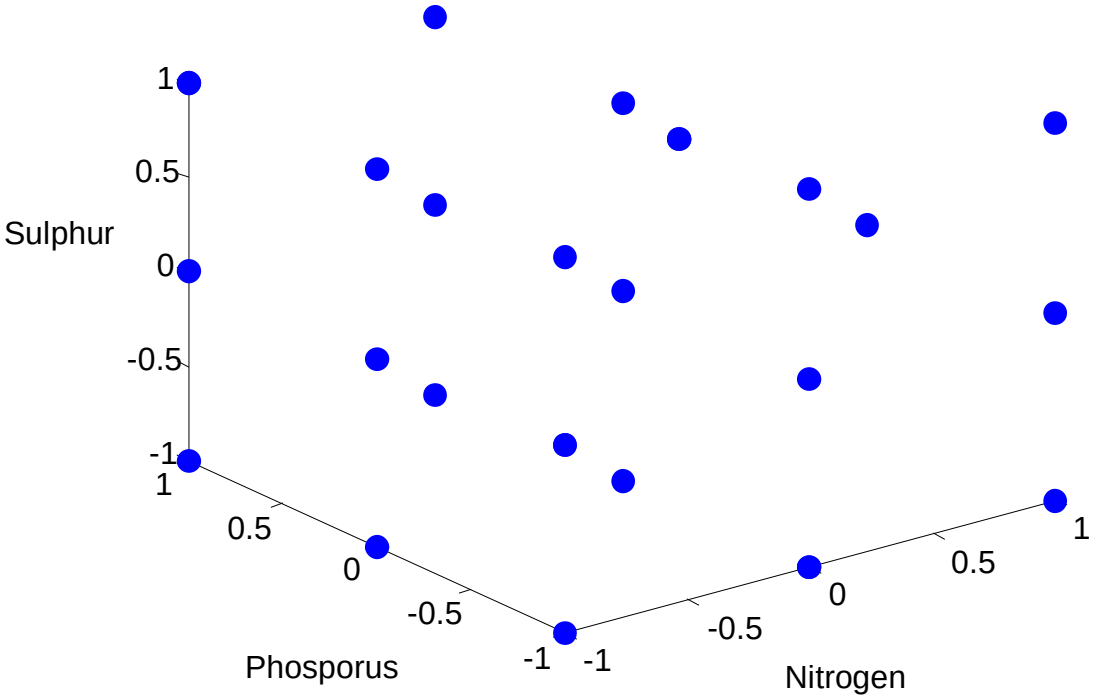


Figure 6.8 show the plot of the final settings of the pure-quadratic model for without control. Twenty three fairly spread optimal design points were generated by the model.

Remark 8: The pure-quadratic model generated 43 optimal design points for with control and 23 optimal design points for without control, although some points are replicated.

6.6 OBSERVATIONS

From remarks 1 through 8 the following observations are made as summarized in the tables below.

Crop	parameters	Model		
		Interaction	**Quadratic**	**Purequadratic**
Maize	**No. of iterations At optimal settings**	2	10	3
	No. of runs (n) At optimal settings	8	42	43
	D-efficiency	100%	100%	100%
Sorghum/ Millet	**No. of iterations At optimal settings**	2	10	3
	No. of runs (n) At optimal settings	8/150	42/150	43/150
	D-efficiency	100%	100%	100%

Table 6.1 Summary of Results for With Control

Crop	Parameters	Model		
		Interaction	**Quadratic**	**Purequadratic**
Maize	**No. of iterations At optimal settings**	2	2	3
	No. of runs (n) At optimal settings	4/32	21/32	23/32
	D-efficiency	100%	100%	100%
Sorghum/ Millet	**No. of iterations At optimal settings**	2	2	3
	No. of runs (n) At optimal settings	4/32	21/32	23/32
	D-efficiency	100%	100%	100%

Table 6.2 Summary of Results for Without Control

From table 6.1, that is the results for with control, we observed that the number of runs n (at optimality), are 8, 42, and 43 (out of 150 initial observations) for interaction, quadratic and purequadratic models respectively. While From table 6.2, the results for without control, we observed that the number of runs n (at optimality), are 4, 21, and 23 (out of 32 initial observations) for interaction, quadratic and purequadratic models respectively.

We recall that the specification for the experiment is that 21 treatment combinations with control are desired. The interaction model produces too few runs (8). The quadratic and purequadratic models generated 42 and 43 runs respectively. Instead of unilaterally selecting any 21 observations out 150, an experimenter may select the 21 observation out of the 42 or 43 generated by the quadratic or purequadratic models. While if interest is in without control, an experimenter can absolutely select all the 21 observations out of the 32 generated by the quadratic model because it generated exactly the number of design points required.

However, if we assess all the models (see table 6.1 and 6.2) and study their graphs (fig. 6.3 to fig. 6.8) quadratic model would clearly be favoured, because the interaction model provides too little runs and purequadratic provides runs higher than quadratic model. Quadratic graph also provided support points that are fairly evenly spread.

Consequent upon favouring the use of the quadratic model, it is incumbent on us to determine the rotatability of the optimal settings (design) generated by the model using Khuri's measure of rotatability described in chapter four.

6.6.1 MEASURE OF ROTATABILITY

We now use the formula given in 4.10 to compute the measure of rotatability of the favoured design. The measure is given by,

$$\Phi_N(D) = \frac{100}{\| U^*(M) \|^2} \frac{(U^{*/}(M)\, W_4)^2}{(W_4)^2}$$

we obtain the values of quantities in the measure as follows.

Design moment	V(M)	UM)	W_0	W_2	W_4	$U^*(M)$
[0]	1	1	1	0	0	0
[1]	-4/27	-0.0323	0	0	0	0
[2]	-1/9	-0.0242	0	0	0	0
[3]	0	0	0	0	0	0
[11]	20/27	-0.0353	0	1	0	0
[22]	23/27	-0.0406	0	1	0	0
[33]	20/27	-0.0353	0	1	0	0
[12]	-2/27	-0.0035	0	0	0	0
[13]	1/27	0.0018	0	0	0	0
[23]	0	0	0	0	0	0
[11]	20/27	0.0353	0	1	0	0
[12]	-2/27	-0.0035	0	0	0	0
[13]	1/27	0.0018	0	0	0	0
[111]	-4/27	-0.0015	0	0	0	0
[122]	-2/27	-0.0008	0	0	0	0
[133]	-1/9	-0.0012	0	0	0	0
[112]	-2/27	-0.0008	0	0	0	0
[113]	-1/27	-0.0004	0	0	0	0
[123]	0	0	0	0	0	0
[22]	23/27	0.0406	0	1	0	0
[23]	0	0	0	0	0	0
[112]	-2/27	-0.0008	0	0	0	0
[222]	-1/9	-0.0012	0	0	0	0
[233]	-2/27	-0.0008	0	0	0	0
[122]	-2/27	-0.0008	0	0	0	0
[123]	0	0	0	0	0	0
[223]	0	0	0	0	0	0
[33]	20/27	0.0353	0	1	0	0
[113]	-1/27	-0.0004	0	0	0	0
[223]	0	0	0	0	0	0
[333]	0	0	0	0	0	0
[123]	0	0	0	0	0	0
[133]	-1/9	-0.0012	0	0	0	0
[233]	-2/27	-0.0008	0	0	0	0

[1111]	20/27	0.0017	0	0	3	0.0017
[1122]	2/3	0.0015	0	0	1	0.0015
[1133]	5/9	0.0013	0	0	1	0.0013
[1112]	-2/27	-0.0002	0	0	0	0
[1113]	1/27	0.0001	0	0	0	0
[1123]	0	0	0	0	0	0
[2222]	23/27	0.0019	0	0	3	0.0019
[2233]	2/3	0.0015	0	0	1	0.0015
[1222]	-2/27	-0.0002	0	0	0	0
[1223]	0	0	0	0	0	0
[2223]	0	0	0	0	0	0
[3333]	20/27	0.0017	0	0	3	0.0017
[1233]	-2/27	-0.0002	0	0	0	0
[1333]	1/27	0.0001	0	0	0	0
[2333]	0	0	0	0	0	0
[1122]	2/3	0.0015	0	0	1	0.0015
[1123]	0	0	0	0	0	0
[1223]	0	0	0	0	0	0
[1133]	5/9	-0.0013	0	0	1	0.0013
[1233]	-2/27	-0.0002	0	0	0	0
[2233]	-2/3	0.0015	0	0	1	0.0015

Now, $(U^{*/}(M)\ W_4)^2 = 6.0025e^{-04}$, $\|U^*(M)\|^2 = 2.1170e^{-05}$

$\|W_4\|^2 = 33.00$

Hence here $\Phi_N(D) = (100/2.1170e^{-05})\ (6.0025e^{-04}/33.00)$

Therefore, $\Phi_N(D) = 83.55\%$.

This shows that the design is near rotatable.

CHAPTER SEVEN

SUMMARY, CONCLUSION AND RECOMMENDATION

7.1 INTRODUCTON

In this chapter we present the summary, conclusion and recommendations based on the results obtained in chapter six.

7.2 SUMMARY AND CONCLUSION

We recall that the main objective of our thesis is to generate with the aid of computer algorithms an optimal settings for a four factor experiment involving nitrogen, phosphorus, sulphur and potassium at 5,5,3 and 2 levels respectively if controls are used, and 4,4,2 and 1 respectively, if there is no control. The factors are to be tested on maize, sorghum and millet. It should also be noted that in the initial experiment 21 treatment combinations are required because of limitation of resources. In chapter six, we started first by generating the treatment combinations for both with and without controls using the algorithms given in chapter five. We used the exchange algorithm also given in chapter five to search for D-optimal settings (designs) for maize, sorghum and millet using the interactions, quadratic and pure-quadratic models. Since it isn't possible plotting the optimal settings for with control, the optimal settings generated for without control were then plotted on a three-dimensional space to depict the distributions of the settings, as shown in fig. 6.3 through 6.8.

The three models interaction, quadratic and pure-quadratic models are compared for the crops. The maize was considered separately while sorghum and millet were considered jointly because they have the same initial and optimal settings.

We favoured the use of quadratic model and evaluated the rotatability of the optimal settings (design) of the model using Khuri's measure of rotatability. It was found that the design was near rotatable with a value of 83.55%.

7.3 RECOMMENDATIONS

Based on our observations in 6.6, we recommend the use of the settings generated by the quadratic model for the initial experiments instead of the ones used. This is because for these type of levels (more than two), the quadratic explains the relationships among factor levels better than the general linear model used for the analysis of the experiment (which only explains relationship of levels for at most two).

The settings used in the initial experiment, where nitrogen, phosphorus, sulphur, and potassium are represented by X1, X2, X3, and X4 respectively are:

7.3.1 The settings for main experiment

The settings for maize in the initial experiment are:

X1	X2	X3	X4
0	40	7.5	60
60	40	7.5	60
120	40	7.5	60
90	20	7.5	60
60	0	7.5	60
30	60	7.5	60
90	60	7.5	60
60	80	7.5	60
0	40	15	60
60	40	15	60
120	0	15	60
30	20	15	60
90	20	15	60
60	0	15	60
30	60	15	60
90	60	15	60
60	80	15	60
60	40	7.5	0
0	0	0	0
60	40	0	60
30	20	7.5	60

While the settings for sorghum and millet in the initial experiment are:

X1	X2	X3	X4
0	20	7.5	30
40	20	7.5	30
80	20	7.5	30
60	10	7.5	30
40	0	7.5	30
20	30	7.5	30
60	30	7.5	30
40	40	7.5	30
0	20	15	30
40	20	15	30
80	20	15	30
20	10	15	30
60	10	15	30
40	0	15	30
20	30	15	30
60	30	15	30
40	40	15	30
40	20	7.5	0
0	0	0	0
40	20	0	30
20	10	7.5	30

The recommended settings generated by the quadratic model (as prespecified model) are:

7.3.2 The recommended settings for Maize with control

X1	X2	X3	X4
0	0	0	60.0000
120.0000	80.0000	0	0
120.0000	80.0000	15.0000	30.0000
0	0	7.5000	30.0000
60.0000	40.0000	15.0000	30.0000
120.0000	80.0000	0	30.0000
0	0	15.0000	30.0000
60.0000	80.0000	7.5000	30.0000
120.0000	40.0000	0	30.0000
0	0	7.5000	30.0000
60.0000	80.0000	7.5000	30.0000
0	0	0	30.0000
120.0000	40.0000	7.5000	30.0000
0	80.0000	0	30.0000
0	40.0000	0	30.0000
120.0000	0	15.0000	30.0000
0	40.0000	15.0000	30.0000
60.0000	80.0000	7.5000	30.0000
0	40.0000	0	30.0000
60.0000	80.0000	15.0000	30.0000
0	40.0000	7.5000	30.0000
60.0000	0	0	30.0000
0	0	15.0000	0

120.0000	0	7.5000	30.0000
0	80.0000	0	0
0	80.0000	0	60.0000
0	80.0000	7.5000	0
0	80.0000	7.5000	60.0000
0	80.0000	15.0000	0
0	80.0000	15.0000	60.0000
0	40.0000	15.0000	30.0000
0	0	0	60.0000
0	0	7.5000	0
60.0000	0	0	30.0000
0	0	7.5000	60.0000
60.0000	80.0000	15.0000	30.0000
0	0	15.0000	60.0000
60.0000	0	15.0000	30.0000
0	40.0000	0	30.0000
120.0000	80.0000	15.0000	30.0000
0	0	15.0000	0
0	40.0000	7.5000	30.0000
0	80.0000	0	0
120.0000	80.0000	7.5000	30.0000
60.0000	0	0	30.0000
0	0	7.5000	60.0000
0	40.0000	15.0000	30.0000
120.0000	80.0000	0	30.0000
0	40.0000	0	0
0	40.0000	0	60.0000
120.0000	0	15.0000	30.0000
0	40.0000	7.5000	0
0	80.0000	15.0000	60.0000
120.0000	0	0	30.0000
0	80.0000	0	0
0	40.0000	15.0000	30.0000
0	0	7.5000	0
0	80.0000	7.5000	60.0000
60.0000	80.0000	7.5000	30.0000
0	80.0000	15.0000	60.0000
120.0000	0	7.5000	30.0000
0	0	0	60.0000
60.0000	0	0	30.0000
0	40.0000	15.0000	30.0000
0	0	15.0000	0
60.0000	0	7.5000	30.0000
120.0000	80.0000	0	30.0000
0	80.0000	7.5000	0
120.0000	80.0000	15.0000	30.0000
0	40.0000	7.5000	30.0000
60.0000	0	15.0000	0
60.0000	0	7.5000	30.0000
0	0	0	60.0000
60.0000	0	0	0
120.0000	80.0000	0	30.0000
0	80.0000	0	0
60.0000	40.0000	0	30.0000
60.0000	0	15.0000	60.0000
0	40.0000	7.5000	60.0000
60.0000	40.0000	0	30.0000
120.0000	0	15.0000	30.0000

7.3.3 The recommended settings for Maize without control

X1	X2	X3
75.0000	20.0000	7.5000
30.0000	20.0000	11.2500
120.0000	80.0000	11.2500
30.0000	20.0000	11.2500
75.0000	80.0000	11.2500
30.0000	50.0000	11.2500
30.0000	80.0000	7.5000
30.0000	80.0000	15.0000
30.0000	50.0000	15.0000
30.0000	20.0000	7.5000
75.0000	20.0000	11.2500
120.0000	80.0000	11.2500
30.0000	50.0000	7.5000
120.0000	50.0000	11.2500
30.0000	20.0000	15.0000
120.0000	20.0000	11.2500
75.0000	20.0000	7.5000
75.0000	20.0000	15.0000
30.0000	80.0000	15.0000
75.0000	50.0000	11.2500
75.0000	50.0000	7.5000
75.0000	50.0000	15.0000
75.0000	80.0000	7.5000
75.0000	80.0000	15.0000
120.0000	20.0000	7.5000
120.0000	20.0000	15.0000
30.0000	80.0000	11.2500

7.3.4 The recommended settings for Sorghum/Millet with control

X1	X2	X3	X4
80.0000	40.0000	7.5000	30.0000
80.0000	20.0000	15.0000	30.0000
0	40.0000	15.0000	15.0000
80.0000	40.0000	0	15.0000
0	20.0000	15.0000	0
40.0000	20.0000	7.5000	15.0000
0	0	0	15.0000
80.0000	0	0	15.0000
80.0000	0	15.0000	15.0000
0	0	0	0
0	0	15.0000	0
0	0	15.0000	30.0000
0	0	0	30.0000
80.0000	40.0000	15.0000	0
0	0	15.0000	15.0000
0	0	0	0
0	0	15.0000	0
0	0	15.0000	30.0000
0	40.0000	0	15.0000
0	0	0	30.0000
80.0000	0	0	15.0000

0	40.0000	0	30.0000
0	40.0000	15.0000	0
0	40.0000	15.0000	30.0000
0	40.0000	0	0
0	40.0000	0	30.0000
0	40.0000	0	0
80.0000	40.0000	15.0000	15.0000
0	40.0000	15.0000	0
0	40.0000	15.0000	30.0000
0	0	0	0
0	0	0	30.0000
0	40.0000	15.0000	30.0000
0	20.0000	7.5000	15.0000
0	0	15.0000	0
0	0	15.0000	30.0000
0	40.0000	15.0000	0
80.0000	0	15.0000	15.0000
80.0000	40.0000	0	15.0000
0	40.0000	0	0
0	0	0	30.0000
0	0	15.0000	0
0	0	0	0
0	40.0000	0	30.0000
0	20.0000	7.5000	15.0000
0	0	15.0000	30.0000
80.0000	0	15.0000	30.0000
80.0000	0	0	0
0	40.0000	15.0000	0
80.0000	40.0000	0	30.0000
80.0000	40.0000	15.0000	0
0	40.0000	0	30.0000
0	20.0000	15.0000	15.0000
0	40.0000	15.0000	30.0000
0	40.0000	0	0
80.0000	40.0000	0	0
80.0000	0	15.0000	0
80.0000	0	0	30.0000
80.0000	40.0000	15.0000	30.0000
40.0000	40.0000	15.0000	15.0000
0	0	0	0
0	40.0000	15.0000	0
0	0	0	30.0000
40.0000	40.0000	7.5000	15.0000
0	40.0000	15.0000	30.0000
0	0	15.0000	30.0000
0	0	15.0000	0
40.0000	0	0	15.0000
0	20.0000	0	15.0000
0	40.0000	0	0
80.0000	0	15.0000	0
0	40.0000	7.5000	30.0000
80.0000	0	0	30.0000
0	0	7.5000	0
80.0000	0	15.0000	30.0000
80.0000	0	0	0
80.0000	40.0000	7.5000	15.0000
40.0000	0	15.0000	15.0000

0	0	7.5000	30.0000
0	20.0000	0	30.0000
80.0000	40.0000	0	30.0000

7.3.5 The recommended settings for Sorghum/Millet without control

X1	X2	X3
50.0000	25.0000	11.2500
20.0000	10.0000	11.2500
80.0000	10.0000	11.2500
20.0000	10.0000	15.0000
20.0000	10.0000	7.5000
20.0000	40.0000	11.2500
20.0000	40.0000	7.5000
20.0000	40.0000	15.0000
80.0000	40.0000	11.2500
20.0000	10.0000	7.5000
20.0000	10.0000	15.0000
20.0000	25.0000	11.2500
20.0000	40.0000	7.5000
20.0000	40.0000	15.0000
50.0000	10.0000	11.2500
80.0000	10.0000	15.0000
80.0000	10.0000	7.5000
50.0000	10.0000	7.5000
20.0000	25.0000	7.5000
50.0000	10.0000	15.0000
80.0000	40.0000	15.0000
50.0000	25.0000	15.0000
50.0000	40.0000	7.5000
50.0000	40.0000	15.0000
80.0000	10.0000	7.5000
80.0000	10.0000	15.0000
80.0000	40.0000	7.5000

Observe that all levels in the recommended settings are feasible because their levels fall within the initial levels that were used. That is, the levels 30-120, 20-80, 7.5-15, and 0-60 for nitrogen, phosphorus, sulphur and potassium respectively for maize. And the levels 20-80, 10-40, 7.5-15 and 0-30 for nitrogen, phosphorus, sulphur and potassium respectively used for sorghum/millet. In fact the recommended settings gave some levels that are not in the initial experiment that could minimize cost of experimentation.

We clearly favoured Quadratic model because it includes constant, linear, cross product and squared terms and this would purposely give a more even distribution of

points in the design region. And as the measure of rotatability indicates the design points are nearly rotatable, i.e. The pure-quadratic has the disadvantage of lacking cross product terms which might be very important in depicting relationships.

Finally, it is our hope that with the aid of our research report there would be tremendous improvement in the production of these staple food products in the savannah zone and any other concerned location(s). Students and experimenters in industries and research centres can adopt the procedures we specified, which has strong degree of fit to the models and design rotatability in generating settings for their respective experiments. This would reduce huge amount of wastes in resources and time. While for those that are only interested in the experimental settings of fertilizer nutrients on maize, sorghum and millet in the savannah zone of Nigeria, we advocate the use of our recommended settings at least for the initial experiment in the sequential process of experimentation.

7.4 Areas of Future Research

This work explores rowexchange algorithms of MATLAB 5.3 to give a procedure for analysing a multi-factor experiment whose design region was of the non-standard type (or restricted). For future research there is the need to consider factors that have three or more levels. Also, the procedure used in generating the treatment combinations for the restricted design region in MATLAB 5.3 is very tedious; there is also the need to devise a simple procedure for this purpose. However, despite the fact that the D-optimal design is established in literature to be the best in applications, there is still the need to compare the performances of the D-optimal designs presented here with the other alphabetic criteria (like A, E, G, V, etc.). One other important area which needs to be explored is the possibility of using the D-optimal designs generated in blocks. This will definitely assist

in situations where the factors are qualitative in nature. It will also be of tremendous importance if the D-optimal design criterion can be used to determine optimal settings for a multiresponse experiment.

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Appendix A
(the program output of 2^2 experiment)

```
[settings,x]=rowexch1(2,4,'l')

z =
    -1    -1
     1    -1
    -1     1
     1     1

fxnew =
     1    -1    -1
     1     1    -1
     1    -1     1
     1     1     1

E =
   -0.5000    0.5000    0.5000
   -0.5000    0.5000    0.5000
   -0.5000    0.5000    0.5000
   -0.5000    0.5000    0.5000

F =
   -0.5000    0.5000    0.5000
   -0.5000   -0.5000    0.5000
   -0.5000    0.5000   -0.5000
   -0.5000   -0.5000   -0.5000

dxold =
    0.7500
    0.7500
    0.7500
    0.7500
dxnew =
    0.7500
    0.7500
    0.7500
    0.7500

dxno =
    0.7500
    0.2500
    0.2500
   -0.2500

d =
    1.0000
    0.5000
    0.5000
    0.5000
```

```
d =

     1

idx =

     1

fxnew =
     1    -1    -1
     1     1    -1
     1    -1     1
     1     1     1

E =
   -0.5000   -0.5000    0.5000
   -0.5000   -0.5000    0.5000
   -0.5000   -0.5000    0.5000
   -0.5000   -0.5000    0.5000


F =
   -0.5000    0.5000    0.5000
   -0.5000   -0.5000    0.5000
   -0.5000    0.5000   -0.5000
   -0.5000   -0.5000   -0.5000


dxold =

    0.7500
    0.7500
    0.7500
    0.7500
dxnew =
    0.7500
    0.7500
    0.7500
    0.7500

dxno =
    0.2500
    0.7500
   -0.2500
    0.2500

d =
    0.5000
    1.0000
    0.5000
    0.5000
```

```
d =

     1


idx =

     2


fxnew =
     1    -1    -1
     1     1    -1
     1    -1     1
     1     1     1


E =
   -0.5000    0.5000   -0.5000
   -0.5000    0.5000   -0.5000
   -0.5000    0.5000   -0.5000
   -0.5000    0.5000   -0.5000


F =
   -0.5000    0.5000    0.5000
   -0.5000   -0.5000    0.5000
   -0.5000    0.5000   -0.5000
   -0.5000   -0.5000   -0.5000


dxold =
    0.7500
    0.7500
    0.7500
    0.7500
dxnew =
    0.7500
    0.7500
    0.7500
    0.7500




dxno =
    0.2500
   -0.2500
    0.7500
    0.2500
```

```
d =
    0.5000
    0.5000
    1.0000
    0.5000

d =
     1


idx =
     3

fxnew =
     1    -1    -1
     1     1    -1
     1    -1     1
     1     1     1

E =
   -0.5000   -0.5000   -0.5000
   -0.5000   -0.5000   -0.5000
   -0.5000   -0.5000   -0.5000
   -0.5000   -0.5000   -0.5000


F =
   -0.5000    0.5000    0.5000
   -0.5000   -0.5000    0.5000
   -0.5000    0.5000   -0.5000
   -0.5000   -0.5000   -0.5000


dxold =
    0.7500
    0.7500
    0.7500
    0.7500


dxnew =
    0.7500
    0.7500
    0.7500
    0.7500


dxno =
   -0.2500
    0.2500
```

```
    0.2500
    0.7500

d =
    0.5000
    0.5000
    0.5000
    1.0000

d =

     1

idx =

     4
```

FINAL SETTINGS

The final settings for the 2^2 experiment, its information matrix x, and graph in fig. 6.1, are as follows:

```
settings =
    -1    -1
     1    -1
    -1     1
     1     1

x =
     1    -1    -1
     1     1    -1
     1    -1     1
     1     1     1
```

Note:

(i) **z** is the matrix of the coded and generated treatment combinations.

(ii) **Fxnew, E, F, dxold, dxnew, dxno and d** are used in the process of updating iteration counter.

(iii) The **idx** and the **d** immediately before it are used to find the maximum change in the determinant.

(iv) The **final settings** are the optimal settings obtained from among the treatment combinations by the row exchange algorithms. The final settings are expected to have a

maximum determinant in comparison to any other settings from within the treatment combinations.

(v) **X** is the information matrix of the optimal settings.

Appendix B
(The program output of 3^2 experiment)

```
[settings,x]=rowexch1(2,9,'q')

settings =

   -1.0000   -1.0000
    1.0000   -1.0000
   -1.4142         0
         0    1.4142
         0   -1.4142
         0         0
   -1.0000    1.0000
    1.0000    1.0000
    1.4142         0

X =
    1.0000   -1.0000   -1.0000    1.0000    1.0000    1.0000
    1.0000    1.0000   -1.0000   -1.0000    1.0000    1.0000
    1.0000   -1.4142         0         0    2.0000         0
    1.0000         0    1.4142         0         0    2.0000
    1.0000         0   -1.4142         0         0    2.0000
    1.0000         0         0         0         0         0
    1.0000   -1.0000    1.0000   -1.0000    1.0000    1.0000
    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
    1.0000    1.4142         0         0    2.0000         0

fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1

E =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
```

```
F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =

    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250

dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250

dxno =
    0.6250
    0.1875
   -0.1250
    0.1875
   -0.0000
   -0.0625
   -0.1250
   -0.0625
    0.1250

Find the changes in the determinant.

d =
    1.0000
    0.5859
    0.6250
    0.5859
```

```
    0.7500
    0.5547
    0.6250
    0.5547
    0.6250

Find the maximum change in the determinant.

d =
     1

idx =

     1

fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1

E =
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066

F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =
    0.6250
    0.6250
    0.6250
```

```
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250

dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250

dxno =

   -0.1250
    0.1875
    0.6250
   -0.0625
   -0.0000
    0.1875
    0.1250
   -0.0625
   -0.1250

Find the changes in the determinant.

d =
    0.6250
    0.5859
    1.0000
    0.5547
    0.7500
    0.5859
    0.6250
    0.5547
    0.6250

Find the maximum change in the determinant.

d =
     1

idx =
     3
fxnew =
     1    -1    -1     1     1     1
```

```
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1

E =
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066
   -0.3333    0.5000    0.0000         0    0.5025   -0.1066

F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250

dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250
```

```
dxno =
    0.3018
   -0.0625
   -0.0518
    0.3643
    0.0000
    0.0107
    0.3018
   -0.0625
   -0.0518

Find the changes in the determinant.

d =
    0.7005
    0.5547
    0.6121
    0.6835
    0.7500
    0.5509
    0.7005
    0.5547
    0.6121

Find the maximum change in the determinant.

d =
    0.7500

idx =
     5

fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1

E =
   -0.3333         0   -0.5000         0   -0.4020    0.3198
   -0.3333         0   -0.5000         0   -0.4020    0.3198
   -0.3333         0   -0.5000         0   -0.4020    0.3198
   -0.3333         0   -0.5000         0   -0.4020    0.3198
   -0.3333         0   -0.5000         0   -0.4020    0.3198
   -0.3333         0   -0.5000         0   -0.4020    0.3198
   -0.3333         0   -0.5000         0   -0.4020    0.3198
```

```
   -0.3333         0   -0.5000         0   -0.4020    0.3198
   -0.3333         0   -0.5000         0   -0.4020    0.3198


F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250

dxno =
   -0.0518
    0.0107
   -0.0518
   -0.0625
    0.0000
   -0.0625
    0.3018
    0.3643
    0.3018

Find the changes in the determinant.

d =
    0.6121
    0.5509
```

```
    0.6121
    0.5547
    0.7500
    0.5547
    0.7005
    0.6835
    0.7005

Find the maximum change in the determinant.

d =
    0.7500

idx =
     5

fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1


E =
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198
   -0.3333         0    0.5000         0   -0.4020    0.3198


F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =
```

```
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250

dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250

dxno =
    0.3018
    0.3643
    0.3018
   -0.0625
    0.0000
   -0.0625
   -0.0518
    0.0107
   -0.0518

Find the changes in the determinant.

d =
    0.7005
    0.6835
    0.7005
    0.5547
    0.7500
    0.5547
    0.6121
    0.5509
    0.6121

Find the maximum change in the determinant.

d =
    0.7500

idx =
     5
```

```
fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1


E =
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333         0         0         0   -0.4020   -0.8528

F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =
    1.0000
    1.0000
    1.0000
    1.0000
    1.0000
    1.0000
    1.0000
    1.0000
    1.0000

dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
```

```
    0.4687
    0.6250
    0.4687
    0.6250

dxno =
   -0.0000
    0.5000
   -0.0000
    0.5000
    1.0000
    0.5000
   -0.0000
    0.5000
   -0.0000

Find the changes in the determinant.

d =
    0.0000
    0.2500
    0.0000
    0.2500
    1.0000
    0.2500
    0.0000
    0.2500
    0.0000

Find the maximum change in the determinant.

d =
     1

idx =
     5

fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1

E =
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
```

```
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066

F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066


dxold =
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250

dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250

dxno =
   -0.1250
   -0.0625
    0.1250
    0.1875
   -0.0000
   -0.0625
    0.6250
    0.1875
   -0.1250
```

```
Find the changes in the determinant.

d =
    0.6250
    0.5547
    0.6250
    0.5859
    0.7500
    0.5547
    1.0000
    0.5859
    0.6250

Find the maximum change in the determinant.

d =
     1


idx =
     7
fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1

E =
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066


F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
```

```
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250

dxnew =
    0.6250
    0.4687
    0.6250
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250


dxno =
    0.1250
   -0.0625
   -0.1250
   -0.0625
   -0.0000
    0.1875
   -0.1250
    0.1875
    0.6250

Find the changes in the determinant.

d =
    0.6250
    0.5547
    0.6250
    0.5547
    0.7500
    0.5859
    0.6250
    0.5859
    1.0000

Find the maximum change in the determinant.
```

```
d =
     1

idx =
     9

fxnew =
     1    -1    -1     1     1     1
     1     0    -1     0     0     1
     1     1    -1    -1     1     1
     1    -1     0     0     1     0
     1     0     0     0     0     0
     1     1     0     0     1     0
     1    -1     1    -1     1     1
     1     0     1     0     0     1
     1     1     1     1     1     1

E =
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
   -0.3333   -0.5000   -0.0000         0    0.5025   -0.1066
F =
   -0.3333    0.3536    0.3536   -0.5000    0.0503    0.1066
   -0.3333         0    0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536    0.3536    0.5000    0.0503    0.1066
   -0.3333    0.3536    0.0000         0    0.0503   -0.4797
   -0.3333         0         0         0   -0.4020   -0.8528
   -0.3333   -0.3536   -0.0000         0    0.0503   -0.4797
   -0.3333    0.3536   -0.3536    0.5000    0.0503    0.1066
   -0.3333         0   -0.3536         0   -0.4020   -0.2665
   -0.3333   -0.3536   -0.3536   -0.5000    0.0503    0.1066

dxold =
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
    0.6250
dxnew =
    0.6250
    0.4687
    0.6250
```

```
    0.4687
    1.0000
    0.4687
    0.6250
    0.4687
    0.6250

dxno =
   -0.0518
   -0.0625
    0.3018
    0.0107
    0.0000
    0.3643
   -0.0518
   -0.0625
    0.3018

Find the changes in the determinant.

d =
    0.6121
    0.5547
    0.7005
    0.5509
    0.7500
    0.6835
    0.6121
    0.5547
    0.7005

Find the maximum change in the determinant.

d =
    0.7500


idx =

     5
```

6.3.1 FINAL SETTINGS

The final settings for the 3^2 experiment, its information matrix x, and graph in fig. 6.2, are as follows:

```
settings =

   -1.0000   -1.0000
    1.0000   -1.0000
```

```
   -1.4142         0
         0    1.4142
         0   -1.4142
         0         0
   -1.0000    1.0000
    1.0000    1.0000
    1.4142         0


x =

    1.0000   -1.0000   -1.0000    1.0000    1.0000    1.0000
    1.0000    1.0000   -1.0000   -1.0000    1.0000    1.0000
    1.0000   -1.4142         0         0    2.0000         0
    1.0000         0    1.4142         0         0    2.0000
    1.0000         0   -1.4142         0         0    2.0000
    1.0000         0         0         0         0         0
    1.0000   -1.0000    1.0000   -1.0000    1.0000    1.0000
    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
    1.0000    1.4142         0         0    2.0000         0
```

Where **z, Fxnew, E, F, dxold, dxnew, dxno, d, idx, final settings and X** are as stated in appendix A.