CONSTRUCTION OF SOME THIRD ORDER OPTIMUM SEQUENTIAL ROTATABLE DESIGNS IN THREE AND FOUR DIMENSIONS

BY

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

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DEDICATION

This thesis is dedicated to my father, Mr. Joshua Bitok, Mr/Mrs William, and my husband Felix, who provided exceptional support during my academic career.

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ABSTRACT

Response Surface Methodology (RSM) is a collection of statistical and mathematical techniques useful for developing, improving and optimizing processes. Response Surface Methodology has gained recognition as a useful tool in a number of fields, including industry, agriculture, and medicine. Given the limited resources currently accessible on the planet, researchers are looking for strategies to maximize resource utilization in order to meet the continually increasing demands at both the individual and society levels. This can only be achieved through an appropriate design of experiments such as in this study. The problem of this study was to construct some third order optimum sequential rotatable designs in three and four dimensions. The specific objectives of the study were; to construct third order sequential rotatable designs in three dimensions by combining pairs of second order rotatable point sets; to construct third order sequential rotatable designs in four dimensions by appending an extra factor in each of the second order rotatable point sets and; to obtain the A-, D-, T-, E- optimality criteria of the sequential third order rotatable designs in three and four dimensions. The third order rotatable arrangement in three and four dimensions were established after all variables were proved to be real and positive and their excess functions were found to be zero. These third order rotatable arrangements formed TORDs after they satisfied the non-singularity conditions required for rotatability, yielding 44, 58, and 46 points TORDs for the three-dimensional designs and 80a and 80b points TORDs for the four-dimensional designs. Most of researches in RSM are theoretical especially in third order rotatability. So, there is need to give hypothetical examples to these designs and existing designs for presentation in applicable formats for the three and four-dimensional rotatable designs to give maximum produce. The study also identified and presented A-, D-, T-, E- optimality criteria in order to obtain the effectiveness of the constructed third order rotatable designs. The design with the smallest (least) optimality criterion among these is considered to be optimal. Design B_{12} was determined to be D-optimal for TORDs in three dimensions, while design $B_{12}^{1}$was identified as the D-optimal design for TORDs in four dimensions. Design B_{12} was found to be T-optimal for TORDs in three dimensions, while design B_{12}^{1} was considered T-optimal for TORDs in four dimensions. Regarding the A-criterion, design B_{13} was deemed optimal in three dimensions, whereas design B_{12}^{1} was identified as the A-optimal design for TORDs in four dimensions. Both designs B_{12} and B_{12}^{1}were found to be E-optimal for the designs in three dimensions and four dimensions, respectively. In order to obtain optimality criteria and confirm the existence of optimal solutions in these and other design settings, the study recommends employing various methodologies. These methods include balanced incomplete block design and pairwise block design.

ABBREVIATIONS AND ACRONYMS

ABBD- Augmented Box-Behnken Design

BIBD- Balanced Incomplete Block Designs

DOE – Design of Experiments

MATLAB - Matrix Laboratory

NFCD - Nested Face Centered Design

PBIBD- Partially Balanced Incomplete Block Design

PBD- Pairwise Block Design

RSM - Response Surface Methodology

SORD - Second Order Rotatable Design

TORD - Third Order Rotatable Design

TOSRD- Third-Order Slope Rotatable Design

SYMBOLS AND NOTATIONS

A - Average Variance Criterion

Ax- Excess function for first order rotatable arrangement

C - Information Matrix

D - Determinant Criterion

E - Eigenvalue Criterion

EX- Excess function for second order rotatable arrangement

HX- Excess function for third order rotatable arrangement

IX- Excess function for third order rotatable arrangement

M - Moment Matrix

M_1 – Block corresponding to linear and quadratic terms

M_2 – Block corresponding to pure cubic terms

M_3 – Block corresponding to cross-product quadratic terms

M_4 – Block corresponding to cubic interaction terms

T - Trace criterion

y - Response variable

DEFINITIONS

Design of Experiments (DOE): A systematic approach to planning experiments so that obtained can be analysed to yield valid and objective conclusions.

Response Surface Methodology (RSM): A collection of statistical and mathematical techniques for modelling and analysing problems where a response variable is influenced by several quantitative factors.

Third- order Model: A response surface model including linear, quadratic, and cubic terms of the independent variables.

Rotatability: A property of a design in which the variance of the predicted response depends only on the distance from design centre and not on the direction.

Sequential Design: An experimental approach where data are collected in stages, allowing additional runs to be incorporated depending on information obtained in earlier stages.

Optimum Design: A design that satisfies some optimality criterion while retaining desirable features such rotatability.

Dimension: The number of independent variables or factors considered in the study.

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CHAPTER ONE: INTRODUCTION

1.0 Introduction

In this chapter the background, statement of the problem, justification, objectives and significance of the study are given.

1.1 Background of the study

1.1.1 Third Order Response Surfaces

Models in which multiple variables influence the response are examined using a statistical technique known as response surface methodology (RSM). It comprises several statistical and mathematical techniques for developing, improving, and maximizing processes. The type of research to be conducted in scientific studies is typically determined by the questions or problems that need to be answered. To address various questions, different methods of collecting data could be employed. Experimental and observational studies are the two categories into which scientific research is subdivided based on methods of data collection. Scientists conducting observational studies are only able to observe the data passively, without influencing the study's progress. Scientists intervene in experimental studies by changing the levels of one or more controllable variables. The purpose of planned experimental studies is to control other noise factors while describing the causal relationship between a process's input(s) and output. Statistical design of experiments techniques is frequently employed in experimental studies to direct the effective distribution of experimental resources with the goal of obtaining the greatest amount of information possible about a process while taking into account the limited resources and inherent variability of the experimental process.

A subfield of applied statistics known as statistical design of experiments (DOE) is used to perform scientific studies of a system, process, or product in which input factors are changed to investigate how they affect the response that is being measured. It is a methodical approach to problem solving in which ideas and strategies are implemented during the data collection phase of an investigation to reduce random fluctuations, control systematic error, improve parameter estimation accuracy, forecast future observation results, and distinguish between competing models. To summarize the data from experiments where one or more quantitative factors are tested at multiple levels, a suitable model that depicts the factor-response relationship can be fitted. The experiment aims to determine how the levels of quantitative factors, such as fertilizer, irrigation, stand density, among others, impact the response, g. The levels $x_{1u}, x_{2u}, \ldots, x_{ku}$ of the k factors, as well as the set of parameters b, can be represented as functions of the response g. An example of a typical model could be

$$g_u = f\,(x_{1u}, x_{2u}, \ldots, x_{ku}\,; b\,) + e_u \qquad (1.1.1)$$

The experimental error of the uth observation is measured by the residual e_u. The function f is known as the response surface. Understanding f gives a comprehensive overview of the experiment's findings and helps determine the best dose combination. It also allows you to predict reactions for x_{iu} values that were not tested during the experiment.

Response surface designs are those that are particularly well suited to fitting response surfaces. Due to its solid mathematical base, it is frequently utilized in industrial process optimization. RSM seeks to investigate the correlation between variables and response with the least amount of work. Because rotatable designs evenly distribute information over the response surface, they are very helpful when prior knowledge about the surface is minimal. A crucial part of any scientific investigation is experimentation. One or more responses are estimated after treatments are assigned to experimental units. An effective way to investigate real-world issues is through a carefully planned and executed experiment. Selecting an appropriate experimental design is a crucial stage in examining the variables that could affect one or more response variables. When making the decision, rotatability is one of the many criteria to consider. A rotatable design will yield information that predicts $\hat{y}$, at every point equally distant from the coded origin of the design with the same degree of precision. To put it another way, the variance of the expected value, or $V(\hat{y})$, will have spherical contours around the design origin. In practical experiments, precise rotatability is not necessary; however, understanding how to achieve it can help achieve approximate rotatability and potentially other desirable design features. To prevent bias in response, response surface designs use random execution of run sequences. The experimenter may find it difficult or expensive to randomize run sequences since it can lead to frequent changes in the factor levels, especially if the experiment involves factors that are difficult to change.

Most of the time, the functional relationship between the response and the input variables is investigated using second order response surface designs. But when there is a noticeable lack of fit or insufficiency in the model, it is better to use a polynomial model of order three to study the relationship. The implementation of third order rotatable designs (TORDs) can be achieved by adding additional runs to the SORDs in a sequential manner. As part of the scientific method, it is necessary to watch and collect data regarding how systems and process's function. In an experiment, certain inputs result in an output with one or more observable responses. Experiments can therefore yield valuable results and conclusions. Several industries, including agriculture, pharmacy, and industry, use Response Surface Methodology (RSM) extensively. For products and processes, most of the responses or yields in these applications come from experiments. The world is experiencing a shortage of resources due to the current economic downturn, which has led scholars to develop reliable strategies to make use of the few resources at hand. The evaluation of available resources, the duration and expense of the experiments, and previous experience with the experimental procedures are a few fundamental factors to take into account when planning and designing experiments. Given the current global food crisis, agricultural fields will inevitably look for better or alternative solutions. Considering the large research effort aimed at improving the statistical tools for response surface investigation, one would think that experimenters would use the highly developed statistical tools more often; however, this is not usually the case. Such experiments could find broad applications in human and veterinary medicine, agriculture, and product research-innovation development for the development of innovative products that optimize resource utilization for an industrialization process that aligns with Kenya Vision 2030.

After selecting a polynomial model with an appropriate order, the researcher must decide which settings to use for the independent variables under his control. An observational framework comprises a predetermined set of parameters, or factor levels, that make up a design. Under certain conditions, a design may become unsuitable and need to have its levels or factors increased in order to be more desirable. For example, in agriculture, ongoing crop cultivation may deplete previously accessible mineral components, requiring a sequential addition of the components that eventually cause the soil to become deficient. Making decisions requires careful experimentation. An apparatus or method for solving the problem at hand is called experimentation. Whenever an experimenter conducts scientific research, they must generally formulate a hypothesis based on the problem for which an answer is sought and then confirm the hypothesis through direct observation or by observing the results of the treatment they have employed. The collection of observations is necessary for this verification, and the experiment's design essentially dictates the pattern of observations that must be made. The focus of classical experimental designs was comparative experiments, which aim to evaluate treatment contrasts, that is, to compare the outcomes of various treatments. Response surface designs, a more recent field, are an exception, where treatments include different combinations of different levels. The nice thing about rotatable designs is that, once the required transformations are applied, the variance of the estimated response stays constant at points that are equally spaced from the center of the design, which is usually considered to be the space origin of the factor. Because rotatable designs generate information about the response surface uniformly in all directions, they are useful when little or no prior knowledge about the nature of the response surface is available.

The fitting of a first order linear surface is aided by first order rotatable designs; a second order quadratic surface is fitted by second order rotatable designs; and a third order cubic surface is fitted by third order rotatable designs. First order rotatable designs yielded second order designs, and second order designs yielded third order rotatable designs. These designs emerged from the need to keep the cost of experimental design to a minimum by minimizing the number of design points. Optimizing the response (output), which is determined by a number of independent factors (input variables), is the goal. In spite of the arguments made by Mead and Pike (1975) that RSM is not just an industrial/statistical tool with rigid definitions; it is a broad methodology that has long existed in biology, but its application requires flexibility in design and interpretation because biological systems are variable, constrained, and often not well-approximated by simple polynomials, there appears to be a consensus that chemical industry invented response surface and the designs used to explore them.

A response variable that is impacted by several independent variables is to be optimized using response surface methodology (RSM). By developing multiple techniques for constructing rotatable designs, including second and third order designs, RSM has advanced the field of research since Box and Wilson (1951) presented it for the first time. RSM was first made popular by their paper. Box and Hunter (1957) investigated the concept, recommended using rotatable designs, and provided both essential and sufficient requirements for a design to be rotatable; they gave moment and non-singularity conditions for second order under which designs for explorering responses surfaces would be rotatable. To make sure every point on a hypersphere has the same prediction variance, they make use of the properties of derived power, product vectors, and Schlaflian matrices. They prove that $N^{-1}X'X=I_{k+1}$, the moment matrix of the first-order rotatable design is precisely the same as moment matrix of the configuration that reduces coefficient variance βi's. As a result, in the context of estimation, a first-order rotatable design is also the "best" design. Popular designs like fractional factorial and full factorial are examples of rotatable designs. The same aspect was used by Box and Draper (1963) to construct the second and third order response model design. Box and his coworkers at Imperial Chemical Industries created Response Surface Methodology (RSM), Box and Wilson (1951) and Box and Youle(1955).

RSM have gained popularity, and numerous authors have written books about it, including Box and Draper (1987) who framed RSM as a structured approach to build empirical models from experimental data and use models to understand and optimize a response(output) influenced by several factors(inputs), Myers et al. (1989) who process and product Optimization using

Designed Experiments, and Myers and Montgomery (1995) who designed experiments efficiently, build models, and optimize responses in complex multivariable systems, without wasting resources and while capturing both main effects and interactions. Although they provide examples from a wide range of applications, the classic works on RSM by Myers and Montgomery (2002) who explained the theorical foundations and practical applications of RSM in industrial, engineering, and product development, they focus on design of experiments, Box and Draper (1987) who pioneered foundational theory of RSM and empirical modeling, and Khuri and Cornell (1996) who provided a strong statistical focus on RSM with detailed mathematical treatment, emphasized on both design theory and analytical methods, still place a strong emphasis on the chemical industry.

Chemical engineering and chemistry have benefited greatly from the most successful uses of Box and Wilson (1951) methods, which have made use of both the steepest ascent techniques and experimental designs. It appears that laboratory and industrial experiments on biotechnological processes are similar to those conducted in chemical engineering. Gardiner, Grandage and Hader (1959) gave moment and non-singularity conditions for TORDs. According to Box and Draper (1959), researchers typically seek to estimate the response in absolute terms perhaps a model's parameters that explains the correlation between the response and the factors. It might also be necessary for researchers to ascertain yield change rates for a specific unit change in input variables. Herzberg (1967) provided alternative method/strategy that consistently yields trustworthy results, doing away with the requirement to throw away the outcome from experiments with (k - l)-dimensional designs. By offering numerous techniques for producing various third order rotatable designs (TORDs), Keny et al (2012) constructed optimal second order rotatable designs and provided a useful hypothetical example. Three-dimensional, third-order rotatable designs were covered by Draper 1960a. Conditions for which a third-order rotatable point arrangement in k dimensions is non-singular are proved as a general theorem. It is demonstrated how some of the constructed second order designs may be paired to produce infinite classes of sequential three-dimensional rotatable designs. Box and Behnken (1960a) developed a class of second-order rotatable designs from first-order designs. Draper (1960b) obtained some three-dimensional third-order rotatable designs and a four-dimensional third-order rotatable design. Das (1961) obtained fractional replicates of factorial designs, including orders two and three, up to eight factors.

Draper (1960a, b, 1961) expanded the theoretical and practical basis of RSM and Gardiner et al. (1959) developed practical designs and application for RSM in chemistry/engineering contexts, both made substantial contributions to the field and increased the possibilities available to researchers looking into RSM. Mutiso (1998) investigated how second order designs may be used to produce precise and sequential three-dimensional rotatable design, by joining pairs of subsequent rotatable designs to construct differential three, four, and five-dimensional calculus optimal designs. Expanding on this concept, Nyakundi and Kilonzo (2021) constructed sequential TORDs in three, four, and five-dimensional by combining the two sets of second order rotatable designs.

Third-order models are employed to approximate the unknown response function, which is anticipated to have cubic effects, just like all other Response Surface Methodology (RSM) approximating functions. Low-order polynomials (first- and second-order) were thought to be appropriate for modeling and optimization studies involving responses and several independent variables until recent studies. The linear function is represented by the first-order main effects model. To improve model fit and adequacy, interaction terms are appended to the first-order main effects model when interactions between the design factors are suspected. When there is a curve in the response function, the first-order modelling including its interaction is inadequate. The second-order modelling becomes essential in such a situation (Koukouvinos et al., 2009). All first-order terms, their cross-product terms, and all pure quadratic terms are included in the second-order model. Moreover, a third-order model needs to be used if it seems that the second-order model lacks fit. First-order terms, cross-product terms, all quadratic terms, cross-products with quadratic terms, and cubic terms make up the third order model. It is generally the case that a (d+1)th-order model is needed to fit the model well when the d-th-order model seems inadequate to accurately convey the real-world relationship that exists between the predictor variables and the response of interest because of higher terms or lack-of-fit. As second-order models and designs fail, more and more researchers are beginning to recognize the necessity of third-order response surface designs.

Authors Landman et al. (2007) are among those who have researched third-order response surface designs. In an exploratory study involving wind-tunnel testing of high-performance aircraft, they formulated a third-order hybrid design known as a Nested Face Centered Design (NFCD). The study was to reduce the test time while accurately characterizing the aerodynamic behavior of an aircraft. Nevertheless, it became clear throughout the investigation that the classic second-order Central Composite designs exhibited inadequate prediction qualities across a cuboidal design space. This resulted in the requirement for a higher order model, which led to the application of third-order design. When the evident lack-of-fit of the second-order polynomial models and designs is confirmed, third-order models and designs become practically necessary. When the response variable's functional relationship with the experimental factors cannot be satisfactorily described by a response surface model, it is said to be out-of-fit. According to Balasubramanian (2010), lack-of-fits can also happen when significant phrases found in the model that involve interactions, quadratic or higher terms, are excluded from the model, or when fitting the model yields multiple abnormally large residuals. The lack-of-fit issue of models biases estimation. A higher model is required for more accurate estimation and approximation. While some second-order models can satisfactorily model many field problems, when the second-order model's reported lack of fit is noted, some demonstrate the need for higher models Seshubabu et al (2014). To overcome the lack-of-fit at this point, third-order or even higher-order models are needed. A third-order model, or even higher, should be taken into consideration as a reasonable solution for second order lack-of-fit. It is in view of such need that this research is carried out to obtain third-order rotatable designs that are simple to construct and can adequately be used in the presence of second-order insufficiency.

The sequentiality of the response surface techniques enables the performance of experiments at various stages, which is an advantage. Therefore, a set of experiments' results can be effectively utilized to successfully prepare the strategy for a subsequent set of experiments (Khuri, 2017). Efficient estimation of first, second, or higher-order terms is made possible by constructing a design sequentially. Previous designs can be augmented to create higher-order models, saving researchers from having to begin experimentation from scratch every time a higher-order design is required. Derringer (1969) examined the use of central composite designs in sequential methods, which has the major benefit that most experimental studies requiring second-order designs employ the central composite design. These designs allow for a sequential progression to higher order surfaces.

Second order rotatable point sets were taken into consideration in this study. According to Draper and Herzberg (1968), a few of these design points are theoretically interesting, and because of the number of points and levels involved, there is currently little chance that they will be used in an experimental investigation. The optimization of certain experimental constraints, including limited time for experimentation, production costs, and input scarcity, necessitates the reduction of these design points. Further development of experimental designs with fewer experimental runs is therefore necessary, particularly in developing nations where living and production costs are high. In the fields of veterinary medicine, human medicine, agriculture, and the chemical industry, experimental designs are frequently employed to obtain valuable information. In addition to providing spherical information contours and enabling easy fitting of a response surface, the design under consideration leads to the most economical utilization of limited resources in pertinent production procedures by offering optimal combinations of treatments in industry, agriculture, and medicine. It should be noted, however, that useful applications for this method are not automatic; judgment is required. If a researcher employs insufficient intelligence to his findings, he will probably suffer as information for any other experimentation technique, and it is always possible to make a poor choice of units, particularly in the new field of experimentation. Constructions of k-dimensional, third-order rotatable designs from those in (k-1) dimensions are performed in a way that experiments in (k-1) dimensions need not to be discarded. Designs of experiments with lower dimensions are performed first and another factor can be appended if it is felt design insufficiency. Although precise rotatability is not necessary in experimental practice, knowing how to achieve it can help make designs more desirable in other ways while also generating approximate rotatability.

Three third-order rotatable designs were constructed in this work using three-dimensional second order rotatable point sets, and two-four dimensional designs were constructed by adding a factor to the point sets. There are specific point sets that are utilized, all of which come from a basic point set that is created when a general point in three dimensions is subjected to a given transformation group. It'll be demonstrated that these generated point sets for third order rotatable designs satisfy all requirements, including the non-singularity condition. The second order and third order rotatability criteria provided by Pukelshein (1993) who came up with rotatability conditions for higher-order polynomial model, including third order, Gardiner *et al.* (1959) gave moment for second order rotatability, Draper (1960a) extended moment conditions to third-order rotatability respectively, were used to evaluate the combination using a three-dimensional transformation.

A transformation group in three dimensions and its generated points sets

Considered is the set of twenty four points provided by Draper (1960a) and Mutiso (1998). (Bose & Draper, 1959) published definitions for particular transformations applied to three dimensional points.

Let W(x, y, z) = (y, z, x). Then W^2(x,y,z)=(z,x,y) and W^3(x,y,z)= (x,y,z)=I

Thus, W,W^2,W^3=I forms a cyclical group of order three. Further,

let R_1(x,y,z)=(-x,y,z), R_2(x,y,z)=(x,-y,z), R_3(x,y,z)=(x,y,-z).

These four transformations W^j, R1, R2, and R3 combine to form a group G of transformations with an order of 24 with elements.

W^j,W^jR_1, W^jR_2, W^jR_3, $W^jR_2R_3$,

$W^jR_3R_1$, $W^jR_1R_2$, $W^jR_1R_2R_3$(j=1, 2, 3)

It is clear that each of the 24 elements is distinct, although R_1,R_2,R_3 commute, W^j and R_i do not commute (j=1, 2; i=1, 2, 3).

All transformations of the group G are applied to any random point (x, y, z) in three dimensions. As a result, getting a set of 24 points with coordinates below is possible.

(±x,±y,±z), (±y, ±z, ±x), (±z, ±x, ±y).

denoted by

G (x, y, z)

Rotatability in Response Surface designs

Allow for v variates, each at s levels. Assume a design will be formed with N of the

s^v treatment combinations are represented as a N x v matrix, also known as the design matrix. The level of appropriateness has been represented by a variable x_i, which is linked to the i^{th} factor. The combinations of treatments here will be referred to as "design points." A design of the aforementioned type will be a rotatable design of order d if a response polynomial surface, according to Box and Hunter (1957).

$$Y=\beta_0+\sum\beta_i x_i+\sum\beta_{ij}x_i x_j+\sum\beta_{ijk}x_i x_j x_k+\ldots \qquad (1.1.2)$$

given a right origin and scale, on the variates $x_i,\ I=1,2,\ldots,v$, of the response y order d as determined by alternative treatments, fit to provide the variance of the predicted response from any given treatment as a function of the treatment combinations' sum squares of the factor levels. Effective fitting of a Polynomial of second order pertaining to the factor-response relationship is made possible by a second order response surface design. Strict limitations are placed on the levels of factors when selecting the design points in order to simplify parameter estimation and produce a design with desired properties that both the model fitted by the design and the resulting design possess. The design's rotatability is one of these features. Rotatable designs accommodate variations in the anticipated response from various treatment combinations in that combination of treatments as a function of the factor levels' sum squares. In other words, if the variance of the expected response at a given set of $x$values solely depends on how far the point defined by the x values is from the design center and not on the direction, then the experimental design is said to be rotatable.

Designs that are rotatable are such in which the variation within the estimated response's $\hat{Y}u$ is solely dependent on the point's distance from the experimental region's center, that is, the variation in the response's estimate at points $x_{ou}, x_{1u}, \ldots, x_{ku}$. Estimating yield differences and response is a major area of study for rotatable design research. It is independent of how the design is oriented in relation to the actual response surface. Box and Draper (1963) made extensive use of this aspect when constructing the response surface models of the second and third orders. Response bias is avoided in response surface designs by randomly executing run sequences. This makes it challenging or costly for experimenters, particularly in cases where variables that are hard to alter are present, since the running sequences' randomization may result in regular variations to the factor levels. Most of the time, the response's functional relationship with the input variables is investigated using designs for second order response surfaces, or SORDs. However, it is preferable to investigate the relationship using a third-order polynomial model when the model's unfitness becomes significant. The implementation of Third-order rotatable designs, also known as TORDs, is achieved by appending additional runs to the SORDs in a sequential manner.

Sequential designs

There are two categories for third-order rotatable designs, sequential and non-sequential. Conversely, non-sequential experiments require all runs to be completed at once in order to enable rotatable least square fitting, designs that are sequential are carried out in segments.

Sequential experiments are more practical and cost-effective, according to Draper (1960). Based on the model's adequacy, third-order rotatable designs can therefore be executed through three phases sequentially utilizing three or four blocks. First order is typically used to run the first part, and an approximation of the response function using the first order model. At this point, the experiment may be stopped if it is determined that the first order model adequately represents the unknown function by observing indications of its good fit. On the other hand, in the event that the first model is deemed insufficient, second order trials are conducted and, should a second order model also prove to be insufficient, a third order model is fitted. The k+1 runs may be found in the first block, the second order runs in the second block, and the third order runs in the third block.

Third-order sequential designs are highly significant due to their pleasant sequential property. When the second order model is not fitting, these designs become even more crucial. To investigate the second order response surfaces, an experimenter may employ a second order design; nevertheless, a lack of fit issue could occur. This presents an opportunity for estimating the third order terms and eliminating the second order model's lack of fit if the sequential third order design is being used. If lack of fit is encountered with the second order model, sequential third order designs suggested by Das and Narasimham(1962) who provided the systematic method for constructing TORDs by combining three dimensions symmetric point sets and extending them to higher dimensions, and Arshad, Akhtar, and Gilmour(2012) who contributed a practical methodology for augmenting Box-Behnken designs to fit third – order models, will be utilized in order to approximate the full third-order model. But the sizes of these designs are enormous. Occasionally, various factors such as the high cost of experimental material make it challenging for an experimenter to use a design of such a large size in a real-world setting. The highly well-liked designs constructed by Box and Behnken(1959) were enhanced and placed third order by Arshad, Akhtar, and Gilmour (2012). These designs, known as augmented Box-Behnken designs (ABBDs), are sequential in nature and can be applied to estimate a full third order model in the event that Second-order models are not fitting.

It is very helpful to build designs sequentially; earlier designs are applicable to models of higher order, saving researchers from having to start from scratch every time they need to conduct research. Furthermore, without having to conduct the experiment again, researchers can review a design for a lower-order model. Response surface techniques were studied by Box and Wilson (1951), who took into consideration the general idea of sequential designs. This resulted in the development of the Central Composite Design, a well-known second-order class of design. Sequential designs have become popular among researchers for a variety of applications over time. Using some existing two dimensional third-order designs as a starting point, some three-dimensional, third-order rotatable designs were created by Huda (1982). The experiments conducted using two-dimensional designs do not require discarding the results with these designs. Sequential design was employed by Bosque-Sendra et al. (2001) to determine formaldehyde from pararosaniline. A second-order design that was defined over the whole experimental domain was used in their methodology. However, a new design that was created by shrinking the original design was used to confirm the response surface's characteristics. Lam (2008) investigated the use of sequential adaptive designs in computer-based studies to fit response surface models. Alaeddini et al. (2013a, 2013b) also took adaptive sequential response surface methodology into consideration for industrial research involving high design optimization performance, little resources for experimentation, and high experimentation cost. Their strategy blended response surface optimization, design of experiments, and nonlinear optimization concepts. A portion of the design space that yields the worst responses based on a specified threshold value is removed from the design by applying the adaptive response surface methodology.

Third-order response surface model

Response Surface Methodology is particularly employed when the true functional relationship between the response y and the independent variables $(x_1, x_2, \ldots, x_j)$ is unknown, and an approximation is sought through polynomial models.

RSM models the system as:

$$y = f\left(x_1, x_2, \ldots, x_j\right) + \varepsilon \qquad (1.1.3)$$

Where f represents the unknown true function relating inputs to the response and ε is the error. In a situation where f has minimal curvature in the region of interest, experimenter approximates it with first-order model. The first-order model for two independent variables is given by:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \qquad (1.1.4)$$

The first-order model only takes into account the two variables' x_1 and x_2, it is occasionally referred to as a main effects model. If these variables interact, it is simple to incorporate them into the model, as shown below:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 \qquad (1.1.5)$$

This model is an interaction-based first-order model. When the interaction term is added, the response function curves. A first-order model is inadequate, even with the interaction term included, due to curvature in the response surface. In such cases, a second-order model which includes quadratic terms, is then used:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 \qquad (1.1.6)$$

In a limited area, this model is probably going to be helpful as an approximation of the actual response surface. Response surface methodology frequently employs the second-order model for a number of reasons.

1. There is a lot of flexibility in the second-order model. Since it can assume a wide range of functional forms, it is frequently a good approximation of the actual response surface.
2. The parameters in the second-order model, the β's, are easily estimated. The method of least squares can be used for this purpose.
3. There is extensive practical experience demonstrating that second-order models are effective.

In general, the first-order model is

$$y=\beta_0+\beta_1 x_1+\beta_2 x_2+\ldots+\beta_k x_k \qquad (1.1.7)$$

and the second-order model is

$$y=\beta_0+\sum_{i=1}^{k}\beta_i x_i+\sum_{i=1}^{k}\beta_{ii} x_i^2+\text{¿}\sum_{i<j=2}^{k}\beta_{ij} x_i x_j\,\text{¿} \qquad \text{for } i<j \qquad (1.1.8)$$

The third-order model is given by the function

$$y=\beta_0+\sum_{i=1}^{k}\beta_i x_i+\text{¿}\sum_{i<j=2}^{k}\beta_{ij} x_i x_j+\text{¿}\sum_{i=1}^{k}\beta_{ii} x_i^2+\sum_{i<j=2}^{k}\beta_{ijj} x_i x_j^2+\text{¿}\sum_{i<j=2}^{k}\beta_{iij} x_{ii}^2 x_j+\text{¿}\sum_{i<j<l=3}^{k}\beta_{ijl} x_i x_j x_l+\text{¿}\sum_{i=1}^{k}\beta_{iii} x_{iii}^3+\varepsilon\,\text{¿¿¿¿¿} \qquad (1.1.9)$$

The response variable (y) is assumed to be normally distributed..

x_i, x_j, x_l are dimensionless coded independent variables; $i < j < l = 3, 4, \ldots, k$.

The least squares method can be used to estimate the unknown parameters (β) in the model. ε is the experimental error.

For k = 2, the full parameter response surface model is given by

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

(1.1.10)

and contains 10 parameters.

For k = 3, the full parameter response surface model is given as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{122} x_1 x_2^2 + \beta_{133} x_1 x_3^2 + \beta_{112} x_{11}^2 x_2 + \beta_{113}$$

(1.1.11)

and contains 20 parameters

1.1.2 Optimum criteria in Experimental Designs

Optimal and classical designs are two common categories for statistical experiment design. The widely used factorial designs, fractional factorial designs, and numerous designs of response surfaces are examples of classical designs. Frequently, they are linked to run sizes and regular design regions (spherical or cuboidal), and they are not flexible enough to accommodate different randomization structures. Nevertheless, there are situations in which classical designs are unable to satisfy the needs of the experiment. Examples of these situations include situations in which the model of interest is in a particular form, the experiment has run size restrictions, or the design region is constrained (i.e., it has an irregular shape).

Conversely, optimal designs offer more versatility for more general design issues and are usually more helpful in scenarios with limited resources, atypical design areas, unique randomization structures, or model formulations. Since they are adaptable and capable of handling a wide range of design issues, the use of optimal designs has grown in popularity in comparison to classical designs. However, the vast majority of existing research focuses on experiments having a single objective or response. There has been little research into the most effective designs for multiple-response experiments. With limited resources, an increasing number of experiments now include multiple response variables that can be described using various models. Selecting an optimal design in this instance would necessitate optimizing design features across several responses.

A category of optimal experimental designs that regard to a statistical criterion is known as an optimal design, or optimum design, in the context of design of experiments. Optimal designs in experiment design enable parameters that should be estimated impartially and with the least amount of variation when estimating statistical models. To determine the parameters as precisely as an optimal design, a non-optimal design needs to undergo a higher number of experimental runs. Experimentation costs can be practically decreased using optimal experiments. A design's optimality is determined by the statistical model and evaluated in relation to a statistical criterion that is connected to the estimator's variance-matrix. Both choosing a proper model and criterion function need an awareness of statistical theory and experience in experiment design.

The study of RSM includes the application of experimental methods to explore the space of independent or process variables, optimization strategies to determine the values of the process variables that will provide an appropriate relationship between the yield and the variables, and empirical statistical modeling to yield desired response values. If the response surface is fitted in a haphazard manner, it can become complicated and time-consuming. It has been suggested that rotatable designs be used. Equitable precision in response estimates is guaranteed by these designs. The field of optimality of designs emerged as a result of the development of computers with high speeds and the realization of the necessity and significance of selecting and implementing the best experimental design based on a well-defined statistical criterion. A category of experimental designs called optimal designs is one that satisfies a certain statistical criterion in the context of experiment design. Optimal designs enable the estimation of parameters with minimal variance and without bias on statistical model estimation experiments. Alphabetic optimality has emerged as a crucial element of experimental design, particularly for the standard linear model. Numerous design criteria have been created to generate the best possible designs, either by response prediction or parameter estimation. Yet, creating designs for the nonlinear model scenario has received comparatively little attention. For a non-optimal design to calculate the parameters as precisely as an optimal design, more experimental runs are needed. A design's optimality is determined by the statistical model and evaluated in relation to statistical criterion that is connected to the estimator's variance-matrix.

Optimal designs have several benefits, such as lower experimentation costs due to fewer experimental runs required for model estimation and the ability to accommodate various types of factors. An optimal design maximizes or minimizes an optimality criterion, which is a mere figure that expresses how impressive a design is. Information-based criteria and distance-based criteria are the two main categories of criteria that are easily available. Information-based criteria include D-optimality and A-optimality that are directly accessible; both are associated with the information matrix of the design. Given the least-squares estimates of the linear parameters in the model, this matrix holds significance because it is proportional to the inverse of the variance-covariance matrix. Suffice it to say, maximizing information and minimizing variance characterize a good design. Smith (1918) introduced the idea of an optimal experimental design when he first suggested optimal criterion and designs for regression problems. Computational algorithms were developed by Kiefer and Wolfowitz (1959) to choose the best statistical inference designs related to regression. These designs are produced utilizing particular optimality criteria that act as markers of good design. Based on the moment matrix, different optimality criteria, also known as alphabetical optimality criteria, are established. A-, D-, E-, and T-criteria a few of the optimality criteria frequently applied to rotatable designs.

Smith(1918) released guidelines that describe how the residual error variance affects an experiment's design where the experiment's data are then used to fit a polynomial model with linear parameters. The contributions made by this paper led to the development of what are now referred to as G-optimal designs for a factor experiment that supports polynomials with degrees one through six. Smith's work is regarded as the foundational paper on optimal design. It was not until the late 1950s that optimal design was rigorously developed theoretically, with major contributions from Kiefer and Wolfowitz (1959). The subject matter of these contributions is the theory of continuous optimal designs, also referred to as approximate or asymptotic designs, or designs that are seen as probability measures. The General Equivalence Theorem, a fundamental mathematical theory of continuous designs, offers a means of confirming the optimality of a proposed design.

While the A- criterion minimizes the trace of the moment matrix's inverse, the D- criterion optimizes the moment matrix's determinant. The minimal eigenvalue of the moment matrix is maximized by the E- criterion, and its trace is maximized by the T- criterion. This study developed A-, D-, T-, and E- optimality criteria for third-order rotatable three- and four-dimensional designs using tried and true methods. When using response surface methods, efficient and effective experiment design depends on an understanding of the optimality criteria. It helps researchers choose and assess rotatable designs in an informed manner, thus improving the accuracy and dependability of the results. To lower the costs associated with experimentation, the TORDs were assessed based on A-, D-, T-, and E-optimality criteria. The opportunities for using rotatable designs in multidimensional situations have increased as a result of these developments in design construction

1.2 Statement of the problem

Second, third, fourth and fifth order rotatable designs have been constructed by various authors. However, while second order rotatable designs are widely used, they may often prove insufficiency, in such cases, predictions based on quadratic models can be misleading, third order rotatable designs in three and higher dimensions are required to overcome this insufficiency. Third order rotatable designs in three and higher order dimensions have not been extensively explored. This study therefore seeks to fill the gap by constructing sequential third order rotatable designs by combining point sets in second order rotatable designs and appending extra factors to the point sets to form third order rotatable design in three and four dimensions, while assessing their optimality under A-, D-, T-, and E- optimality criteria.

1.3 Justification of the present study

TORDs may be run sequentially depending on the model adequacy. One part is second order rotatable design which may be run first; then, if the second order polynomial approximation is found to be inadequate, the trials of the second part may be run, and third order surface may be fitted. In situations where SORD model inadequacy arises further SORD experiments are carried out without discarding SORDs original model observations so that when the pairs of observations are combined TORD model can be checked. TORDs not only ensure rotatability but also allow reliable estimation of cubic effects. Evaluating designs under A-, D-, T-, and E-optimality criteria is essential to ensure that estimates of model parameters are precise. The present study is therefore justified, as it bridges the insufficiency of quadratic designs, extension to higher dimension, sequential construction framework and evaluation of A-, D-, T-, and E-optimality criteria.

1.4 Objectives of the study

1.4.1 General objective

To construct some third order optimum sequential rotatable designs in three and four dimensions respectively.

1.4.2 Specific objectives

1. To construct sequential third order rotatable designs in three dimensions by combining pairs of second order rotatable point sets.
2. To construct sequential third order rotatable designs in four dimensions by appending an extra factor in each of the second order rotatable point sets.
3. To obtain the A-, D-, T-, E- optimality criteria of the sequential third order rotatable designs in three and four dimensions.

1.5 Significance

The construction of third order optimum rotatable designs in three and four dimensions was the aim of this study. SORDs point sets enables prove the existence of TORDs in three dimensions in situations where the experimenter experiences inadequacy in second order polynomial approximation, appending extra factor to SORDs point sets gives TORDs in four dimensions. Examining the A-, D-, T- and E- optimality criteria allows experimenters to choose the design that has the least optimality criterion as being the most suited.

CHAPTER TWO: LITERATURE REVIEW

2.0 Introduction

This chapter contains literature review on the construction of some third order optimal rotatable designs in three and four dimensions from pairs of second order rotatable point sets.

2.1 Construction of rotatable designs in three dimensions

Response surface methodology encompasses three main methods: applying empirical statistical modeling to establish an appropriate approximation relationship between the yield and the process variables, as well as optimization methods to determine the values process variables that yield desired response values, and a methodical approach to investigate the domain of the procedure or independent factors. Designs that are rotatable possess the advantage of ensuring that the variance of the expected responses depends only upon the location of the points within the experimental region. This concept guarantees that experimental data is collected uniformly in all directions from the origin within the space of the design variables. Because it allows for precise measurements at every point, it is useful when constructing designs for second- and third-order response surface models.

According to Hill and Hunter (1966) review of the literature, Box and Wilson (1951) were the ones who first developed and described Response surface methodology, and Box (1952, 1954) improved its desirability and profitability. Mead and Pike (1975) felt that this implied a very limited perspective on the subject. Many experimental programs aim to interpret the relationship between a quantifiable characteristic of a study process, according to Box and Behnken (1959). Utilizing response surface techniques makes achieving this goal simple (Myers et al., 2009). The association between the response variable and a group of independent variables is provided by the function. This helps to clarify that response surface designs, also known as d-th order designs, come in carrying orders. d-th order designs, according to Box and Behnken (1959), are designs that enable the experimenter to estimate every model coefficient connected to a model of d-th order. The choice of the d-th order of the design is very much dependent on its ability to realistically and satisfactorily interpret the relationships between the responses of interest as well as the group of independent variables (Arshad et al., 2020). Empirically, in certain subject areas, the order relating response surface design is more prevalent.

Applications for designs of second-order response surfaces can be found, for instance, in the domains of industry, agriculture, biology, and pharmaceuticals. Morshedi and Akbarian (2014) reported using designs for second-order response surfaces in greenhouse experiments and snap bean production. In order to model the post weld heat treatment process under Industrial Technology, Peasura (2015) used designs of response surfaces of second order. Response surface designs of second order were applied in the field of food sciences by Khuri (2017). Third-order response surface models and designs have wide applicability in the domains of chemistry, physics, meteorology, and industry, especially when considering the rates of changes of the response surfaces, such as rates of changes in process yields. Seshubabu et al. (2014) considered using third-order response surface models in response to the rising need for higher order designs. They used Balanced Incomplete Block Designs (BIBD) to construct Third-Order Slope Rotatable Designs (TOSRD). SeshuBabu et al. (2014) documented numerous studies that necessitated the use of third-order models and designs because the second-order models and designs did not fit. Third order constructed designs can be sequential or non-sequential.

Box and Wilson (1951) took into consideration the general idea of sequential designs in the study of response surface methods. According to their method of sequential experimentation, axial points are added when the test for lack of fit detects the system's curvature, and Points of experimentation are moved sequentially in the gradient-based directions using a 2k factorial design or its fractions. The majority of response surface research was focused on the rotatable classes of designs of the second and third orders, as demonstrated by the works of Draper (1960), Box (1954), Box and Hunter (1957), and Gardiner et al. (1959). For example, without considering the orthogonality of the designs, Gardiner et al. (1959) obtained rotatable designs that were of third-order.

Third-order designs have been constructed using a variety of methods, such as split plot designs, simplex designs, double balanced incomplete block designs, partially balanced incomplete block designs (PBIBDs) and balanced incomplete block designs (BIBDs), among others. The following are some helpful sources that detail these methods: Das and Narasumham (1962) early pioneers in constructing rotatable designs using BIBDs, Baker and Bargmann (1985) developed orthogonal third- order central composite designs, Yang (2008) provided a systematic study of multiple- criteria third-order response surface designs, Koske et al. (2011) extended the construction of slope- rotatable third- order designs, SeshuBabu et al. (2015) proposed new methods for third-order slope rotatable designs , Rotich et al (2017) applied third order models in optimization problem, and Oguaghamba and Onyia (2019) extended RSM to generalized full cubic(third order) polynomial models for mixture experiments.

Through various experimental designs, RSM offers a framework for accurately and economically estimating these relations. Response surface methodology looks at how one or more response variables relate to several explanatory variables. Box and Hunter(1957) were the first to introduce the idea of rotatability. It has proven to be a crucial design criterion since its inception. Response Surface Methodology is most used in meticulous situations where several input variables have the potential to control some process quality feature or performance measure. The area of Response Surface Methodology includes the use of experiments to determine the process's or independent variables' space; experience with statistical modeling to develop a workable relationship between the yield and the process variable, as well as an optimization technique to determine the values of the process variables that produce the desired response values. RSM was initially created to simulate experimental responses, as stated by Box and Draper (1987). Later, it was extended to simulate numerical experiments. The distinction lies in the type of error generated by the response. Box and Hunter(1957) were the first to introduce the concept of rotatable designs and are set up so that the estimate response's variance at a given point is a function of the point's distance from the origin (the design's center), and thus invariant when the design is rotated orthogonally, using geometric configuration, they created these designs, with the goal of achieving constant variances of response estimates on equidistant circles, spheres, or hyper-spheres centered on the design. They also ascertained the moment requirement for a d-th order rotatable design in their seminal work. Clearly, one of the most desired characteristics of Response Surface Methodology is rotatability. Following this, several writers provided techniques for building second order and third order designs, including Box & Behnken (1960), Gardiner et al. (1959), and Bose and Draper (1959). When analyzing growth rates in pig nutrition studies, Wishart (1938, 1939) provided an illustration of orthogonal polynomials, while Winsor (1932) employed the Gompertz curve in a scenario where it was thought that the relative growth rate would decline exponentially over time.

Response curves were initially applied in the agronomic study of crop yield in relation to levels of fertilizer applied or crop spacing. According to Mitscherlich (1930), there is an asymptotically and biologically plausible relationship between the supply of a necessary growth factor (in this case, space) and plant yield. Crowther and Yates (1941) utilized Mitscherlich (1930) response equations to investigate arable crop response to multiple fertilizers. Box & Wilson (1951) study explored experimental designs whose objective is to locate the point on a response surface where the optimum is reached with the fewest number of observations. They also mentioned the possibility of simultaneous changes in several factors during a response surface study's exploration phase. They expanded upon the widely recognized experimental design factorial principle by introducing the idea of composite designs, which are applicable in the response surface methodology. These designs comprise the 2k and 2k vertices of a k-dimensional cube and a k-dimensional octahedron and are meant to be used for fitting a complete quadratic model once they reach a nearly stationary region. Making use of Taylor series expansion, they developed the convention for coded levels and talked about the steepest ascent or descent in search of the nearest stationary region around the optimal representation of the models.

Box (1952) published a paper on designs with first-order multifactors, and Box (1954) studied response surfaces using generic examples. Box and Youle (1955) showed the relationship between the fitted surface and the underlying mechanism of the system. They introduced rotatable designs to investigate the geometric configurations of the response surfaces. Carter's (1957) construction of a few second-order rotatable, two-dimensional designs came right after this. Box and Draper (1963) used the same approach to create designs for the response models of the second and third orders. Third order rotatable designs can be grouped as sequential or non-sequential. While non-sequential experimentation requires all runs to be completed at once in order to enable rotatable least square fitting, sequential designs are carried out in segments or blocks. Sequential experiments are more practical and cost-effective, according to Draper (1960). Depending on the adequacy of the model, third order rotatable designs can be executed in three stages sequentially with three or four blocks. First order models are typically used to approximate the response function after the first part, which is first order, has been run. The experiment may end at this point if it is determined that the first order model represents the unknown function adequately, as demonstrated by evidence of the goodness of fit. On the other hand, in the event that the first model is deemed insufficient, second order trials are conducted and, should a second order model also prove to be insufficient, a third order model is fitted.

The variability of the difference between expected responses at any two sites is defined by the angles and separation of the points from the center, according to Herzberg (1967). By combining particular groups of point sets, Bose and Draper (1959) and Draper (1960a) showed how to construct an infinite number of classes of second order rotatable three-dimensional designs. Herzberg (1967) developed an alternate technique for creating k-dimensional second order rotatable designs. In contrast to Draper's method, Herzberg's approach produced designs that had a lot of points, but did not require any conditions to be met. The moment and non-singularity conditions for third order rotatability were given by Gardiner et al. (1959). The moments and non-singularity conditions for fourth order rotatability were also provided by Patel and Arap Koske (1985), who conducted research after them. Fifth-order rotatability's moments and non-singularity conditions were given by Njui and Patel (1988).

Three dimensional rotatable designs of third order were constructed by Draper (1960b). He presented a general theory for the non-singularity requirement in k-dimensions and further devised a technique for constructing sequential third order rotatable designs by combining particular second order designs. Second order rotatable point sets in this study were taken from Draper (1960) and Mutiso (1998) SORDs, new classes of sequential TORDs were obtained beyond those obtained in Draper (1960b). An alternate technique for creating certain third order rotatable designs was provided by Huda (1982a, 1982b). Kosgei et al (2013) used balanced incomplete block design to construct a modified third order rotatable design with five levels. Otieno et al (2016) conducted a cost-effectiveness analysis to determine the optimal malaria controls methods in Kenya. In their study on additional investigation of second order rotatability, Draper and Herzberg (1968) proposed that a researcher could construct reduced second order rotatable designs by carefully combining fractions of the current point set with other point sets. In the current study, the aforementioned articles underwent in-depth reviews.

Mutiso (1998) was able to develop designs that satisfy the requirements of optimality and rotatability by utilizing calculus-based approaches, which increased the options for experimental designs in several dimensions. This development in design construction benefits statistical experimentation and gives researchers more options for planning experiments that are more effective and precise. Calculus was utilized to get the optimal values and to estimate the design moments λ_2 and λ_4. Koske et al., (2008) have provided a helpful example with twenty four points and a particular optimum sequential rotatable design with an example to illustrate how coded levels could become natural levels. This paper shows developments in the rotatable designs' construction in many dimensions, providing researchers with useful instruments for carrying out tests successfully and quickly using BIBD.

2.2 Construction of rotatable designs in four or more dimensions

In response surface designs, run sequences are executed at random to prevent response bias. Given that the run sequence randomization may result in frequent variations in the factor levels, which, particularly when hard-to-change variables are involved in the experiment, make it challenging or costly for the investigator. Most of the time, the functional relationship between the response and the input variables is investigated using second order response surface designs, or SORDs. However, it is preferable to investigate the relationship using a polynomial model of order three when the model's lack of fit becomes significant. The implementation of third order rotatable designs (TORDs) can be achieved by adding additional runs to the SORDs in a sequential manner.

Constructing second-order rotatable designs in four dimensions or more required a general method, which was provided by Draper (1960a), who also provided the conditions that had to be met for k-dimensional second-order rotatable designs to exist. Draper (1960b) obtained third order rotatable designs in four dimensions and from Draper’s designs Thanker and Das obtained both second and third orders designs with up to eight factors (Thaker & Das, 1961).

Three-dimensional third-order rotatable designs were developed by Huda (1982) based on the already-existing two-dimensional third order rotatable designs. Experimental outcomes conducted in accordance with the designs of two dimensions do not have to be discarded when these designs are utilized. Some of these designs can be performed one after the other in each of the three factors, beginning with a design with one dimension. Additionally, compared to the majority of the existing rotatable designs in three dimensions of the third order these TORDs require fewer points, and a few components of his designs are shared by those constructed by Herzberg(1967)

Following Huda 's works Patel and Mutiso (1992) constructed designs of third order in four dimensions. From constructed third order rotatable designs in four dimensions Koske and Mutiso (2005) constructed five-dimensional third order rotatable designs. Some cues from Draper and Herzberg (1985) were utilized by Arap Koske (1987) to construct a four-dimensional, fourth-order rotatable design following the construction of a fourth order rotatable design in three dimensions by Arap Koske and Patel (1986). In three, four, and five dimensions, Mutiso (1998) constructed rotatable designs that are both specific and sequentially optimal. Mutai, Koske and Mutiso (2012) constructed a four-dimensional TORD using BIBDs. Mutai (2012) constructed k-dimensional third order rotatable designs under balanced incomplete block designs using Huda's (1982b) method. Eighty points four- dimensional TORD was constructed by combining two, four-dimensional SORDs by Nyakundi and Matunde (2019), they also gave practical hypothetical case study. (Nyakundi 2019) added a factor to a second-order rotatable four-dimensional design to form fifty six points TORD. Second, third, fourth and fifth order rotatable designs have been constructed by various authors, however, third order rotatable designs in three and higher order dimensions have not been explored, most researchers have largely been on second-order rotatable designs. Following above citations, this study therefore seeks to fill the gap by constructing sequential third order rotatable designs by combining point sets in second order rotatable designs and appending extra factors to the point sets to form third order rotatable design in three and four dimensions.

2.3 Optimality Criteria for Response Surface Designs

RSM is now a standard tool for analyzing experimentation data. Response surface models of the first or second order, as they are commonly referred to, are utilized in these models to examine the impact of multiple input variables regarding a response variable by identifying intricate functional relationship through "simple" linear or quadratic multivariate polynomial regression, Myers, Montgomery, and Anderson Cook (2009). The creation of effective and ideal experimental designs for response surface models has been the focus of numerous authors' efforts. According to the D-, G-, and I-optimality criteria, the resolution III 2k factorial and fractional factorial 2kkp designs are optimal for models of the first order (Anderson-Cook, Borror, and Montgomery 2009). Conversely, in the case of the response surface model of second order, the circumstances are more intricate, and designs that seem reasonable on the surface but are not optimal, like central composite designs, are not. According to Kiefer (1974), approximate designs has been studied for this model by a number of authors; optimality criteria and the design space being evaluated (usually a k-dimensional cube, ball, or simplex) determine the differences in methodology and optimal designs.

Based on explicit determinations by Kiefer (1959, 1961b) who laid the foundation of optimal experimental design through the development of optimality criteria and the equivalence theorem, Kiefer and Wolfowitz (1959) who extended Kiefer’s (1959, 1961b) work by jointly formalizing the concept of optimality in regression models, Kono (1962) who pioneered the movement from purely theoretical optimal design toward practical rotatable designs, Farrell, Kiefer, and Walbran (1967) who extended optimal design theory with emphasis on variance properties and criteria for optimality, the second-order model of polynomial regression for the ball and cube has D-optimal approximate designs moreover, Rafajlowicz and Myszka (1988), as well as Dette and R¨oder (1997) who established optimal product designs for multivariate polynomial regression models in broader contexts. Specifically, it is demonstrated that D-optimal designs on a ball are also rotatable designs. Other criteria for optimality have received comparatively less attention. The A- and Q-optimal designs were studied numerically by Laptev (1974) was first to to study A-optimality in quadratic response surface designs, Denisov and Popov (1976) extended Laptev's work by considering Q- optimality as an alternative to A- and D- criteria, and Golikova and Pantchenko (1977) carried the numerical investigations further, giving systematic comparisons of A- and Q- optimal designs in higher-dimensional. Galil and Kiefer (1977b) found optimal designs that can be rotated numerically for the model of second-order response surface. The optimal design problems in second-order mixture models were studied by Draper, Heiligers, and Pukelsheim (2000) extended the scope of optimality criteria to restricted-response surface and mixture models, broadening their practical applicability and Draper and Pukelsheim (2003) provided a framework for applying optimality criteria when the model has linear parameter restrictions. However, it appears that determining the optimal designs explicitly among all approximation designs in terms of criteria other than the D-criterion is a challenging task that has only occasionally been resolved. The E-optimality criterion, one of Kiefer's criteria Kiefer (1974), cannot be distinguished if the multiplicity of the least eigenvalue of the optimal design's information matrix is greater than 1. This feature makes figuring out which designs are E-optimal very difficult and demanding. Analytically constructing designs that are E-optimal for linear regression models are actually quite challenging, only a few linear and nonlinear models in the one-dimensional case have been successfully constructed (Melas (1982) investigated E-optimal designs for polynomial regression models, Dette (1993) focused on optimal designs beyond D- optimality, Pukelsheim and Studden (1993)developed all major optimality criteria, Dette and Haines (1994) provided explicit constructions of E- optimal designs for quadratic response surface models). Results for models with multiple predictors are rare in the literature. Cheng (1987), and Dette and Studden (1993) for instance, identified chemical balance weighing designs and E-optimal spring balance designs. Among all designs in the class, the E-optimal designs whereby the corresponding information matrix possesses a minimum eigenvalue of multiplicity k(k + 1)/2, were identified by Galil and Kiefer (1977a) after considering the response surface model of second order on the k-predictor cube.

The book "Optimal Experimental Designs" by Atkinson and Donev (1992) is the source of the literature on optimal design. Pukelsheim (1993), who authored a book on the optimal design of experiments, closely followed this. For statistical model estimation experiments, optimal designs enable parameter to be approximated using minimal variation and impartially. For a non-optimal design to estimate the parameter as precisely as an optimal design, more experimental runs are needed. A statistical model determines a design's optimality, which is then evaluated in relation to a statistical criterion that is connected to the estimator's variance matrix. Panda and Das (1994) started an investigation into rotatable designs of the first order under the assumption that the model contains correlated errors. Das (1997) investigated rotatable designs of second order under the assumption of correlated errors in the model. Das (1999) introduced a procedure for constructing second order rotatable designs, a method for constructing second order rotatable designs with correlated errors, and an initial method for constructing second order rotatable designs.

In 2006, Kosgei, Koske, Too and Mutiso investigated the optimality of a SORD in three dimensions. They derived the information matrix of the design by estimating the relevant moments and the evaluated its performance under several classical optimality criteria, including the determinant D-, average-variance A-, eigen value E- and trace T- criteria. According to Montgomery (2009) and Myers et al. (2009), there are a variety of design experiments that can be used in food or chemical industries to evaluate ingredients, prepare or rework a new food product, or even optimize the conditions to produce an optimal process in many experimental investigations. In cases like these, it could be necessary to conduct experiments on the design of interest with optimal settings. Choosing the optimum design of experiments is regarded as among the greatest crucial steps in design experimentation process. Selecting the appropriate design for an experiment is a necessary step before beginning any experiment. Analyzing the designs' optimality criteria helps achieve this Given the availability of generalized inverses, the small technical issue of the moment matrix's rank deficiency is totally irrelevant. Keifer(1974) optimality criteria, for instance, are merely understood to be the mean of order P of the positive eigenvalues of moment matrix, Pukelsheim (1993), these technical variations are the exact reason why the eigenvalues dissection of the moment matrix for the Kronecker representation adopts a nearly explicit form for rotatable designs of the third order, Draper and Pukelsheim (1994).

The family of matrix means, ϕ (p), was first presented by Kiefer (1974), and Pukelsheim (1993) provided a detailed discussion of it. Pukelsheim's thorough explanation is mostly theoretical and filled with technical terms from mathematics. There are essentially two approaches to building design criteria that take into account the various experiment goals. One method is to average multiple competitive design criteria to create new optimality criteria. According to Dette and

Franke (2000), an alternative would be to strive to maximize one main optimality criterion while adhering to restrictions for particular minimum efficiencies of other criteria. The term "optimal design of experiments" (G-optimality) was first used by Smith (1918), used to maximize the local power of the F-ratio and later popularized by Kiefer and Wolfowitz (1959). Wald (1943) proposed increasing the determinant, placing a focus on the accuracy of the estimated parameters. The determinant criterion is another name for the D-optimality criterion. D-optimality's primary goal is to estimate parameters. D-optimality was introduced by Kiefer and Wolfowitz (1959) following the proposed designs for obtaining weighing designs. According to Kiefer (1960), the class of rotatable designs is very rich because it contains the optimal designs that can be found for polynomial regression models over hyperspherical regions under a number of widely used criteria, including D-optimality.

The most researched criterion, as evidenced by the works of Kiefer (1959) who established the general theory for constructing and evaluating designs in regression models, Fedorov (1972) who developed algorithms for finding optimal designs numerically, Silvey (1980) who offered a rigorous mathematical framework for the theory of optimal design, focusing on criteria such as D- and A- optimality for parameter estimation in linear models, Pázman (1986) who extended the theory of optimality criteria, Pukelsheim (1993) who provided a comprehensive and rigorous exposition of optimal experimental design, unifying the general theory of optimality criteria and information matrices and Mandal (2000) who worked on construction of higher-order optimum rotatable designs in three and four dimensions. Mandal (2000) examined the process of creating D-optimal designs in multiple scenarios that are utilized in the moment matrix's determinant, or conversely, minimizing determinant of the moment matrix's inverse. Over the past few years, it has been acknowledged such even with designs for response surfaces, the experimenter's primary focus may not always be on the response at specific individuals. The variations in responses at different places can occasionally be more interesting (Herzberg, 1967).

Chernoff (1953) used Fisher's information matrix to introduce the A-optimality criterion. Within the framework of generalized linear models Ehrenfeld (1955), but Heiligers (1996) introduced computational procedures for the E-optimal polynomial regression design. The method used here is based on identifying the design that maximizes the moment matrix's minimum eigenvalue, or alternatively, minimizes its maximum eigenvalue. The goal of E-optimality is to minimize the maximum variance among all normalized linear combinations of parameter estimates that are possible. The field of optimum design in experiments has substantially advanced because of these contributions.

In three dimensions, Mutiso (1998) constructed optimal designs of order two, but the optimization criteria for the construction were not stated. As per Pukelsheim (2006), functions possessing suitable properties to measure the largeness of information matrices are considered real optimality criteria. These functions are upper semi-continuous, positively homogeneous super additive, non-negative, and non-constant. Such criteria are called information functions. For different classes of designs with blocking, Morgan (2007) has been studying design optimality. Selecting a design that will yield a well-fitting model to the data is important when limiting the response surface problem to response optimization. Specifically, a design that yields dependable parameter estimates needs to be chosen, which can be utilized to make accurate predictions.

The A- and D-rotatability of two-dimensional third-order designs was examined by Huda et al. (2007). They were able to determine the variance-covariance matrix expression of the approximate axial slopes in the factor space at a particular point for a third order, symmetrically balanced design in two dimensions. Huda continued by deriving the matrix's trace and determinant to demonstrate that symmetry and balance are insufficient for the design to be either A-rotatable or D-rotatable. Based on Pukelsheim (2006) methods, Kosgei, (2002) obtained a criterion for third-dimensional second order designs by taking the A-, E-, D-, and T- criteria into account. The D- optimal criterion is the most common optimality criterion for generation of a design Goos and Jones (2011), in which the determinant of the covariance matrix of the estimators of the model parameters is minimized. Goos and Jones (2007) went into great detail about D-optimal split-plot designs. Some three-, four-, and five-dimensional third-order rotatable designs were constructed by Nyakundi(2016). Determination of the information matrix regarding the second-order model featuring the linear, quadratic and interaction factors and the construction of the 20 points three-dimensional second order rotatable designs were obtained by Tum (2012). In three dimensions, Nicholas (2016) assessed G- and I-optimal second-order rotatable designs. Nyakundi (2019) evaluated D-, A-, and E- optimality criterion. Nyakundi and Kilonzo (2021) developed optimal sequential TORDs in three, four and five dimensions. Hemavathi, Jaggi, and Varghese (2021) compared efficiencies under D- and A- criteria. Hemavathi, Varghese, Shekhar and Jaggi (2022) checked prediction variance properties under sequential augmentation.

In 2023, Ponte et al develop efficient algorithms to find D- optimal RSM designs for large or structured problems. Application focused contributions showing how D- optimal second order designs enhance estimation precision in small-sample experiments. The information matrix is used to determine the optimality criteria as well as precise values of the following criteria are obtained for the particular designs: the determinant criterion D-, the average-variance criterion A-, the eigenvalue criterion E-, and the trace criterion T-. The information matrix parameter estimates' optimality for the generalized variance is determined by the smallest of the criteria. These criteria assess the desirableness of a design, T-optimum design has not been used much due to the T-criterion's linearity attribute, while the ellipsoidal confidence region's content is minimized in D-optimal design for the parameters of the linear model parameters, A-optimal design minimizes the sum (or average) of the variance of the parameter estimate, and E-optimal design minimizes the variance of every single parameter estimate. After these criteria were evaluated, it was found that the more homogeneous the design, the more optimal it was. Thus, optimum designs obtained provide quite important instruments for use in a variety of fields, including industry, agriculture, and medicine. Determining the "largeness" of a definite information matrix that is nonnegative is the ultimate goal of any optimality criterion.

An optimal design maximizes or minimizes an optimum criterion, which is a criterion that sums up the value of a design. The optimality of designs is assessed using a number of alphabetical optimality criteria. Model discrimination criteria, parameter estimation criteria, and other criteria are the three categories into which these criteria are divided. Earlier works often emphasized on either rotatability or optimality. Current study integrates both ensuring variance properties are optimized while preserving rotatability. Evaluating designs under A-, D-, T-, and E- optimality criteria is essential to ensure that estimates of model parameters are precise. This led to evaluation of A-, D-, T-, and E- optimal design strategies for third-order rotatable three- and four-dimensional designs.

CHAPTER THREE: METHODOLOGY

3.0 Introduction

This chapter explains how the 44, 58, 46, 80a, and 80b points optimum sequential rotatable designs in three and four dimensions are constructed.

3.1 Construction of sequential third order rotatable designs in three dimensions.

Investigating the construction of third order specific and sequential rotatable designs in three dimensions using the existing second order rotatable set of points designs is the first steps

Consider the following sets of points given by;

B_1= S(f, f, 0)+ S(a, a, a)+S(c_1, 0, 0), (3.1)

B_2= S(f, f, 0)+S(c_2, 0, 0), (3.2)

B_3= S(f, f, 0)+ S(a, a, a)+2S(c, 0, 0) (3.3)

B_4= S(c_2, 0, 0)+ S(a, a, a)+S(c, 0, 0) (3.4)

The following third order rotatable configurations in three dimensions are produced by combining these sets of points in pairs:

B_{12}= (2S(f, f, 0)+ S(a, a, a)+S(c_1, 0, 0)+S(c_2, 0, 0)) (3.5)

B_{13}= (2S(f, f, 0)+ 2S(a, a, a)+2S(c, 0, 0)+S(c_1, 0, 0)) (3.6)

B_{14}= (S(f, f, 0)+ S(a, a, a)+S(c_1, 0, 0)+S(c_2, 0, 0)+ S(a, a, a)+S(c, 0, 0)) (3.7)

Each of the aforementioned designs gives 44, 58, and 46 points.

Provided that all excess functions are zero, the points in each set of combinations form a sequential rotatable arrangement in three and four dimensions, respectively. From equations of excess functions, one variable is estimated using MATLAB so that, following substitution, the other variable is real and non-negative.

If the moment conditions for third are reached, the point sets are regarded as constituting a rotatable arrangement.

The moment and the conditions for second order rotatability's non-singularity are as follows.

i. $\sum_{u=1}^{n} x_{iu}=0$

ii. $\sum_{u=1}^{n} x_{iu}^2=N\lambda_2$

iii. $\sum_{u=1}^{n} x_{iu}^4=¿3\sum_{u=1}^{n} x_{iu}^2 x_{ju}^2=3N\lambda_4$

iv. $\sum_{u=1}^{n} x_{iu}^6=15\sum_{u=1}^{n} x_{iu}^2 x_{ju}^2 x_{lu}^2=5\sum_{u=1}^{n} x_{iu}^4 x_{ju}^2=15N\lambda_6$

v. The excess function given is zero (3.8)

The third order rotatable arrangements generate third order rotatable designs in three dimensions if non-singularity conditions for third order rotatability are satisfied.

i. $\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$ and

ii. $\frac{\lambda_2 \lambda_6}{\lambda_4{}^2} > \frac{k+2}{k+4}$ are satisfied, for k=3,4 is number of factors. (3.9)

Table 3.1: A Summary of the excess functions for 44, 58, and 46 points TORDs in three dimensional designs

Point set	$S(f,f,0)$	$S(a,a,a)$	$S(c_1,0,0)$	$S(c_2,0,0)$	$S(c,0,0)$
No.of points	12	8	6	6	6
AX	$8f^2$	$8a^2$	$2c_1^2$	$2c_2^2$	$2c^2$
EX	$-4f^4$	$-16a^4$	$2c_1^4$	$2c_2^2$	$2c^4$
HX	$8f^6$	$-112a^6$	$2c_1^6$	$2c_1^6$	$2c^6$
IX	$4f^6$	$-16a^6$	0	0	0

3.2 Construction of sequential third order rotatable design in four dimensions.

The four-dimensional sequential third-order rotatable designs are created by adding a factor into each of the forty four and forty six points above (3.5) and (3.7) to produce;

$$B_{12}^{1}=\left(2S(f,f,0,0)+S(a,a,a,a)+S(c_1,0,0,0)+S(c_2,0,0,0)\right) \quad (3.10)$$

B_{14}^{1}= (S(f, f, 0, 0)+ S(a,a,a,a)+S(c_1, 0, 0, 0)+S(c_2, 0, 0, 0)+ S(a,a,a,a)+S(c, 0, 0, 0)). (3.11)

The above points give 80a and 80b points respectively.

If the moment conditions for third order rotatability are met and the excess functions should be zero, as stated in equation (3.8), the supplied points are third order rotatable arrangements in four dimensions. To be regarded as third-order rotatable four-dimensional designs, these arrangements must also satisfy the non-singularity conditions for third order rotatability given in equation (3.9).

Table 3.2: A Summary of the excess functions for 80a, and 80b points TORDs in four dimensional designs.

Point set	$S(f,f,0,0)$	$S(a,a,a,a)$	$S(c_1,0,0,0)$	$S(c_2,0,0,0)$	$S(c,0,0,0)$
No.of points	24	16	8	8	8
AX	$12f^2$	$16a^2$	$2c_1^2$	$2c_2^2$	$2c^2$
EX	0	$-32a^4$	$2c_1^4$	$2c_2^2$	$2c^4$
HX	$12f^6$	$-448a^6$	$2c_1^6$	$2c_2^6$	$2c^6$
IX	$4f^6$	$-64a^6$	0	0	0

3.3 Evaluation of the A-, D-, T-, E- optimality criteria for sequential third order rotatable designs in three and four dimensions

A design may perform exceptionally well in one criterion while falling short in another, according to Kosgei (2002). This is due to the specific roles that these criteria play in enhancing parameter estimates, which ultimately aim to maximize response (yield). If an experimenter wants to use a D-optimal third order rotatable design in three and four dimensions, they can do so by analyzing all of the designs' D-optimality in three and four dimensions and choosing the least D-optimal design for that design. For all other criteria, the same case applies. Evaluation of the A-, D-, T-, E- optimality criteria of the five rotatable designs in three and four dimensions using the A-, D-, T-, E- optimality criterion. The commonly utilized criteria for the design of the experiment are the Determinant Criterion (D-), Average Variance Criterion (A-), Eigenvalue Criterion (E-), and Trace Criterion (T-). The following definitions apply to these conventional optimality criteria:

3.3.1 D- Optimality

The variance-covariance matrix's determinant is minimized by the runs selected by the D-optimal algorithm. This minimizes the volume of the coefficients' joint confidence ellipsoid.

This is the information matrix minimization criterion that has received the most research.

D-criterion= $¿M\vee¿^{\frac{1}{s}}¿$, where M is overall moment/information matrix and s is number of parameters

The ellipsoidal confidence region's content is minimized for the linear model's parameters in D-optimal design. By taking the s^{th} root that, according to the determinant criterion $\varnothing(c)$, both functions cause the information functions, the version $\varnothing_0$(C) = $(det\ C)^{\frac{1}{S}}$ suitable for comparing various criteria and applying information function theory. Due to the formula (det $C¿¿^{-1}$ = (det C^{-1}) , minimizing the determinant of the information matrices equals maximizing the determinant of the dispersion matrix.

According to Nyangweso (1995), for third order rotatability the determinant criterion is given by;

$|M| = \cap \lambda_2^k \lambda_6^{(k^2+k)} \lambda_4^{(2k-1)} ¿$ (3.12)

for $\cap ¿ 2^{k^2+k-1} \times 3^k$ and k is the number of factors

3.3.2 A- Optimality

The trace of the variance-covariance matrix is minimized in an A-optimal design. This minimizes the polynomial model coefficients' average prediction variance.

By minimizing the total or the average of the estimated variances, the average-variance criteria (A-criterion) are used.

The average variance $\varnothing_{-1}$(C) (which is how large, on average, the variance are) is given by $\varnothing_0$

(C) $= (\frac{1}{s} trace\, C^{-1})^{-1}$ an expression for the average variance of the estimated regression coefficients (if C is positive definite).

It is the standardized variances' average of the optimal estimators for the scalar parameter systems formed by the columns of K, $c_1 \beta, c_2 \beta \; . \; . \; . \; c_k \beta$,.

The evaluation of the Nyangweso (1995) A-criterion for third order rotatable designs is provided by;

A-criterion = $\left(\frac{1}{s} tr\left(M^{-1}\right)\right)^{-1}$ (3.14)

$tr\left(M^{-1}\right) = tr\left(M_1^{-1}\right) + tr\left(M_2^{-1}\right) + tr\left(M_3^{-1}\right) + tr\left(M_4^{-1}\right)$ where; (3.15)

$$tr\left(M_1^{-1}\right)=\frac{2(k+2)\lambda_4^2+k(k+1)\lambda_4-k(k-1)\lambda_2^2}{2\lambda_4[(k+2)\lambda_4-k\lambda_2^2]}, \tag{3.16}$$

$$tr\left(M_2^{-1}\right)=\frac{6(k+4)\lambda_6^2+k\left(3k^2+7k-8\right)\lambda_2\lambda_6-k(k-2)\left(2k+10\lambda_4^2\right)}{6\lambda_6[(k+4)\lambda_2\lambda_6-(k+2)\lambda_4^2]}, \tag{3.17}$$

$$tr\left(M_3^{-1}\right)=\frac{k(k-1)}{2\lambda_4} \text{ and} \tag{3.18}$$

$$tr\left(M_4^{-1}\right)=\frac{k(k-1)(k-2)}{6\lambda_6} \tag{3.19}$$

3.3.3 T- Optimality

The trace criterion, T-, $\varnothing_0(C) = \frac{1}{s}$ trace C

Although the trace criterion is commonly employed for model discrimination, its applicability in parameter estimation has not been as extensive as it could be due to the T-criterion's linearity, which leaves room for interpolation. The other matrix means are concave without being linear. The trace criterion is evaluated as follows:

$$\varnothing_{-\infty}(C) = \frac{1}{s} \text{ trace C} \tag{3.20}$$

Where s is the number of parameters and C is the information matrix. Where,

$$tr(M)=tr\,M_1+tr\,M_2+tr\,M_3+tr\,M_4 \text{ and} \tag{3.21}$$

$$tr\,M_1=1+k(3\lambda_4), \tag{3.22}$$

$$tr\,M_2=k\left(\lambda_2+15\lambda_6+3\lambda_6(k-1)\right), \tag{3.23}$$

$$tr\,M_3=\lambda_4\begin{bmatrix}k\\2\end{bmatrix} \text{and} \tag{3.24}$$

$$tr\,M_4=\lambda_6\begin{bmatrix}k\\3\end{bmatrix} \tag{3.25}$$

for third order rotatable designs according to Nyangweso (1995). Where k is number of factors and λ_2, λ_4, and λ_6 are normalized second, fourth and sixth moment constants respectively.

3.3.4 E- Optimality

The E-Criteria aims to lower the variance of each parameter estimate by reducing the information matrix's largest Eigenvalue.

$\varnothing_{-\infty}(C) = \lambda_{min}(C^{-1})$

It is equivalent to minimizing the information matrix's largest eigenvalue.

According to Nyangweso (1995), the eigenvalues of the moment matrix's determinant for TORDs are as follows:

The smallest Eigen value criterion, E-,

$\varphi_{-\infty}(M) = \alpha^2 - [(k+4\lambda_6+\lambda_2)]\alpha + [(k+4)\lambda_2\lambda_6 - (k+2)\lambda_4^2]$ for α is an eigenvalue of the information matrix (3.26)

The quadratic equation in (3.26) is determined, and the value that is the smallest is chosen as E-criterion.

CHAPTER FOUR: RESULTS AND DISCUSSIONS

4.0 Introduction

This chapter gives results and discussions on the construction of 44, 58 and 46 TORDs in three and four dimensions and 80a and 80b TORDs in four dimensions. To assess the designs, A-, D-, T-, E- optimality criteria are obtained.

4.1 Construction of TORDs in Three Dimensions

4.1.1 Construction of 44 Points TORDs in Three Dimensions

The combination denoted by B_{12}, containing forty-four points given in (3.5) is considered.

Substituting B_{12} to the moment conditions provided in 3.8 gives;

$$\sum x_{iu}^2 = 16f^2 + 8a^2 + 2c_1^2 + 2c_2^2 = 44\lambda_2\ , \quad (4.1)$$

$$\sum x_{iu}^4 = 16f^4 + 8a^4 + 2c_1^4 + 2c_2^4 = 132\lambda_4\ , \quad (4.2)$$

$$\sum x_{iu}^2 x_{ju}^2 = 8f^4 + 8a^4 \quad (4.3)$$

$$\sum x_{iu}^6 = 16f^6 + 8a^6 + 2c_1^6 + 2c_2^6 = 660\lambda_6 \quad (4.4)$$

$$\sum x_{iu}^4 x_{ju}^2 = 8f^6 + 8a^6 \quad (4.5)$$

$$\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 8a^6 \quad (4.6)$$

These moment conditions give excess functions as follows;

Ex = $\sum x_{iu}^4 - 3\sum x_{iu}^2 x_{ju}^2 = 0$

$$16f^4 + 8a^4 + 2c_1^4 + 2c_2^4 - 3(8f^4 + 8a^4) = 0$$

$$2c_1^4 + 2c_2^4 - 16a^4 - 8f^4 = 0 \quad (4.7)$$

Hx = $\sum x_{iu}^6 - 15\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 0$

$$16f^6 + 8a^6 + 2c_1^6 + 2c_2^6 - 15(8a^6) = 0$$

$$16f^6 + 2c_1^6 + 2c_2^6 - 112a^6 = 0 \quad (4.8)$$

Ix = $\sum x_{iu}^4 x_{ju}^2 - 3\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 0$

$$8f^6 + 8a^6 - 3(8a^6) = 0$$

$$8f^6 - 16a^6 = 0$$

$$f^6 = 2a^6 \quad (4.9)$$

Let $c_1^2 = xa^2 \wedge c_2^2 = ya^2$ (4.10)

It follows from this that

$x^2 + y^2 = 14.3496$. (4.11)

$x^3 + y^3 = 40$ (4.12)

Making x the subject in equation (4.11) gives

$x = (14.3496 - y^2)^{1/2}$ and $x^3 = (14.3496 - y^2)^{3/2}$

Substituting the values of x^3above to equation (4.12) gives;

$2y^6 - 43.0482y^4 - 80y^3 + 617.715841y^2 - 1354.7408 = 0$ (4.13) Equation (4.13) is solved using MATLAB as follows:

For equation (4.13) to satisfy roots command, a coefficient 0 is put in an intermediate power that is not present in the equation. To give

$2y^6 + 0y^5 - 43.0482y^4 - 80y^3 + 617.715841y^2 + 0y - 1354.7408 = 0$ (4.14)

Taking p to be a vector with 7 polynomial coefficients of y in equation (4.14) above gives

$p = (2\,0 - 43.0482 - 80\,617.715841\,0 - 1354.7408)$

Finding the roots of p in MATLAB, input

$p = [2\,0 - 43.0482 - 80617.715841\,0 - 1354.7408];$

Then

$r = roots(p)$

Gives complex roots, taking real and positive values, gives

$y = 2.1954$ and $x = 3.0871$. (4.15)

Because the values of x and y are both real and positive, the set of points has a rotatable arrangement.

Substituting x and y values in (4.15) to (4.10) gives;

$c_1^2 = 3.0871a^2$ and $c_2^2 = 2.1954a^2$ (4.16)

Substituting (4.16) and (4.9) to (4.1), (4.2) and (4.4) gives;

$\lambda_2 = 0.880084\,a^2, \lambda_4 = 0.47044\,a^4$ and $\lambda_6 = 0.18182\,a^6$ (4.17)

Substituting (4.13) to the non-singularity conditions provided in [3.9] for k=3, gives,

$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$ =0.6073724309¿ 0.6 and

$\frac{\lambda_2 \lambda_6}{\lambda_4{}^2} > \frac{k+2}{k+4}$ =0.72303245133 ¿ 0.71428571429 (4.18)

Which satisfy the non-singularity conditions for TORDs. The forty four points design denoted by B_{12} forms TORD in three dimensions.

4.1.2 Construction of 58 Points TORD in Three Dimensions

The combination denoted by B_{13}, containing fifty eight points given in (3.6) is considered.

Substituting B_{13} to the moment conditions given in 3.8 gives;

$\sum x_{iu}^2 = 16 f^2 + 16 a^2 + 4 c^2 + 2 c_1^2 = 58 \lambda_2$, (4.19)

$\sum x_{iu}^4 = 16 f^4 + 16 a^4 + 4 c^4 + 2 c_1^4 = 174 \lambda_4$, (4.20)

$\sum x_{iu}^2 x_{ju}^2 = 8 f^4 + 16 a^4$ (4.21)

$\sum x_{iu}^6 = 16 f^6 + 16 a^6 + 4 c^6 + 2 c_1^6 = 870 \lambda_6$ (4.22)

$\sum x_{iu}^4 x_{ju}^2 = 8 f^6 + 16 a^6$ (4.23)

$\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 16 a^6$ (4.24)

These moment conditions give excess functions as follows;

$\sum x_{iu}^4 - 3 \sum x_{iu}^2 x_{ju}^2 = 0$

$16 f^4 + 16 a^4 + 4 c^4 + 2 c_1^4 - 3\left(8 f^4 + 16 a^4\right) = 0$

$4 c^4 + 2 c_1^4 - 8 f^4 - 32 a^4 = 0$ (4.25)

Hx = $\sum x_{iu}^6 - 15 \sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 0$

$16f^6+16a^6+4c^6+2c_1^6-15(16a^6)$

$2c_1^6+4c^6+16f^6-224a^6=0$ (4.26)

Ix = $\sum x_{iu}^4 x_{ju}^2 - 3\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 0$

$8f^6+16a^6-3(16a^6)=0$

$8f^6-32a^6=0$

$f^6=4a^6$ (4.27)

Let $c_1^2=xa^2$ and $c^2=ya^2$ (4.28)

It follows from this that

$x^2+y^2=26.0794$. (4.29)

$x^3+y^3=80$ (4.30)

Solving equation (4.29) and (4.30) using MATLAB gives;

$x=3.27704$ and $y=2.1265$. (4.31)

The set of points forms a rotatable arrangement because x and y have real, positive values. Substituting x and y values in (4.31) to (4.28) gives;

$C_1^2=3.27704a^2$ and $c^2=2.11265a^2$ (4.32)

Substituting (4.32) and (4.27) to (4.19), (4.20) and (4.22) gives;

$\lambda_2=1.01309615227a^2$,$\lambda_4=0.62251403875a^4and\lambda_6=0.275862632$

Substituting (4. singularity conditions provided 33) to the non- in [3.9] for k=3 $13a^6$ (4.33)

, gives,

$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$=0.60652375933¿0.6 and

$\frac{\lambda_2\lambda_6}{\lambda_4{}^2} > \frac{k+2}{k+4}$ =0.72118260292¿0.71428571429 (4.34)

Which satisfy the non-singularity conditions for TORDs. The fifty eight points design denoted by B_{13} forms TORD in three dimensions.

4.1.3 Construction of 46 Points TORD in Three Dimensions

The combination denoted by B_{14}, containing forty six points provided in (3.7) is considered. Substituting B_{14} to the moment conditions provided in 3.8 gives;

$$\sum x_{iu}^2 = 8f^2 + 2c_1^2 + 8a^2 \,, \tag{4.35}$$

$$\sum x_{iu}^2 = 2c_2^2 + 8a^2 + 2c^2 \tag{4.36}$$

$$\sum x_{iu}^2 = 8f^2 + 2c_1^2 + 16a^2 + 2c_2^2 + 2c^2 = 46\lambda_2 \tag{4.37}$$

$$\sum x_{iu}^4 = 8f^4 + 2c_1^4 + 8a^4 \,, \tag{4.38}$$

$$\sum x_{iu}^4 = 2c_2^4 + 8a^4 + 2c^4 \tag{4.39}$$

$$\sum x_{iu}^4 = 8f^4 + 2c_1^4 + 16a^4 + 2c_2^4 + 2c^4 = 138\lambda_4 \tag{4.40}$$

$$\sum x_{iu}^2 x_{ju}^2 = 4f^4 + 8a^4 \tag{4.41}$$

$$\sum x_{iu}^2 x_{ju}^2 = 8a^4 \tag{4.42}$$

$$\sum x_{iu}^6 = 8f^6 + 2c_1^6 + 16a^6 + 2c_2^6 + 2c^6 = 690\lambda_6 \tag{4.43}$$

$$\sum x_{iu}^4 x_{ju}^2 = 4f^6 + 16a^6 \tag{4.44}$$

$$\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 16a^6 \tag{4.45}$$

These moment conditions give excess functions as follows;

$$\sum x_{iu}^4 - 3\sum x_{iu}^2 x_{ju}^2 = 0$$

$$8f^4 + 2c_1^4 + 8a^4 - 3\left(4f^4 + 8a^4\right) = 0$$

$$2c_1^4 - 4f^4 - 16a^4 = 0 \tag{4.46}$$

$$\sum x_{iu}^4 - 3\sum x_{iu}^2 x_{ju}^2 = 0$$

$$2c_2^4+8a^4+2c^4-3(8a^4)=0$$

$$2c_2^4+2c^4-16a^4 \quad (4.47)$$

$$\text{Hx} = \sum x_{iu}^6-15\sum x_{iu}^2 x_{ju}^2 x_{lu}^2=0$$

$$8f^6+2c_1^6+16a^6+2c_2^6+2c^6-15(16a^6)$$

$$2c_1^6+2c_2^6+2c^6+8f^6-224a^6=0 \quad (4.48)$$

$$\text{Ix} = \sum x_{iu}^4 x_{ju}^2-3\sum x_{iu}^2 x_{ju}^2 x_{lu}^2=0$$

$$4f^6+16a^6-3(16a^6)=0$$

$$4f^6-32a^6=0$$

$$f^6=8a^6 \quad (4.49)$$

Let$c^2=xa^2$ and $c_2^2=ya^2$ (4.50)

It follows from this that,

$$x^2+y^2=8 \,. \quad (4.51)$$

$$x^3+y^3=16 \quad (4.52)$$

Solving equation (4.51) and (4.52) using MATLAB gives;

$x=2$ and $y=2$. (4.53)

The set of points forms a rotatable arrangement because x and y have real, positive values.

Substituting x and y values in (4.53) to (4.50) gives;

$c^2=2a^2$ and $c_2^2=2a^2$ (4.54)

Substituting (4.49) and (4.54) to (4.37), (4.40) and (4.43) gives;

$\lambda_2=1.04347826087a^2$,$\lambda_4=0.69565217391a^4and\lambda_6=0.34782608696a^6$ (4.55)

Substituting (4.55) to the non-singularity conditions given in (3.9) for k=3, gives,

$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2} = 0.638888888889¿0.6$ and

$\frac{\lambda_2 \lambda_6}{\lambda_4^2} > \frac{k+2}{k+4} = 0.75000000564 ¿0.71428571429$ (4.56)

Which satisfy the non-singularity conditions for TORD. The forty six points design denoted by B_{14} forms TORD in three dimensions.

4.2 Construction of TORDs in Four Dimensions

4.2.1 Construction of 80a Points TORD in Four Dimensions

The combination denoted by B_{12}^1 , containing 80a points provided in (3.10) is considered.

Substituting B_{12}^1 to the moment conditions provided in 3.8 gives;

$$\sum x_{iu}^2 = 24 f^2 + 16 a^2 + 2 c_1^2 + 2 c_2^2 = 80 \lambda_2 , \quad (4.57)$$

$$\sum x_{iu}^4 = 24 f^4 + 16 a^4 + 2 c_1^4 + 2 c_2^4 = 240 \lambda_4 , \quad (4.58)$$

$$\sum x_{iu}^2 x_{ju}^2 = 8 f^4 + 16 a^4 \quad (4.59)$$

$$\sum x_{iu}^6 = 24 f^6 + 16 a^6 + 2 c_1^6 + 2 c_2^6 = 1200 \lambda_6 \quad (4.60)$$

$$\sum x_{iu}^4 x_{ju}^2 = 8 f^6 + 16 a^6 \quad (4.61)$$

$$\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 16 a^6 \quad (4.62)$$

These moment conditions give excess functions as follows;

Ex = $\sum x_{iu}^4 - 3 \sum x_{iu}^2 x_{ju}^2 = 0$

$$24 f^4 + 16 a^4 + 2 c_1^4 + 2 c_2^4 - 3\left(8 f^4 + 16 a^4\right) = 0$$

$$2 c_1^4 + 2 c_2^4 - 32 a^4 = 0 \quad (4.63)$$

Hx = $\sum x_{iu}^6 - 15 \sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 0$

$$24 f^6 + 16 a^6 + 2 c_1^6 + 2 c_2^6 - 15(16 a^6)$$

$24f^6+2c_1^6+2c_2^6-224a^6=0$ (4.64)

Ix = $\sum x_{iu}^4 x_{ju}^2 - 3\sum x_{iu}^2 x_{ju}^2 x_{lu}^2 = 0$

$8f^6+16a^6-3(16a^6)=0$

$8f^6-32a^6=0$

$f^6=4a^6$ (4.65)

Let $c_1^2=xa^2 \wedge c_2^2=ya^2$ (4.66)

This implies that,

$x^2+y^2=16$. (4.67)

$x^3+y^3=64$ (4.68)

Solving equation (4.67) and (4.68) using MATLAB gives;

$x=4$ and $y=0$ (4.69)

The set of points forms a rotatable arrangement because x and y have real, positive values.

Substituting x and y values in (4.69) to (4.66) gives;

$c_1^2=4a^2$ and $c_2^2=0$ (4.70)

Substituting (4.65) and (4.70) to (4.57), (4.58) and (4.60) gives;

$\lambda_2=0.77622031559a^2$, $\lambda_4=0.4519842a^4$ and $\lambda_6=0.2a^6$ (4.71)

Substituting (4.71) to the non-singularity conditions given in [3.9] for k=4, gives,

$\frac{\lambda_4}{\lambda_2^2}>\frac{k}{k+2}$=0.7501588604¿0.66666666667 and

$\frac{\lambda_2\lambda_6}{\lambda_4{}^2}>\frac{k+2}{k+4}$ =0.75992108346¿0.75 (4.72)

Which satisfies the non-singularity conditions for TORD. The 80a points design denoted by B_{12}^1 forms TORD in three dimensions.

4.2.2 Construction of 80b Points TORD in Four Dimensions

The combination denoted by B_{14}^{1}, containing 80b points given in (3.11) is considered.

Substituting B_{14}^{1} to the moment conditions provide in 3.8 gives;

$$\sum x_{iu}^{2}=12f^{2}+2c_{1}^{2}+16a^{2}\ , \quad (4.73)$$

$$\sum x_{iu}^{2}=2c_{2}^{2}+16a^{2}+2c^{2}, \quad (4.74)$$

$$\sum x_{iu}^{2}=12f^{2}+2c_{1}^{2}+32a^{2}+2c_{2}^{2}+2c^{2}=80\lambda_{2}, \quad (4.75)$$

$$\sum x_{iu}^{4}=12f^{4}+2c_{1}^{4}+16a^{4} \quad (4.76)$$

$$\sum x_{iu}^{4}=2c_{2}^{4}+16a^{4}+2c^{4} \quad (4.77)$$

$$\sum x_{iu}^{4}=12f^{4}+2c_{1}^{4}+32a^{4}+2c_{2}^{4}+2c^{4}=240\lambda_{4} \quad (4.78)$$

$$\sum x_{iu}^{2}x_{ju}^{2}=4f^{4}+16a^{4} \quad (4.79)$$

$$\sum x_{iu}^{2}x_{ju}^{2}=16a^{4}$$

(4.80)

$$\sum x_{iu}^{6}=12f^{6}+2c_{1}^{6}+32a^{6}+2c_{2}^{6}+2c^{6}=1200\lambda_{6} \quad (4.81)$$

$$\sum x_{iu}^{4}x_{ju}^{2}=4f^{6}+32a^{6} \quad (4.82)$$

$$\sum x_{iu}^{2}x_{ju}^{2}x_{lu}^{2}=32a^{6} \quad (4.83)$$

These moment conditions give excess functions as follows;

$$\sum x_{iu}^{4}-3\sum x_{iu}^{2}x_{ju}^{2}=0$$

$$12f^{4}+2c_{1}^{4}+16a^{4}-3\left(4f^{4}+16a^{4}\right)=0$$

$$2c_{1}^{4}-32a^{4}=0$$

$$c_{1}^{4}=16a^{4} \quad (4.84)$$

$$\sum x_{iu}^{4}-3\sum x_{iu}^{2}x_{ju}^{2}=0$$

$$2c_2^4+16a^4+2c^4-3(16a^4)=0$$

$$2c_2^4+2c^4-32a^4=0 \qquad (4.85)$$

$$Hx = \sum x_{iu}^6-15\sum x_{iu}^2 x_{ju}^2 x_{lu}^2=0$$

$$12f^6+2c_1^6+32a^6+2c_2^6+2c^6-15(32a^6)$$

$$2c_1^6+2c_2^6+2c^6+12f^6-448a^6=0 \qquad (4.86)$$

$$Ix = \sum x_{iu}^4 x_{ju}^2-3\sum x_{iu}^2 x_{ju}^2 x_{lu}^2=0$$

$$4f^6+32a^6-3(32a^6)=0$$

$$4f^6-32a^6=0$$

$$f^6=16a^6 \qquad (4.87)$$

Let $c_2^2=xa^2$ and $c^2=ya^2$ (4.88)

This implies that,

$$x^2+y^2=16 \,. \qquad (4.89)$$

$$x^3+y^3=64 \qquad (4.90)$$

Solving equation (4.89) and (4.90) using MATLAB gives;

$x=4$ and $y=0$. (4.91)

The set of points forms a rotatable arrangement because x and y have real, positive values.

Substituting x and y values in (4.91) to (4.88) gives;

$c^2=4a^2$ and $c_2^2=0$ (4.92)

Substituting (4.84), (4.87) and (4.92) to (4.75), (4.78) and (4.81) gives;

$$\lambda_2=0.97797a^2, \lambda_4=0.71748a^4 \text{and} \lambda_6=0.4a^6 \qquad (4.93)$$

Substituting (4.93) to the non-singularity conditions given in (3.9) for k=4, gives,

$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$=0.7501683449¿0.66666666667 and

$\frac{\lambda_2 \lambda_6}{\lambda_4{}^2} > \frac{k+2}{k+4}$ =0.75991658862¿0.75 (4.94)

Which satisfies the non-singularity conditions for TORD. The eighty points design denoted by B_{14}^1 forms TORD in three dimensions.

4.3 Evaluation of A-,D-, T-,E- optimality criteria in three and four dimensions

4.3.1 Optimality criteria for the 44 points TORD in three dimensions

4.3.1.1 D- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.17) to general formula given in (3.12) for D-criterion gives;

D - criterion =0.221460522 (4.95)

4.3.1.2 T- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.17) to (3.22) (3.23) (3.24) and (3.25) then add as per (3.21) and substitute the answer to the general formula given in (3.20) for T-criterion gives;

T- criterion = 1.04610075 (4.96)

4.3.1.3 A- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.17) to (3.16) (3.17) (3.18) and (3.19) then add as per (3.15) and substitute the answer to the general formula given in (3.14) for A-criterion gives;

A- criterion = 0.140772405 (4.97)

4.3.1.4 E- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.17) to general formula given in (3.26) for E-criterion gives;

α= 0.002943 or 4.60442208672

taking the smallest eigenvalue gives;

E - criterion =0.002943 (4.98)

4.3.2 Optimality criteria for the 58 points TORD in three dimensions

4.3.2.1 D- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.33) to general formula given in (3.12) for D-criterion gives;

D - criterion =0.32959516 (4.99)

4.3.2.2 T- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.33) to (3.22) (3.23) (3.24) and (3.25) then add as per (3.21) and substitute the answer to the general formula given in (3.20) for T-criterion gives;

T- criterion = 1.45823276 (4.100)

4.3.2.3 A- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.33) to (3.16) (3.17) (3.18) and (3.19) then add as per (3.15) and substitute the answer to the general formula given in (3.14) for A-criterion gives;

A- criterion = 0.05518542 (4.101)

4.3.2.4 E- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.33) to general formula given in (3.26) for E-criterion gives;

α= 0.00365911or 5.11288757

taking the smallest eigenvalue gives;

E - criterion =0.00365911 (4.102)

4.3.3 Optimality criteria for the 46 points TORD in three dimensions

4.3.3.1 D- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.55) to general formula given in (3.12) for D-criterion gives;

D - criterion =0.56756981 (4.103)

4.3.3.2 T- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.55) to (3.22) (3.23) (3.24) and (3.25) then add as per (3.21) and substitute the answer to the general formula given in (3.20) for T-criterion gives;

T- criterion = 1.73695621 (4.104)

4.3.3.3 A- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.55) to (3.16) (3.17) (3.18) and (3.19) then add as per (3.15) and substitute the answer to the general formula given in (3.14) for A-criterion gives;

A- criterion = 0.324559608 (4.105)

4.3.3.4 E- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=3 given in (4.55) to general formula given in (3.26) for E-criterion gives;

α= 0.02235287 or 5.4124293

taking the smallest eigenvalue gives;

E - criterion =0.02235287 (4.106)

4.3.4 Optimality criteria for the 80a points TORD in four dimensions

4.3.4.1 D- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=4 given in (4.71) to general formula given in (3.12) for D-criterion gives;

D - criterion =0.143116714 (4.107)

4.3.4.2 T- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k= given in (4.71) to (3.22) (3.23) (3.24) and (3.25) then add as per (3.21) and substitute the answer to the general formula given in (3.20) for T-criterion gives;

T- criterion = 1.61202978 (4.108)

4.3.4.3 A- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=4 given in (4.71) to (3.16) (3.17) (3.18) and (3.19) then add as per (3.15) and substitute the answer to the general formula given in (3.14) for A-criterion gives;

A- criterion = 0.0110405042 (4.109)

4.3.4.4 E- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=4 given in (4.71) to general formula given in (3.26) for E-criterion gives;

α= 0.00290916803 or 5.77331083195

taking the smallest eigenvalue gives;

E - criterion =0.00290916803 (4.110)

4.3.5 Optimality criteria for the 80b points TORD in four dimensions

4.3.5.1 D- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=4 given in (4.93) to general formula given in (3.12) for D-criterion gives;

D - criterion =0.433798618 (4.111)

4.3.5.2 T- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k= given in (4.93) to (3.22) (3.23) (3.24) and (3.25) then add as per (3.21) and substitute the answer to the general formula given in (3.20) for T-criterion gives;

T- criterion = 2.891326 (4.112)

4.3.5.3 A- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=4 given in (4.93) to (3.16) (3.17) (3.18) and (3.19) then add as per (3.15) and substitute the answer to the general formula given in (3.14) for A-criterion gives;

A- criterion = 0.163481589 (4.113)

4.3.5.4 E- criterion

Substituting the moments λ_2, λ_4 and λ_6 and k=4 given in (4.93) to general formula given in (3.26) for E-criterion gives;

α=(0.00621427505 or 6.57175572495

taking the smallest eigenvalue gives;

E - criterion =0. 00621427505 (4.114)

4.4 Discussions

4.4.1 Construction of 44, 58, 46, 80a and 80b points three- and four-dimensional third order rotatable design

Table 4.4.1: Summary of moment and non-singularity condition for 44, 58, 46, 80a and 80b points three- and four-dimensional third order rotatable designs.

Design	B_{12}	B_{13}	B_{14}	B_{12}^{1}	B_{14}^{1}
Number of points	44	58	46	80a	80b
No. of factors	3	3	3	4	4
λ_2	$0.880084a^2$	$1.0130961527a^2$	$1.04347826087a^2$	$0.7762203155a^2$	$0.97797a^2$
λ_4	$0.47044a^4$	$0.62251403875a^4$	$0.69565217391a^4$	$0.4519842a^4$	$0.71748a^4$
λ_6	$0.18182a^6$	$0.2758626323a^6$	$0.3478260869a^6$	$0.2a^6$	$0.4a^6$
$\frac{\lambda_4}{\lambda_2^2}$	0.6073724309	0.60652375933	0.638888888889	0.7501588604	0.7501683449
$\frac{\lambda_2\lambda_6}{\lambda_4^2}$	0.72303245133	0.72118260292	0.75000000564	0.75992108346	0.75991658862
	0.6	0.6	0.6	0.66666666667	0.66666666667

$\frac{k}{k+2}$					
$\frac{k+2}{k+4}$	0.7142857142 9	0.71428571429	0.71428571429	0.75	0.75

The results for the construction of three- and four-dimensional for the five TORDs are summarized in the table 4.4.1 above. It presents three sets of points: 44, 58, and 46 points in three dimensions and two sets of points: 80a and 80b points in four dimensions which satisfy the moment and non-singularity conditions for rotatability for third order specified in equations 3.8 and 3.9.

4.4.2 Evaluation of A-, D-, T-, E- optimality criteria for 44, 58, 46, 80a and 80b points third order rotatable designs in three and four dimensions

The results for the evaluation of the optimality criteria for the five TORDs are summarized in the table below.

Table 4.4.2: Summary of Optimality criteria for 44, 58, 46, 80a and 80b points three- and four-dimensional third order rotatable designs.

Design	**Number of points**	**Number of factors**	**D- criterion**	**T- criterion**	**A- criterion**	**E- criterion**
$\mathbf{B_{12}}$	44	3	0.221460522	1.0461007 5	0.140772405	0.002943
$\mathbf{B_{13}}$	58	3	0.32959516	1.4582327 6	0.05518542	0.00365911
$\mathbf{B_{14}}$	46	3	0.56756981	1.7369562 1	0.324559608	0.0223528039 5
B_{12}^{1}	80a	4	0.143116714	1.6120297	0.0110405042	0.0029091680

				8		3
B_{14}^{1}	80b	4	0.433798618	2.891326	0.163481589	0.0062142750 5

According to table 4.4.2, the optimality criteria for design B_{12}, B_{13} and B_{14} in three dimensions, and B_{12}^{1} and B_{14}^{1} in four dimensions are provided. As the number of elements rises, T- optimality's suitability declines whereas D-, T- and E- optimality's suitability rises as the number of factors rises. Although D- optimality is frequently advised, this study did not find it to be appropriate. Alternative optimality criteria, however, showed promise for playing the function of D-optimality, as the study found.

The 80a and 80b design points were two designs that had the same number of points. Using the least optimality value among these two designs, an experimenter would select the design with 80a points, which is the optimal design.

CHAPTER FIVE: CONCLUSIONS AND RECOMMENDATIONS

5.0 Introduction

This chapter provides conclusions, and recommendations based on construction of 44, 58, 46, 80a, and 80b points three- and four-dimensional third order optimum sequential rotatable designs

5.1 Conclusions

5.1.1 Construction of 44, 58, 46, 80a and 80b points three- and four-dimensional third order rotatable design

The constructed point sets satisfy both the moment and non-singularity conditions, thereby confirming the validity of obtaining higher-order rotatable designs in three-and four-dimensional cases. In three dimensions, designs with 44, 58, and 46 points were successfully generated through combination of pairs of existing second order point sets. In four dimensions, 80a and 80b points designs were obtained by appending an extra factor to the second order point sets. However, it is worth noting that one of the three-dimensional TORD (B_{13}) with 58 points does not correspond to a four-dimensional TORD, indicating that the method is dimension- dependent rather than universally applicable.

5.1.2 Evaluation of A-, D-, T-, E- optimality criteria for sequential third order rotatable designs in three and four dimensions

Design B_{12} was determined to be D-optimal for TORDs in three dimensions, while design $B_{12}^{1}$was identified as the D-optimal design for TORDs in four dimensions. Design B_{12} was found to be T-optimal for TORDs in three dimensions, while design B_{12}^{1} was considered T-optimal for TORDs in four dimensions. Regarding the A-criterion, design B_{13} was deemed optimal in three dimensions, whereas design B_{12}^{1} was identified as the A-optimal design for TORDs in four dimensions. Both designs B_{12} and B_{12}^{1}were found to be E-optimal for the designs in three dimensions and four dimensions, respectively.

5.3 Recommendations

5.3.1 Construction of 44, 58, 46, 80a and 80b points three- and four-dimensional third order rotatable design

The present study showed how third order rotatable designs can be constructed successfully in three and four dimensions, though one third order rotatable design in three dimensions did not correspond to a four-dimensional TORD. Based on this finding, future research should aim to develop construction strategies that extend more consistently across higher dimensions. Practical implementation of these designs in real-world experimental settings would provide valuable validation of their utility.

5.3.2 Evaluation of A-, D-, T-, E- optimality criteria for sequential third order rotatable designs in three and four dimensions

The study recommends that other methods be used to obtain A-, D-, T- and E- optimality criteria such as BIBD and PBD to prove the existence of optimal designs also other optimality criteria such as G-, I-, V-, U-, C-, CD-, DT- and IV- criteria be established for TORDs in this study.

In practical, optimal designs are known to reduce the cost of experimentation. Hence, optimal TORDs in three and four dimensions be applied in real life experiments.

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APPENDIX: MATLAB PROGRAMS

In this appendix, MATLAB function for complex roots is given, in every equation a coefficient 0 is put in any intermediate power that is not present. A vector representing polynomial is created before finding roots. Taking P as a column vector with a number of polynomial coefficient to find roots; input

$P = [polynomial\, coefficients];$

Now, taking r to be its solution; input

$r = roots(p)$

Gives complex roots, real and positive roots are selected.