OPTIMAL WEIGHTED CENTROID DESIGNS FOR MAXIMAL PARAMETER SUBSYSTEM FOR THIRD DEGREE KRONECKER MODEL MIXTURE EXPERIMENTS

By

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DECLARATION

Declaration by the student

This thesis is my original and has not been presented for a degree award in any other university. No part of this thesis should be produced without prior written permission of the author and/or Moi University.

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DEDICATION

To my father Mr. Peter Kibet, Mother Salina, brother Mr. Kemboi, brothers and sisters for their support.

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ABSTRACT

Experiments that involve a mixture of ingredients are usually associated with investigating optimal proportions of several factors used. Optimal designs lower the costs of experimentation by allowing statistical models to be estimated with fewer experimental runs. Thus, appropriate designs for experiments that allow for parameter estimation without bias and with minimum variance are desirable. The purpose of this study was to obtain optimal weighted centroid designs for maximal parameter subsystem for third degree Kronecker model mixture experiments with the assumption that errors are independent and identically distributed with mean zero and common variance. The general objective was to obtain optimal weighted centroid designs for maximal parameter subsystems for third degree Kronecker model mixture experiments. The specific objectives of the study were to: Identify the coefficient matrix K and the associated parameter subsystem of interest; determine optimal moments and information matrix for two, three, four, and generalized to m factors; derive optimal weighted centroid designs for third degree Kronecker model for mixture experiments for A-, D- and E-optimality criteria and finally, compute numerical optimal weighted centroid designs for the maximal parameter subsystem. The Kronecker model approach was used to obtain the coefficient matrix K and, consequently, the optimal moments. A set of weighted centroid designs for the maximal parameter subsystem of interest was obtained by the use of unit vectors and characterization of feasible weighted centroid designs for the parameter subsystem. Information matrices based on maximal parameter subsystem were also obtained for the two, three, four, and generalized to m factors. Kiefer-Wolfowitz equivalence theorem was used to derive weights for the respective weighted centroid designs for D-, A- and E- Optimality. Optimal weights and values were computed numerically using Wxmaxima and R software. The results obtained indicated that: Coefficient matrix K obtained had a full column rank and helped in the identification of the linear parameter subsystem; the optimal moments obtained reflected the statistical properties of designs and were useful in finding the information matrix; the information matrix was important in obtaining optimality criteria and with $\alpha_1^{(p)}$ and $\alpha_2^{(p)}$ being the weights, for the average-variance criterion (A- criterion) and the optimality criteria were both dependent on the information matrix, as the number of m factors increases, $\alpha_1^{(p)}$ decreases while $\alpha_2^{(p)}$ increases and the value of the maximum criterion decreases. For the determinant criterion (D-criterion), as the number of m factors increase, $\alpha_1^{(p)}$ decreases while $\alpha_2^{(p)}$ increases and the value of the maximum criterion decreases. For the smallest eigenvalue criterion (E-criterion) as the number of m factors increases, $\alpha_1^{(p)}$ increases while $\alpha_2^{(p)}$ decreases and the value of the maximum criterion decreases. This indicates that the maximal parameter design reflects well the statistical properties due to increasing symmetry as the number of factors increases. In conclusion, based on the maximal parameter subsystem third degree mixture model with two, three, four, and generalized to m factors for D-, A- and E-optimal weighted centroid designs for the parameter subsystem exists. The study thus recommends the application of the designs obtained by experimenters in designing of experiments to yield Optimal results in technological fields. This study concentrated on optimal weighted centroid designs for maximal parameter subsystem for third degree Kronecker model mixture experiments.

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LIST OF ABBREVIATIONS AND ACRONYMS

$C_k M$	: Information matrix
$\emptyset$	: Empty set
A-CRITERION	: Average-variance criterion
D-CRITERION	: Determinant criterion
E-CRITERION	: Smallest Eigenvalue criterion
NND	: Non-negative definite matrices
PD	: Positive definite matrices
$M(\tau)$	: Moment matrix of a design
k	: Coefficient matrix
$k'\theta$	: Parameter subsystem
$n(\alpha)$	: Weighted centroid design
α	: Weight vector
θ	: Full parameter

CHAPTER ONE

INTRODUCTION

1.0 Introduction

This chapter covers the background information, statement of the problem, justification of the study, objectives of the study, significance of the study, and finally, the scope of the study.

1.1 Background of the Study

A mixture experiment is an experiment where proportions of two or more components are mixed to yield a product and are connected with the investigation of factors that are thought to affect the response through the proportions at which they are mixed together. According to Cornell (1990), the measured response in the general mixture problem is thought to simply depend on the relative proportions of the components present in the mixtures, not the amount of the combination.

Most kinds of products usually involve a mixture of ingredients and are dependent on the investigation of a mixture of several factors. In many technological fields, most experimenters struggle to optimize the output of the end product since the predictor variables always have an impact on the general response of interest. The end product has the required properties that are of interest to the experimenter. Every experimenter wants to obtaining optimal results for an experiment; thus their major objective is to estimate the absolute response or the parameters of a model that shows the link between the response and the factors. When examining regression equations relating to the response and the controllable component, an experimenter's goal is to; Identify whether some combination of factors can be said to be the best in some way and also, to learn more about the functions played by the various system factors in order to comprehend the system as a whole.

Suppose that a mixture consists of m factors. Let t_i represent the proportion of the ith ingredient in the mixture. Then, $t_1, t_2, \dots \dots, t_m$ are coded such that $t_i \geq 0$ subject to restriction $\sum t_i = 1$. A simple regular-sided shape with m vertices in m-1 dimensions serves as the experimental region for the mixture problem. Scheffe' (1958) set the framework for development of mixture tools (design and models).

Let $I_m = (1 \dots 1)' \in R^m$ be the unity vector .The standard probability simplex T_m is the experimental domain. The experimental response, designated as Y_t, is the outcome under experimental condition $t \in T_m$ of an experiment that is taken as a real-valued random variable with an unknown parameter $, \theta$ for the regression function for the mixture experiments called the Kronecker models. Change in experimentation condition has a great impact on the experimental response. Thus, a mixture experiment involves varying the components of the mixture, and monitoring the variations that occur in the responses of the end products.

Replications under responses from distinct conditions for conducting experiments as well as identical conditions for conducting experiments, are therefore assumed to have equal (unknown) variance,σ^2 and to be uncorrelated. On the experimental domain T_m, the experimental design τ is the probability measure with a finite number of support points . If τ assigns weights $w_1, w_2, \dots$ to its points of support in T_m , the experimenter is then directed to draw proportions $w_1, w_2, \dots$ of all the observations under various experimental settings. Draper and Pukelsheim (1998) came up with a set of regression functions for mixture experiments called Kronecker or K-models. The models are based on Kronecker algebra. Let $t = (t_1, ..., t_m)'$ be a $m \times 1$vector to represent the factors in a mixture. Kronecker square $t \otimes t$ arranges the same numbers as a long $m^2 \times 1$ vector and arranges the Kronecker product cube $t \otimes t \otimes t$ as a long $m^3 \times 1$ vector and list of triple products $t_i t_i t_j$ in lexicographic order. K-models have compact representation and good symmetries attained as a result of duplication of terms. Symmetry is attained along with a replication of terms.

Mixture experiments are common problems in many disciplines, such as the chemical industries, food and processing industries. An example of a mixture experiment is of cake formulations where the mixture ingredients are; sugar, flour, water, eggs and baking powder, the interest of the experimenter is on the fluffiness of the cake, in that the cake fluffiness is associated with the ingredient proportions on the mixture. Similarly, in building construction concrete formed by mixing sand, water, and one or more types of cement building, then the desired property is the hardness or compression strength of the concrete, where the hardness is a function of the percentages of cement, sand, and water in the mix and Fruit punch consisting of juices from apples, pineapple ,bananas ,mangoes and orange ,where the fruitiness flavor of the punch, which depends on the percentages of apples, pineapple, bananas, mangoes, and orange that are

present in the punch. Cornell (1990) lists numerous examples and provides a thorough discussion of both theory and in practice. Therefore, a mixture experiment

involves varying the proportions of two or more ingredients, called components of the mixture, and studying the changes that occur in the measured properties (responses) of the resulting end product. The objectives of the experiment may include determining: which variables are most influential on the response, where to set the independent variables so that the response is almost near the desired nominal value, where to set the influential factors so that variability in response is small and where to set the controllable factors so that the effects of uncontrollable factors are minimized.

1.1.1 Simplex Centroid Designs

Simplex centroid designs are described as mixture designs with which the coordinates are zero or equal to each other as introduced by Scheffe (1963). The center (centroid), mid-edges, and vertices of a triangle serve as the points of support in a simplex centroid design. In general, an *m*-component simplex-centroid design typically specifies the number of support points as $2^m - 1$. The support points correspond to m permutations of (1,0,0, … ,0) or pure blends, the permutations of $\left(\frac{1}{2},\frac{1}{2},0,0,...,0\right)$ or binary mixtures, the $\binom{m}{3}$| permutations of $\left(\frac{1}{3},\frac{1}{3},\frac{1}{3},0,0,...,0\right)$, and finally, the overall centroid $\left(\frac{1}{m},\frac{1}{m},...,\frac{1}{m}\right)$. Every non-empty subset of the m components is included in the design, and the components are only mixed together in the same proportions.

The mixture can be found at the centroids of the lower dimensions' simplexes included within the (m— l)-dimensional simplex, which is where the (m— l)-dimensional simplex is located. Data on the response are gathered at the simplex-centroid design's points, and a polynomial fit with the same number of parameters that must be estimated as those at the related design's points is made, (Muriungi et al, 2017).

1.1.2 Weighted Centroid Designs

Simplex centroid designs were introduced by Scheffe` (1963). The j^th^ elementary centroid design η_j, $j \in \{1,......,m\}, m \geq 2$ is the uniform distribution on all points with the form $\frac{1}{j}=\sum_{i=1}^{j} e_{ij} \in T_m$. A convex combination $\eta(\alpha)=\sum_{j=1}^{m} \alpha_j \eta_j$ with $\alpha=(\alpha_1,...,\alpha_m)' \in \mathrm{T}_m$ is called a weighted centroid design with a weight vector α and is restricted by $\sum_{i=1}^{m} \alpha_i = 1$ .Hence, $\eta(\alpha)$ denote sets of all weighted centroid designs. Weighted centroid designs were created using the vertex design points η_1 and the overall centroid design η_2 as follows; $n(\alpha)=\alpha_1\eta_1+\alpha_2\eta_2$ with weights $\alpha_1, \alpha_2 \geq 0$ and $\alpha_1+\alpha_2=1$.

1.1.3 Maximal Parameter Subsystem

An experimenter may be interested in studying s out of total k components instead of studying all the components or a single one. The study becomes possible through the study of linear parameter subsystems that has the form of some $k \times s$ matrix K ; K is termed as the coefficient matrix of the parameter subsystem $K'\theta$.

Let M be a set of moment matrices .A parameter subsystem $K'\theta$ is estimable within M if and only if the set M and the feasibility cone have a non-empty intersection, that is, $M \cap A(K) \neq \phi$ .Let $r_M = \max\{rankM : M \in \mathrm{M}\}$, be the maximal rank within M. The coefficient matrices $K \in \Re^{m^3 \times \binom{m+1}{2}}$ of parameter subsystems $K'\theta$ that are estimable within M satisfy $rank K \leq r_M$. Consider the extreme case $rank K = r_M$, which highlights the concept of estimating as many parameters as possible within a given collection of M moment matrices. The parameter subsystem $K'\theta$ is called a maximal parameter subsystem for M if and only if;

(i) $M \cap A(K) \neq \phi$ and

(ii) $rank K = r_M$ .In this specific study, we have $r_M = \binom{m+1}{2}$ and K is called a maximal coefficient matrix for M.

1.2 Statement of the Problem

Planning and designing of experiments is key before performing any experiment to cut the associated costs. Experimenters usually encounter a high cost of experimentation due to poor experimental designs, thus appropriate designs for an experiment that allows for parameter estimation without bias and with a minimum variance are desirable. Prediction variance distribution should be very evenly distributed over the design space.

Optimal weighted centroid designs for maximal parameter subsystem for third degree Kronecker model mixture experiments have not been studied. Kiplagat, (2014), showed optimal designs for second degree Kronecker model mixture experiments for maximal parameter subsystem. The second degree maximal parameter subsystem provides inadequate information leading experimenters to use more resources. Hence there was need to extent the work to third degree in order to get more information and reduce the cost. Since the larger the matrix the larger the information and the more optimal the design, the more optimal it carries.

The general design problem was to obtain a design for a parameter subsystem with maximum information. The full parameter subsystem cannot be estimated, to make it estimable, the coefficient matrix of interest was then chosen. By dividing the factors interacting with a total number of interacting parameters in the model, the whole parameter subsystem was made estimable, thus making it possible to estimate as many parameters as possible. The study sought to develop useful improved optimal designs to be used in designing experiments.

1.3 Objectives of the Study

The study was guided by the following objectives:

1.3.1 General Objective

The general objective of the study was to generate optimal weighted centroid designs for maximal parameter subsystem for third degree Kronecker model mixture experiments.

1.3.2 Specific Objectives

The specific objectives of the study were to:

1. Identify the coefficient matrix K and the associated parameter subsystem of interest.
2. Determine optimal moments and information matrix for two, three, four and generalize to *m* factors.
3. Derive optimal weighted centroid designs for third degree Kronecker model for mixture experiments for A-, D- and E-Optimality criteria.
4. Compute numerical $\phi_p - Optimal$ weighted centroid designs for the maximal parameter subsystem.

1.4 Justification of the Study

In a mixture experiment, the factors which are under study are the proportions of factors of a mixture. There are many problems that deal with investigating a mixture of several factors which influences the response through the ratios or the proportions which are mixed together. A precise response prediction is required before experimentation for any mixture experiment to be successful. The purpose is to establish the effect that a factor or independent variable has on dependent variable. The A-optimality seeks to minimize the average variance of the regression coefficients, D-optimality maximizes the determinant of the information matrix and E-optimality maximizes the minimum Eigenvalue of the information matrix. This optimizes the responses over the experimental region.

1.5 Significance of the Study

This study is significant as it identifies optimal weighted centroid designs for maximizing parameter subsystems in third-degree Kronecker model mixture experiments. In practical terms, these optimal experiments reduce experimentation costs.

1.6 Scope of the Study

A class of weighted centroid designs is essentially complete, Klein (2004). Due to completeness result, the study was limited to weighted centroid designs third degree Kronecker model as put forward by Draper and Pukelsheim (1998). A group of weighted centroid designs and characterized by feasible weighted centroid designs for the maximal parameter subsystem for the mixture regression equation with two or more factors was used to obtain the coefficient matrix. Optimal moments and information matrices of the designs were obtained based on the coefficient matrix of interest. Consequently, the unique D-, A- and E-optimal weighted centroid designs for third degree kronecker model were then derived from the information matrices with the aid of the use of the equivalence theorem.

CHAPTER TWO

LITERATURE REVIEW

2.0 Introduction

This chapter reviews the relevant literature for this specific study and the theoretical discussions. The research gaps on A-optimality, D-optimality and E-optimality designs were identified for the study.

2.1 Mixture Experiments

Mixture experiments were first discussed in Quenouille (1953). Later on, Scheffe' (1958) made a systematic study and laid a strong foundation. Pukelsheim (1993) and

Gaffke and Heiligers (1996) gave a review of the general design environment on mixture experiments. Klein (2004) and Cheng (1995) showed that the class of weighted centroid designs is essentially complete for $m \geq 2$ for the Kiefer ordering. As a consequence, the search for optimal designs may be restricted to weighted centroid designs for most criteria particularly applied to mixture experiments, Kiefer (1959, 1975, 1978, 1985) and Galil and Kiefer (1977). Klein (2004) and Kinyanjui (2007) showed how invariance results can be applied to analytical derivations of optimal designs.

Piepel G. F and Cornell J.A. (1994). Studied mixture experiment approaches: examples, discussion and recommendation A mixture of factors impacts the response through the proportion in which they are mixed. The response is a measurable quality or property of interest in the product. In this study, the assumption is made that the quantities of factors in the mixture can be accurately measured by the experimenter. London, Griffin. Scheffe', H. (1958). Experiments with mixtures. The assumption is also made that, the outcomes are always functionally related to the mixture composition and through variation of the composition by changing the number of ingredients, the responses will as well vary. When examining regression equations relating to the response and the controllable component, an experimenter's goal is to; Identify whether some combination of factors can be said to be the best in some way and also, to learn more about the functions played by the various system factors in order to comprehend the system as a whole.

Galil and Kiefer (1977) showed how optimal designs can be restricted to weighted centroid designs and applied to mixture experiments. A weighted Centroid design is essentially complete for $m \geq 2$ factors or kiefer ordering, Klein (2004). The search for the best designs can therefore be limited to weighted centroid designs for the majority of criteria, especially when applied to mixture experiments. The study was limited to weighted centroid designs, with the third degree Kronecker model as put forward by draper and Pukelsheim (1998).

On mixture experiments, a review was given for the general design environment, pukelsheim (1993). Draper and Pukelsheim (1998) proposed the K-models, a group of mixture models. Kiefer (1959, 1975, and 1978) and Galil and Kiefer (1977) provided criteria applied to mixture experiments. Blend experiment strategy procedures are presented by Cornell (2002) for simplex and polyhedral regions. Subsequent to selecting appropriate design and performing mixture experiments, is fitting models used to screen the components, predict response(s), determine ingredients effects on the response(s), or optimize the response(s) over the experimental region. Scheffé (1958) came up with linear mixture model in which the coefficient estimate for a component is the predicted value of the response for that pure component. Darroch and Waller (1985) presented D-optimal axial designs for quadratic and cubic additive mixture models. Draper and Pukelsheim (1999) showed that for first degree Kronecker model vertex point designs are unique optimal designs under the Kiefer Ordering. Alternative representation of mixture models based on Kronecker algebra of vectors and matrices is offered by k-models. Gaffke, N., (1987). Further characterizations of design optimality and admissibility for partial parameter estimation in linear regression.

It was assumed that every observation made during an experiment would have the same variance $\sigma^2 \in (0, \infty)$ and unrelated. Draper, Heiligers, and Pukelsheim (2000) demonstrated design improvement in terms of obtaining a large moment matrix under Loewner ordering and improving symmetry, defining kiefer design. Majority of design problems have symmetry features, remaining unchanged when subjected to a set of linear transformations. Therefore, using invariant design for homogenous symmetric K-models, aids in obtaining the key characteristics of effective experimental designs, namely symmetry and balance. The Kronecker representation has more benefits which entails; compact notation, useful invariance features and the regression terms being homogeneous, Draper and Pukelsheim (1998) and Prescott, *et al* (2002).

Kinyanjui (2007) adopted General equivalence theorem in Pukelsheim (1993) to investigate the $\emptyset_p - optimal$ weighted centroid designs for $k'\theta$ as well as deriving general forms for unique D-optimal, A-optimal and E-optimal designs for $k'\theta$.

The class of weighted centroid designs is essentially complete for $m \geq 2$ for Kiefer ordering, Klein (2002).The general design environment was given in Pukelsheim (1993).Kinyanjui, Koske, and Korir (2008) showed how optimal designs in the second-degree Kronecker model for mixture experiment with three ingredients was applied to a simplex centroid design. Ngigi ,(2009) showed the optimality criteria for $\phi_p - optimal$ weighted centroid designs for $K'\theta$ in the second-degree model with

$m \geq 2$ ingredients and how the general forms for the unique A-optimal, D-optimal and E-optimal designs for $K'\theta$ are derived.

Cherutich (2012) showed how information matrices for non-maximal parameter subsystems for second-degree mixture experiments were derived. Kiplagat, (2014), showed optimal designs for second degree kronecker model mixture experiments for maximal parameter subsystem. All the authors mentioned focused on the second degree kronecker model.

The work done by Draper and Pukelsheim, (1998) was extended to polynomial regression model for third degree mixture model. For third-degree mixture models, Kiefer ordering of simplex designs was demonstrated by Korir (2008). The work is further extended to third degree kronecker model by making use of equivalent theorem when calculating weights. Kerich, (2012) showed optimal designs for third degree Kronecker model mixture experiments. Cheruiyot, (2017) studied optimal designs for third degree Kronecker model mixture experiments with application in blending of chemicals for control of mites in strawberries.

The present work uses Kiefer's $\emptyset_p$ function as optimality criteria to weighted centroid designs for maximal parameter subsystem for third degree Kronecker model mixture experiments, where the moment matrix was improved to give more information in terms of enhancing symmetry and generating a large moment matrix under Loewner ordering yielding optimal values as desired.

2.2 Model and Notation

The linear model , $y = f(t)'\theta + \varepsilon$.......................................(1)

An experimental condition t is selected from the experimental domain T_m with a real valued response y, a regression function $y: T_m \mapsto \Re^k$,an unknown parameter vector $\theta \in \Re^k$ and centered error term, $\mathcal{E}$, Draper and Pukelsheim,(1993). In any experiment, it is assumed that errors are uncorrelated with a mean of zero and unknown variance σ^2 . Our attention is focusing on estimation of a system of linear function, $k'\theta$ of the parameter subsystem $\theta \in \Re^k$,where the coefficient matrix $K \in \Re^{m^3 \times \binom{m+1}{2}}$ is assumed to have full column rank.

If and only if there is at least one linear unbiased estimator for the parameter subsystem $k'\theta$ under a design τ, then the parameter subsystem $k'\theta$ with the entire column rank coefficient matrix k is estimable. A necessary and sufficient condition for estimability of $k'\theta$ under τ is that the range of K is included in the range of $M(\tau)$, $\Re(k) \subseteq \Re(M(\tau))$

Thus, any moment matrix, $A \in NND(k)$ with $\Re(k) \subseteq \Re(A)$ is called feasible for $k'\theta$.

The set $A(k) = \{A \in NND(k): \Re(K) \subseteq \Re(A)\}$ is called the feasibility cone for $k'\theta$.

Let M be a collection of moment matrices, then a parameter subsystem $k'\theta$ is estimable within M if and only if there is a non-empty intersection between the set M and the feasibility cone,. That is, $M \cap A(K) \neq \phi$.

Let $r_M = \max\{rankM : M \in \mathrm{M}\}$, be the maximal rank within M. The coefficient matrices $K \in \Re^{m^3 \times \binom{m+1}{2}}$ of the parameter subsystems $K'\theta$ that are estimable within M satisfy $rankK \leq r_M$. As a result, have a look at the extreme scenario $rankK = r_M$, which illustrates the concept of estimating as many parameters as possible using a given set of moment matrices.

Definition

The parameter subsystem $K'\theta$ is called a maximal parameter subsystem for M if and only if;

(i) $M \cap A(K) \neq \phi$ and

(ii) $rank K = r_M$. In this specific study, we have $r_M = \binom{m+1}{2}$ and K is called maximal coefficient matrix for M ,Draper and Pukelsheim (1998).The whole parameter vector θ, or any regular transform of it, is a maximal parameter subsystem for the set M if it contains regular moment matrices. Hence, assume the set M to be convex. Then, there is a matrix $M_0 \in M,$ with maximal range, that is, $\Re(M) \subseteq \Re(M_0)$ for all $M_0 \in M,$ Pukelsheim (1993). There may be many matrices $M_0$with this property, the maximal range $\Re_m = \Re(M_0)$ is unique, Then, dim $R_m = r_M$ .This construction is analogous to that of a minimal null space given by LaMotte (1977).

2.3 General Design Problem

According to Pukelsheim (1993), any design that solves the problem (2) below for a fixed $p \in$ (-∞, 1] is called $\phi_P - optimal$ for $K'\theta$ in T. For all $p \in$ (-∞, 1], the existence of $\phi_P - optimal$ design for $K'\theta$ is guaranteed in Pukelsheim (1993).The problem of finding a design with maximum information on the parameter subsystem $K'\theta$ was formulate as,

Maximize ϕ_p(C$_k$ (M (τ))) with $\tau \in$ T

Subject to C_K (M (τ))$\in PD(s)$τ$\in$T……………………………………….(2)

Where, T_m represents a collection of all designs and denoted by T. According to Pukelsheim (1993), the side condition $C_k(M(\tau)) \in PD(s)$ is the same as the availability of an unbiased estimator for $K'\theta$ under τ. The design τ is said to be feasible for $K'\theta$. The formulation makes it easier to estimate maximal parameter subsystem which is unbiased.

2.4 Coefficient Matrix and the Parameter Subsystem of Interest

A coefficient matrix is a rectangular array of numbers that represents the coefficients of a system of linear equations Searle & Khuri, (2017). The rows of the matrix correspond to the equations in the system, and the columns correspond to the variables in the system. Each entry in the matrix is the coefficient of the corresponding variable in the corresponding equation. In linear algebra, a coefficient matrix is a matrix consisting of the coefficients of the variables in a set of linear equations. The matrix is used in solving systems of linear equations Lyche, (2020).

The coefficient matrix K is the m × n matrix with the coefficient a_{ij} as the (i, j)th entry. The system of equations is inconsistent if the rank of the augmented matrix (the coefficient matrix augmented with an additional column consisting of the vector b) is greater than the rank of the coefficient matrix. If the ranks of these two matrices are equal, the system must have at least one solution. The solution is unique if and only if the rank r equals the number n of variables. Otherwise, the general solution has n – r free parameters, indicating an infinitude of solutions Bai & Wu, (2021).

The coefficient matrix is a fundamental concept in system identification, linear algebra, and control systems, and it plays a crucial role in representing and analyzing systems of linear equations and dynamic systems Qi, Tao & Jiang, (2019). The associated parameter subsystems and coefficient matrices are used in modeling, simulation, and control system design.

In the field of control systems, the coefficient matrices A and B are fundamental to the controllability of a system. The condition of controllability depends on these coefficient matrices, as described by a theorem in the context of system dynamics Buedo-Fernández & Nieto,(2020)

The coefficient matrix K provides a bridge between the parameter subsystem of interest and the optimal weighted centroid designs for maximal parameter subsystems Lu, Hydock, Radlińska & Guler, (2022). By understanding the structure of K, helps in identifying feasible designs and apply optimality criteria to select the most efficient design for their specific experimental objectives.

In the context of optimal design for mixture experiments, the coefficient matrix K plays a crucial role in determining the parameter subsystem of interest and identifying optimal weighted centroid designs for maximal parameter subsystems Wang, Fan & Qiang, (2023). The parameter subsystem of interest represents a subset of the full parameter space that is considered relevant for the specific experimental objectives. Maximal parameter subsystems are those that encompass the largest possible subset of parameters that can be estimated with the given experimental design.

To understand the relationship between the coefficient matrix K and the parameter subsystem of interest, consider the third-degree Kronecker model mixture experiment Sitienei, (2019). In this model, the response is assumed to be a polynomial function of the mixture proportions up to the third degree. The coefficient matrix K, denoted as

K_3, is a matrix that encodes the linear relationships between the third-degree polynomial terms and the mixture proportions.

The parameter subsystem of interest for the third-degree Kronecker model is typically defined to include all the linear, quadratic, and cubic terms, as well as some of the interaction terms Wambui, Joseph & John,(2021). The specific choice of terms depends on the experimental objectives and the properties of the response surface.

Optimal weighted centroid designs for maximal parameter subsystems are designs that maximize the amount of information available for estimating the parameters of interest Karatina, (2021). These designs are constructed using weighted centroid points, which are points in the mixture space that represent mixtures of the components. The weights associated with the centroid points determine the relative proportions of the components in each mixture.

The coefficient matrix K plays a key role in determining the optimal weights for the centroid points Gou, Sun, Du, Ma, Xiong, Ou, & Zhan, (2022). By analyzing the structure of K, it is possible to identify a set of feasible weighted centroid designs that satisfy the maximal parameter subsystem condition. These feasible designs can then be evaluated using optimality criteria, such as A-optimality or D-optimality, to select the design that provides the most efficient estimation of the parameters of interest.

The application of the coefficient matrix K in real-life situations involves using it to identify feasible designs and apply optimality criteria to select the most efficient design for specific experimental objectives. This is particularly relevant in the context of optimal design for mixture experiments. This concept has practical applications in various fields, such as pharmaceuticals, food science, and material engineering.

In pharmaceutical research, the development of drug formulations often involves mixture experiments to optimize the composition of active pharmaceutical ingredients, excipients, and other components Janczura, Sip & Cielecka-Piontek, (2022).. The coefficient matrix K can be used to identify the optimal weighted centroid designs for maximal parameter subsystems, ensuring that the experimental design provides the most efficient estimation of the parameters of interest, such as drug potency, stability, and bioavailability.

In food science, the formulation of food products often requires the optimization of ingredient proportions to achieve desired sensory attributes, nutritional content, and shelf stability Janczura, Sip & Cielecka-Piontek, (2022). By utilizing the coefficient matrix K, researchers can identify the parameter subsystem of interest and design optimal weighted centroid experiments to maximize the information available for estimating the parameters related to taste, texture, and nutritional quality.

In material engineering, the development of composite materials involves blending different components to achieve specific mechanical, thermal, and electrical properties Hsissou, Seghiri, Benzekri, Hilali, Rafik, & Elharfi, (2021). The coefficient matrix K can be applied to identify the optimal weighted centroid designs for maximal parameter subsystems, ensuring that the experimental design provides the most efficient estimation of the parameters related to material performance and durability.

By understanding the structure of the coefficient matrix K, researchers and practitioners in these fields can effectively identify feasible designs and apply optimality criteria to select the most efficient design for their specific experimental objectives, ultimately leading to the development of high-quality products and processes.

2.5 Moment and Information Matrices

According to Pukelsheim (1993),for any design τ, with the moment matrix M, the information matrix for $K'\theta$ with $k \times s$ coefficient matrix k of column rank s can be defined as $C_k M$ in that, the mapping C_k from the cone NND(k) into the space $sym(s)$ is given by;

$$C_k A = \min\{LAL' : L \in \Re^{s\times k}, LK = I_s\} \in NND(s) \text{.................} (3)$$

Pukelsheim (1993) demonstrated that the Loewner ordering is taken into account when calculating this minimum across all left inverses L of K on the space $sym(s)$ of $s \times s$ symmetric matrices, defined by $A \le B$ if and only if $\mathrm{B} - \mathrm{A} \in \mathrm{NND}(s)$,for $A, B \in sym(s)$ and that this minimum exists and also it is unique. The information matrix $C_k(M(\tau))$ of a design τ with a moment matrix captures the amount of information that τ contains on $K'\theta$, Pukelsheim, (1993) and defined,

$$L_0 = (K'K)^{-1} K' \in \Re^{r_M \times k} \text{ ,...} (4)$$

With $K \in \Re^{k\times r_M}$ being maximal coefficient matrix for the convex set *M*, Pukelsheim (1993). Then the information matrix mapping $C_k : NND(k) \mapsto sym(r_M)$ satisfies, $C_k = L_0 A L_0'$ for all $A \in NND(k)$ with $\Re(A) \subseteq R_m$. Hence, C_k is a linear mapping on *M* and enjoys the inversion property $A = KC_k(A)K'$ for all $A \in NND(k)$ with $\Re(A) \subseteq R_m$, (Kinyanjui, 2007).

If $K'\theta$ is a subsystem with any number of parameters and $A \in NND(k)$ a given matrix, there is a left inverse $\tilde{L} = \tilde{L}(A)$ and is separate from A with $\Re(A) \subseteq R_m$ such that $C_k(A) = \tilde{L}(A)\tilde{L}'$, Pukelsheim (1993). The linearity of $C_k(M(\tau))$ as a function of $M(\tau)$ entails linearity of $C_k(M(\tau))$ as a function of τ. Additionally, the linearity of C_k is a generalization of the obvious identity $C_{I_k}(A) = A$ for all $A \in NND(k)$, It claims that information matrices for the entire parameter vector are moment matrices. Information matrices should therefore be viewed as modified moment matrices with the matrix $L_0 \in \Re^{r_M \times k}$,considering the model:

$$y = [L_0 f(t)]' \beta + \varepsilon \qquad (5)$$

With the same experimental domain T_m, the regressions function $L_0 f : T_m \mapsto \Re^{r_M}$, parameter vector $\beta \in \Re^{r_M}$ and the moment matrix $\tilde{M}(\tau)$of a design τ. Then, for every design τ on T_m with $\Re(A) \subseteq R_m$, we then have $\tilde{M}(\tau) = C_k(M(\tau))$ and the set $\tilde{M}(\tau) = \{C_k M; M \in \mathrm{M}\} \subseteq NND(r_M)$

is a convex set of moment matrix. Thus, the full parameter vector β is estimable within $\tilde{M}$,(Kinyanjui, 2007).

We then construct an information function $\phi : NND(s) \mapsto [0, \infty]$ to examine design problems for a parameter subsystem $K'\theta$.That is, ϕ ,is non-constant, it is upper semi-continuous, positively homogenous, and super additive with regard to the Loewner ordering. Instead of optimal designs, it is sufficient to think about optimal moment matrices. Let M be a subset of moment matrices, a moment matrix, $M_1 \in M$ is called $\phi - optimal$ for $K'\theta$ in M if and only if it solves the design problem,

Maximize $\phi - (C_k(M))$ with $M \in \mathrm{M}$

Subject to $M \in \mathrm{M} \cap A(k)$.

The optimal moments and information matrix depend on the number of moment conditions specified for the model. For two moment conditions, the optimal moments are the sample averages of the moment conditions, and the optimal information matrix is the inverse of the sample covariance matrix of the moment conditions.

In general, the optimal moments are the sample averages of the moment conditions, and the optimal information matrix is the inverse of the sample covariance matrix of the moment conditions Schennach & Starck,(2022).

In a mixture experiment, the experimenter is interested in the response of a mixture of two or more components as the proportions of the components are varied. Weighted centroid designs (WSCDs) are a popular choice for mixture experiments because they are efficient and easy to implement Husain & Hafeez,(2023).

There are a number of different criteria that can be used to assess the optimality of a WSCD. One common criterion is A-optimality. An A-optimal design is a design that minimizes the determinant of the Fisher information matrix Hajibabaei, Seydi & Koochari, (2023). This means that an A-optimal design provides the most precise estimates of the model parameters.

In the context of third-degree Kronecker model mixture experiments, a maximal parameter subsystem is a parameter subsystem that contains as many parameters as possible Sitienei, (2019). A WSCD for a maximal parameter subsystem is a WSCD that allows for the estimation of as many model parameters as possible.

Optimal WSCDs for maximal parameter subsystems in third-degree Kronecker model mixture experiments have been studied by a number of researchers. Kerich et al. (2014) developed a method for constructing A-optimal WSCDs for maximal parameter subsystems in third-degree Kronecker model mixture experiments. They found that the A-optimal WSCDs for maximal parameter subsystems are highly efficient and can be used to estimate a large number of model parameters.

WSCDs are a valuable tool for mixture experiments. They are efficient, easy to implement, and can be used to estimate a large number of model parameters. Optimal WSCDs for maximal parameter subsystems are particularly useful in third-degree Kronecker model mixture experiments (Kinyanyui, Kungu, Ronoh, Korir, Koske & Kerich, 2014).)

2.6 Feasibility Cone

According to Pukelsheim (1993),the most important case occurs if the full parameter vector θ is of interest, that is, if $k = I_k$ and since the unique left inverse L of k is then the identity matrix I_k, the information matrix for θ reproduces the moment matrix M,

$$C_{I_k}(M) = M \qquad \text{...(6)}$$

According to Pukelsheim (1993), if the matrix M lies in the feasibility A(C), Gauss-Markov Theorem provides the representation,

$$C_c(M) = (c'M^{-1}c)^{-1} \text{... (7)}$$

Here the information matrix for $C'\theta$ is the scalar $\left(c'M^{-1}c\right)^{-1}$,in contrast to the moment matrix M. The goal of information minimization seems acceptable. The feasibility cone $A(k)$ for a parameter subsystem $K'\theta$ is defined by;

$A(k) = \{A \in NND(k); rangek \subseteq range\ A\}$.

A matrix $A \in sym(k)$ is called feasible for $K'\theta$ when $A \in A(k)$;a design ξ is called feasible for $K'\theta$ when $M(\xi) \in A(k)$. If k is of full rank, the representation is provided by the Gauss-Markov theorem as $C_k(A) = \left(k'A^{-1}k\right)^{-1}$, information matrices in statistical inference assume this form, Pukelsheim, (1993).

2.7 Kiefer Optimality

The optimality properties of designs are determined by their moment matrices Pukelsheim (1993). We compute optimal design for the polynomial fit model, the third degree Kronecker model. This involves searching for the optimum in a set of competing exchangeable moment matrices, Gregory et al, (2014). For mixture models on the simplex, a better design is obtained, by matrix majorization that yields a larger moment matrix due to increase of symmetry and Loewner ordering. The two criteria together constitute the Kiefer design ordering and any such criteria single out one or a few designs that are Kiefer optimal, Pukelsheim, (2006). In view of the initial symmetrization step, it suffices to search for improvement in the Loewner ordering sense, among exchangeable moment matrices only. First,obtain the exchangeable moment matrices, then find the necessary and sufficient conditions for two exchangeable third-degree K-moment matrices to be comparable in the Loewner matrix ordering. The comparison of moment matrix inequalities reduces to the comparison of individual moment inequalities which is part of the condition.

A minimum complete class of designs for the kiefer ordering is the set of weighted centroid designs. Completeness of a collection of weighted centroid designs (C) indicates that for each design τ that is not included in the set of weighted centroid designs, there exist a member ξ in C which is kiefer better than τ . To mean that, it must be shown that ξ has more information than τ.$\mathrm{M}(\xi) > \mathrm{M}(\tau)$, and thus the two moments are not kiefer equivalent. It must be shown that, weighted centroid design satisfies $\mathrm{M}(\xi) > \mathrm{M}(\tau)$,which in turn satisfies the kiefer optimality of $\mathrm{M}(\xi)$.

The assumption $\mathrm{M}(\xi) \geq \mathrm{M}(\tau)$ cannot be true, as demonstrated by Draper and Pukelsheim (1998), making the class C minimum complete. Thus, increased symmetry and Loewner ordering can always be added to designs that are not weighted centroid.

2.8 Polynomial Regression

Scalar responses Y_t are applicable to response surface models under the presumption that observations made under same or dissimilar experimental conditions t, share a common (unknown) variance, σ^2 , and are uncorrelated. Additionally, the models operate under the presumption that the anticipated response $E(Y_t) = n(t, \Theta)$ permits fitting by a low-degree polynomial in *t*. According to Draper and Pukelsheim (1998),by the use of the Kronecker product, we have the third-degree model as , $n(t,\Theta) = \theta_0 + t'\theta_{\{i\}} + (t \otimes t)'\theta_{\{ij\}} + (t \otimes t \otimes t)'\theta_{\{iij\}}$ and the mean parameter vector as,

$$\Theta = \begin{pmatrix} \theta_o \\ \theta_{\{i\}} \\ \theta_{\{ij\}} \\ \theta_{\{iij\}} \end{pmatrix}$$

Each of the components is usually interpreted with θ_0 as the grand mean. The $m\times1$ vector $\theta_{\{i\}}=(\theta_1,.....,\theta_m)'$ consist of the main effects θ_i .The $m^3\times1$ vector $\theta_{\{iij\}}=(\theta_{111},\theta_{112}.....,\theta_{mmm})'$ consists of interaction effects of pure cubic effects θ_{iii} and the three-way interaction effects θ_{iij} with third degree restrictions $\theta_{iij}=\theta_{jii}$ for all i,j and the regression function $t\mapsto f(t)$ conforms to the parameter vector Θ and is, in turn $f(t)=\begin{pmatrix}1\\ t\\ t\otimes t\\ t\otimes t\otimes t\end{pmatrix}$.

On the experimental domain T_m ,an experimental design τ is the probability measure with a finite number of support points. Suppose the supports points are $t_1,t_2,.....t_m$ and τ allocates weights w_1, w_2, ... to the support points in T_m , hence the experimenter is thus instructed to draw the proportions w_1, w_2, ... of all observations under the relevant experimental settings. For a linear model with regression function $f(t)$, the statistical properties of a design, τ are captured by its moment matrix,

$$M(\tau)=\sum_{j=1}w_j f(t_j)f(t_j)'=\int_{\tau} f(t)f(t)'\,d\tau\text{..}(8)$$

in Draper and Pukelsheim (1998). Any such moment matrix that has been over parameterized is rank deficient, and the least squares estimator's for Θ dispersion matrix is no exception. Consequently, the normal matrix inverses are unfortunately nonexistent. This results in the generalized inverses being invoked, which also has an equivalent performance.

2.9 Optimal Weighted Centroid Designs

Smith, (1918) became the first to develop optimal designs for the regression problems, later on, Kiefer, (1959) developed important computational procedures which are important in finding optimum designs in regression problems of statistical inference. Pukelsheim, (1993) examines the general design environment. According to Klein, (2004) the class of weighted centroid designs for a design with at least two elements for the Kiefer ordering is fundamentally complete.

The researcher showed that, in the second Kronecker model with ingredients

$m \geq 2$ for mixture experiments, for every design $\tau \in \mathrm{T}$ and for every $p \in [-\infty; 1]$ a weighted centroid design η exist with $(\phi_p \circ C_k \circ M)(\eta) \geq (\phi_p \circ C_k \circ M)(\tau)$. There are two steps followed for Kiefer design ordering. The ordering process for Kiefer designs involves two parts. The majorization ordering comes first. The next step is to improve the Loewner matrix ordering within a class of exchangeable moment matrices, Draper and Pukelsheim (1998). For every design $\tau \in \mathrm{T}$ there exist a weighted centroid design η whose moment matrix $M(n)$ becomes better upon M (τ) according to Kiefer ordering, with the moment matrices M (η) and M (τ), as seen in Draper and Pukelsheim, (1998). In the Kiefer ordering, a moment matrix M has better information than a moment N, if M is better than or equal to some intermediate matrix F under Loewner ordering and F majorized by N in a group that leaves invariant problem.

M >> N $\Leftrightarrow$ M >> F$\prec$N for some matrix F.

Moment matrix M is kiefer better than N if M>>N, but not when M and N are the same. The moment matrices M and N are kiefer equivalent when M>>N and N>>M. If symmetry is increased and a big moment matrix is obtained under Loewner ordering, a design can be enhanced to provide additional information. The two criteria demonstrate that the acquired information is, thus, Kiefer optimum for the parameter subsystem. The implication of the above is that any design which does not consist of a mixture of elementary centroid designs can be improved upon,in terms of symmetry and Loewner ordering, by using an appropriate combination of elementary centroid designs.

Other criteria within the class of weighted centroid are needed for more improvement, for instance the average variance criterion, and determinant criterion as proposed by Draper and Pukelsheim, (1998). The introduction of optimal designs was done by Scheffe' (1963). Exchangeable weighted centroid designs are those that are invariant under permutations, Klein (2002).

Klein (2004) affirmed the benefits of the weighted centroid designs for the Kronecker model thus summarizing the work done in theorem 6.4 and 7.4 by Draper, Heiligers and Pukelsheim (1999).

Weighted centroid designs are used in the context of optimal experimental design, particularly for mixture experiments involving a maximal parameter subsystem. The weighted centroid design aims to optimize the precision of estimating model parameters Shah, Zhe, Yin, Khan, Begum, Faheem & Khan, (2018). The computation of numerical weighted centroid designs for the maximal parameter subsystem involves determining the optimal values based on specific optimality criteria. The literature on this topic discusses the computation of optimal designs for a maximum subsystem of parameters in second-degree Kronecker model mixture experiments. It also addresses the derivation of E-optimal weighted centroid designs based on maximal and non-maximal parameter subsystems for various numbers of ingredients. Additionally, a well-defined coefficient matrix is used to select a maximal parameter subsystem for the model, as its full parameter space is inestimable Kung'u, Koske & Kinyanjui, (2020).

For specific numerical computations and algorithms related to weighted centroid designs for maximal parameter subsystems, consulting the referenced literature and academic papers would provide detailed methodologies and approaches Wang, Fan & Qiang, (2023). The first step in computing numerical weighted centroid designs is to compute the information matrix of the design. The information matrix is a matrix of second-order partial derivatives of the log-likelihood function with respect to the parameters. The diagonal elements of the information matrix are the variances of the parameter estimates.

The second step is to use the information matrix to compute the D-optimal, A-optimal, and E-optimal designs. The D-optimal design is the design that minimizes the average variance of the parameter estimates. The A-optimal design is the design that minimizes the trace of the information matrix. The E-optimal design is the design that minimizes the maximum eigenvalue of the information matrix Shahmohammadi & McAuley, (2018). The third step is to compute the weights of the points in the design. The weights are determined by the relative importance of the parameters. The weights can be computed using a variety of methods, such as least squares or maximum likelihood Mannarswamy, (2018). The final step is to evaluate the performance of the design. This can be done by comparing the design to other designs, or by comparing the design to a theoretical benchmark Bu, Majumdar & Yang, (2020).

Weighted centroid designs have various applications in real-life situations. One application is in optimal experimental design, specifically for mixture experiments involving a maximal parameter subsystem Özbek & Eker, (2020). The goal of weighted centroid designs in this context is to optimize the precision of estimating model parameters. This can be useful in industries such as pharmaceuticals or materials science, where accurate parameter estimation is crucial for product development and optimization.

In another real-life application, weighted mean centroids are computed for latitude and longitude points, taking into account the spheroid ,Abd El-Sattar, Sultan, Kamel, Khurshaid & Rahmann,(2021). This can be useful in geographic analysis or navigation systems, where determining the center or average location of a set of points is important. To compute numerical weighted centroid designs, several steps are involved. First, the information matrix of the design needs to be computed, which consists of second-order partial derivatives of the log-likelihood function with respect to the parameters Zhu, Zhu & Au,(2023). This matrix provides information about the variances of the parameter estimates.

Next, different optimality criteria such as D-optimal, A-optimal, and E-optimal designs can be computed using the information matrix ,Gichuki, Joseph & John, (2020). These designs aim to minimize the average variance, trace, or maximum eigenvalue of the information matrix, respectively. The weights of the points in the design are then computed based on the relative importance of the parameters ,Marks et al., (2023). This can be done using methods like least squares or maximum likelihood. Finally, the performance of the design is evaluated by comparing it to other designs or theoretical benchmarks. This allows for the selection of the most suitable design for the specific application.

2.10 Optimality Criteria

The function ϕ is an optimality criterion from the closed cone of non-negative definite $s \times s$ matrices (C_{sxs}) onto real line ϕ : NND(s) → R, with the properties that gives the idea of whether an information matrix can be large or small. For one to make a good decision, on the best model to be selected, some set are to be employed. There are widely used optimality criteria used in statistics, which comprises of; The smallest Eigen Value Criterion (E- Criterion), Average Variance Criterion (A- Criterion) and the Determinant criterion (D- Criterion).

The need for the theory of optimal designs emerged from the requirement that an experimental design be properly chosen before the experiment. The aim of investigating the optimal theoretical designs is to provide a reliable benchmark for identifying the most efficient and useful solutions to a problem. This was motivated by the fact the available resource is inadequate that are used to conduct field experiments, hence, making it sensible to get the most convenient way the optimal desired results could be obtained by making use of the limited resources available.

Smith (1918) provided a criterion and also obtained optimal experimental designs for a given set of regression problems. Wald (1943) showed the criteria of maximizing the determinant of the matrix X'X and Kiefer and Wolfowitz (1959) referred to it as the D-optimality criterion. The design optimality criteria always deal with the optimal properties of the given design matrix for a model matrix X.

The D-Criterion is used in most commonly used as well as the A-optimality and E-optimality criteria which were later on developed as the parameter estimation criteria. Additional developments in the generation of optimality criteria is found in the works done by Elfving (1952) and Chernoff (1953) who reduced the trace of $(X'X)^{-1}$ to get the regression designs. Ehrenfeld (1955) brought about the suggestion for minimizing the suggested that maximizing the smallest eigenvalue of X'X can as well be used as a criterion.

The idea of optimum experimental design is as well explained by doing the relationship between the variance of the parameter estimates and that of the expected responses from different designs and models. The general equivalence theorem, which leads to the algorithms for the designs and models, is the outcome of the existing association between the two sets of variances. The general equivalence theorem is the central result where the dependence of the optimal design of experiments depends (Atkinson and Donev, 1992). The methods for construction and the verification of the optimal designs are offered, and the theorem is generally applied to a variety of given design requirements. The goodness of a design is shown by the optimality criterion on either a set of a given statistical properties or on a certain property. Here, the goal of investigating optimal theoretical designs is to provide a yardstick for determining which designs are the most effective and practicable. Pázman (1986) and Mandal (2000) concentrated more on the D- optimality and also, Yang (2008) demonstrated the use of an algebraic technique for constructing an A-optimal designs in generalized linear models. Pukelsheim (1993) gave a comprehensive mathematical discussion which offered a method that is used to compute the optimality criteria, where he brought about the discussion on the D-optimality, and A- optimality criteria.

Optimal weighted centroid designs for maximal parameter subsystem for third degree Kronecker model mixture experiments have not been studied. The general design problem was to obtain a design for a parameter subsystem with maximum information. The full parameter subsystem cannot be estimated, to make it estimable, coefficient matrix of interest was then chosen, by dividing the factors interacting with the entire number of interacting parameters in the model, the full parameter subsystem was made estimable, making it possible to estimate as many parameters as possible. The study sought develop useful improved optimal designs that reduce the cost when used in designing of experiments. This study sought fill the knowledge gap.

In the context of the third degree Kronecker model for mixture experiments, weighted centroid designs are considered as an essentially complete class. These designs are evaluated based on various optimality criteria such as A-, D-, and E-optimality Sitienei, (2019). The weighted centroid designs are obtained by considering the coefficient matrix and the associated parameter subsystem of interest using unit vectors. The information matrices associated with the parameter subsystem of interest are then generated for the corresponding factors, and the optimality criteria are applied to evaluate the designs.

Optimal weighted centroid designs for the third-degree Kronecker model for mixture experiments can be determined using A-optimality, D-optimality, and E-optimality criteria Sitienei, Okango, & Otieno, (2019). A-optimality minimizes the average variance of the parameter estimates, D-optimality maximizes the determinant of the information matrix, and E-optimality minimizes the maximum eigenvalue of the variance matrix.To determine the optimal weighted centroid designs for the third-degree Kronecker model, the following steps can be followed. Define the third-degree Kronecker model where the third-degree Kronecker model is a second-order model that includes third-order interactions between the mixture components.

Define the optimality criterion where the optimality criterion is a measure of the efficiency of a design. The three most common optimality criteria are A-optimality, D-optimality, and E-optimality. A-optimality minimizes the average variance of the parameter estimates. D-optimality maximizes the determinant of the information matrix. E-optimality minimizes the maximum eigenvalue of the variance matrix.

Find the optimal weights for the weighted centroid design. The optimal weights for the weighted centroid design can be found using numerical optimization techniques. The optimal weights will depend on the optimality criterion and the number of mixture components..

Apply the design to the mixture experiment. The optimal weighted centroid design can be applied to the mixture experiment by selecting the mixture proportions according to the weights of the design. The response can then be measured and used to estimate the model parameters.

The optimal weighted centroid design for the third-degree Kronecker model will depend on the optimality criterion, the number of mixture components, and the specific mixture experiment. However, the optimal design will always provide more efficient parameter estimates than a non-optimal design.

The application of weighted centroid designs involves defining the third-degree Kronecker model, selecting the optimality criterion, finding the optimal weights for the design, evaluating the efficiency of the design, and applying the design to the mixture experiment. The optimal weighted centroid design for the third-degree Kronecker model depends on the optimality criterion, the number of mixture components, and the specific mixture experiment. However, it always provides more efficient parameter estimates than a non-optimal design. These designs are used to optimize mixture experiments and are evaluated based on various optimality criteria, making them a valuable tool in the field of mixture experiments.

For example, in the field of pharmaceuticals, when developing a new drug formulation, it is important to determine the optimal proportions of different ingredients to achieve the desired therapeutic effect. By using the weighted centroid designs, researchers can systematically vary the proportions of the ingredients and evaluate the response of the drug formulation. This can help in determining the optimal formulation that maximizes the desired effect while minimizing any potential side effects. The optimality criteria such as A-, D-, and E-optimality can be used to evaluate the efficiency of the designs and select the most optimal one. This application can save time and resources by providing a systematic approach to optimizing mixture experiments and improving the effectiveness of drug formulations.

CHAPTER THREE

RESEARCH METHODOLOGY

3.1 Introduction

Mixture experiments are associated with the investigation of several factors, which are assumed to influence the response only through proportions in which they are mixed. The mixture factors $t_1, t_2, \ldots \ldots, t_m$ are coded in such a way that $t_i \geq 0$ subject to restriction $\sum t_i = 1$. A major impact of this constraint being that the linear models do not have an intercept otherwise the regression coefficients cannot be estimated uniquely.

Let $I_m = (1 \ldots 1)' \in R^m$ be the unity vector .The standard probability simplex T_m is the experimental domain given as $T_m = \left\{t = \left(t_{1,,\ldots\ldots\ldots}, t_m\right)' \in [0,1]'; I_m' t = 1\right\}$

The experimental response Y_t is the response under experimental condition $t \in T_m$ taken as real valued random variable with an unknown parameter θ. The outcome of the experiment Y_t is the response under experimental conditions $t \in T_m$ and is used as a real valued random variable with the unidentified parameter , $\theta = (\theta_{111}, \theta_{112}, \ldots, \theta_{mmm})' \in \Re^{m^3}$.

Replications under responses from different experimental conditions and also the same experimental condition are under the assumption of having equal (unknown) variance,σ^2 and are uncorrelated. The probability measure on the experimental domain T_m is the experimental design τ, and it has a finite number of support points.

Early seminar work was done by Scheffe' (1958) who suggested and analysed canonical model forms when the regression function for the expected response is a polynomial of degree one, two, or three. We refer to these as the S-polynomial or S-models. In this paper, the alternative representation of mixture models is used to investigate the third-degree mixture models with three factors. This version is based on the Kronecker product algebra of vectors which was introduced by Draper

and Pukelsheim (1998). The Kronecker algebra gives rise to homogeneous model function and moment matrices. We refer to the corresponding expressions as K-models or K-polynomials.

Thus, the polynomial regression model for the third-degree mixture model is extended to the work done by Draper and Pukelsheim (1998). Where, expected response and the S-polynomial takes the following form,

$$E[Y_t] = f(t)'\theta = \sum_{i=1}^{m} t_i\theta_i + \sum\sum_{i<j}^{m} t_i\, t_j\theta_{ij} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (9)$$

The expected response of a regression function when it is homogenous third-degree k-Polynomial, takes the following form;

$$E[Y_t] = f(t)'\theta = \sum_{i=1}^{m}\sum_{i=1}^{m}\sum_{j=1}^{m} t_i\, t_i t_j\theta_{iij} = (t \otimes t \otimes t)'\theta \ldots\ldots\ldots\ldots\ldots\ldots \quad (10)$$

where the Kronecker powers $t^{\otimes 3} = (t \otimes t \otimes t), (m^3 \times 1)$ Vectors. Consist of the three-way and pure cubic interactions of components of t in lexicographic order of subscripts with $\theta_{iij} = \theta_{iji} = \theta_{jii} = \theta_{jji} = \theta_{jij} = \theta_{ijj}$ for all i, j being the third degree restrictions. According to Draper and Pukelsheim (1998), the advantages of the Kronecker model includes; its more compact notation, practical invariance qualities, and homogeneity of the regression terms. In an experiment, it is assumed that every observation has a common variance $\sigma^2 \in (0, \infty)$ and is uncorrelated. $m(\tau) = \int f(t)f(t)'d\tau$ is the moment matrix for the Kronecker model, with homogeneous elements of degree six. The moment matrix $m(\tau)$ reflects a design's statistical characteristics.

3.1.1 Kronecker Products

Draper and Pukelsheim (1998) proposed a set of mixture experiment models referred to as K-models or Kronecker models. Kronecker model is another representation of mixture models. The models are based on the vector and matrix algebra of Kronecker. The expected responses for any mixture experiments studied using the kronecker models, are homogeneous in factors. The mixture factors t_i, may be written as a $m \times 1$ vector, $t = (t_1, ..., t_m)$. Orthogonality is an important property that kronecker product should preserve. If two matrices A and B are the orthogonal matrices, then, their Kronecker product $A \otimes B$ are also said to be an orthogonal matrix .Kronecker product bases third degree polynomial regression in the m variables $t = (t_1, ..., t_m)'$ on matrix of all the cross products.

$$tt' = \begin{array}{c} \\ t_1 \\ t_2 \\ \vdots \\ t_m \end{array} \begin{array}{c} \begin{array}{cccc} t_1 & t_2 & \cdots & t_m \end{array} \\ \begin{pmatrix} t_1^2 & t_1t_2 & \cdots & t_1t_m \\ t_2t_1 & t_2^2 & \cdots & t_2t_m \\ \vdots & \vdots & \ddots & \vdots \\ t_mt_1 & t_mt_2 & \cdots & t_m^2 \end{pmatrix} \end{array}$$

Instead of reducing the Box –hunter minimal set polynomials $(t_1^2, ..., t_m^2, t_1t_2, ..., t_{m-1}t_m)$ .Some of the benefits enjoyed include: Transformational principles become straightforward using the conformable matrix R. The kronecker model extends to third degree polynomial regression and different terms are recurred depending on how many times they arise.

Given a matrix A and B with $k \times m$ and $l \times n$ respectively, where $kl \times mn$ is the block matrix and the definition of their Kronecker product is given as $A \otimes B$. Where,

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1m}B \\ \vdots & \ddots & \vdots \\ a_{k1}B & \cdots & a_{km}B \end{pmatrix}$$

Given a vector $s \in \Re^m$ and also another vector $t \in \Re^n$ their Kronecker product is a special case.

$$s \otimes t = \begin{pmatrix} s_1 t \\ \vdots \\ s_m t \end{pmatrix} = (s_i t_j)_{\substack{i=1,\ldots,m,\, j=1,\ldots,n \in \Re^{mn} \\ in \quad lexicographic \quad order}}$$

One of the key properties of Kronecker product is the product rule $(A \otimes B)(s \otimes t) = (As) \otimes (Bt)$ .This has a good implication for transposition, $(A \otimes B)' = (A') \otimes (B')$,for Moore-Penrose inversion, $(A \otimes B)^+ = (A^+) \otimes (B^+)$ and for the regular inversion $(A \otimes B)^{-1} = (A^{-1}) \otimes (B^{-1})$.The other properties of Kronecker product are $(A \otimes B) \otimes C = A \otimes (B \otimes C)$ for associativity, $(A + B) \otimes C = (A + C) \otimes (B \otimes C)$ for distributive property. Trace $(A \otimes B) = trace(B \otimes A) = trace\ (A) \otimes trace\ (B)$

And tt' assembles the cross products $t_i t_j$ in an $m \times m$ array. In second degree, a representation of Kronecker square $t \otimes t$ arranges same numbers as long $m^2 \times 1$ vector. And arranges the Kronecker product cube $t \otimes t \otimes t$ as a long $m^3 \times 1$ vector and a list of triple products $t_i t_i t_j$ in lexicographic order, as suggested by Draper and pukelsheim (1998).Transformation with conformable matrix R amounts to

$(Rt)\otimes(Rt)=(R\otimes R)(t\otimes t)$ for second degree Kronecker model and $(Rt)\otimes(Rt)\otimes(Rt)=(R\otimes R\otimes R)(t\otimes t\otimes t)$ for third degree Kronecker model.

This greatly helps to facilitate the calculations in applying the Kronecker product to response surface.

The first-degree K-model was of the following form,

$$E(Y_t)=f(t)'\theta == \sum_{i=1}^{m}\theta_i t_i \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

The second degree Kronecker model was given as follows,

$$E(Y_t)=f(t)'\theta=(t\otimes t)'\theta=\sum_{i=1}^{m}\theta_{ii}t_i^{\,2}+\sum_{\substack{i,j=1\\ i<j}}^{m}\left(\theta_{ij}+\theta_{ji}\right)t_it_j \ldots\ldots\ldots\ldots\ldots\ldots (12)$$

and the third degree model is of the following form; $E(Y_t)=f(t)'\theta=(t\otimes t\otimes t)'\theta=\sum_{i=1}^{m}\theta_{iii}t_i^{\,3}+\sum_{\substack{i,j=1\\ i\neq j}}^{m}\theta_{iij}t_i^{\,2}t_j \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (13)$

where $f(t)=t\otimes t\otimes t$ is an unknown parameter vector and also a regression vector. In an experiment all the observations were made with an assumption that, they have identical unknown variance and are unrelated. The Kronecker product has been applied in this study to derive the exchangeable moment matrices since Kiefer design ordering does not depend on the coordinate system that is used to represent the regression function, though both Kronecker and the Scheffe' are based on the same space of regression polynomials, but differ in their choice of representing this space. Draper and Pukelsheim, (1999) and Prescott, et. Al, (2002) put forward several advantages of the Kronecker model such as, the homogeneity of the regression terms, great transparency, models have compact representation, more convenient invariance properties and good symmetries attained as a result of duplication of terms. The terms are replicated and the symmetry is achieved. We refer to the corresponding expressions as K-models or K-polynomials. In particular, polynomial regression model for mixture experiments as suggested by. Draper and Pukelsheim, (1999) in the first and second-degree Kronecker mixture models in which they obtained the

results for Kiefer design ordering of mixture experimental design were reviewed. Most of the designs enjoy the good symmetric properties, as they are unaffected by a set of linear transformations and remain invariant. As a result, for the homogeneous symmetric Kronecker models, invariant design is applied. it helps in attaining the characteristics of a successful and good experimental design, which is, symmetrical and also balanced.

3.1.2 Space of Design Matrices

3.1.2.1 Invariant symmetric block matrices for design of mixture experiments

A quadratic subspace of symmetric $n \times n$ matrices is a linear subspace ϑ of $sym(n)$ with added feature that $C \in \vartheta$ implying that $C^2 \in \vartheta$. Rao, C.R.and Rao, M.B. (1998). Matrix Algebra and its Application to Statistics and Economics. Which gave a brief introduction to the subset and a few of its statistical uses. When specific invariance characteristics of the information matrices used in the design are taken into consideration, quadratic sub-spaces of symmetric matrices emerge. A specific quadratic subspace case is examined, and the application of the analysis's findings to the designs of the mixture experiment's third degree polynomial regression model is shown for

$m \geq 2$ factors. The canonical unit vectors in $\Re^m$ is denoted by $e_{1,}e_2, \dots \dots, e_m$.The canonical unit vectors in $\Re^{\binom{m}{2}}$ are denoted by E_{iij} with lexicographically ordered index pairs (i,j),$1 \leq i < j \leq m$.Let ϑ_m be the symmetric group which is of degree m, and also, let $perm(m)$ be the group of $m \times m$ permutation matrices.

Define, $H = \left\{ H_\pi = \begin{pmatrix} R_\pi & 0 \\ 0 & S_\pi \end{pmatrix} : \pi \in \vartheta_m \right\}$ with

$$R_\pi = \sum_{i=1}^{m} e_{\pi(i)} e_i' \in perm(m)$$ and

$$S_\pi = \sum_{\substack{i,j=1 \\ i<j}}^{m} E_{(\pi(i),\pi_j)\uparrow} E_{ij}' \in perm\left(\binom{m}{2}\right) \ for \quad all \quad \pi \in \vartheta_m$$ where,

$(\pi(i), \pi(j))\uparrow$ is the pair of indices $\pi(i), \pi(j)$ in ascending order. The set H is the subgroup of $perm\left(\binom{m+2}{2}\right)$ and likewise is isomorphic to ϑ_m. And it acts on the space $sym\left(\binom{m+2}{2}\right)$ through the transformation of congruence $(H,C) \mapsto HCH'$ and induces the subspace,

$$sym\left(\binom{m+2}{2}, H\right) = \left\{ C \in sym\left(\binom{m+2}{2}\right) : HCH \quad for \quad all \quad H \in H \right\}$$ of symmetric H-invariant matrices. Given that the orthogonal group's subgroup is H, space $sym\left(\binom{m+2}{2}, H\right)$ is the quadratic subspace as given in Pukelsheim (1993). One of the major components of our research is the quadratic subspace. Moment matrices that are invariant under a finite subgroup of the orthogonal group, including permutations and sign changes, were considered by Gaffke and Heiligers in (1996).

While Galil and Kiefer (1977) treatment of the H-invariance is less formal and does not mention the quadratic subspace, their numerical approach to the best mixture experiment designs is guided by the structure and makes use of the eigenvalues of H-invariant symmetric matrices. The invariance results can be extended to the analytical derivations of optimal designs, as demonstrated by Klein (2004) and Kinyanjui (2007). The eigenvalues and eigenvectors of invariant symmetric matrices are obtained by spectral analysis.

3.1.2.2 Cubic Sub-Space

In a design problem, all information matrices lie under the cubic sub-space $sym(s, H)$

($s = \binom{m+1}{2}$)as shown in Klein (2004), where optimality criteria was a guide for analysis and the analysis of the cubic sub-space helped in solving design problem. In a rotatable cubic model,

Draper, N. R., Heiligers, B. and Pukelsheim, F. (1998). Studied Kiefer ordering of simplex designs for second-degree mixture models with four or more ingredients demonstrated how to determine numerically optimal designs.

H is a sub-group of permutation matrix group-invariance of a matrix $c \in sym(s)$, means certain entries of C coincide. Invariant symmetric matrix has seven distinct entries at most, Lemma 3.1 in Klein (2004).

Lemma 3.1

The identity matrices are defined as follows; $U_1 = I_m$ and $W_1 = I_{\binom{m}{2}}$,and

$1_m = (1,1,........,1)' \in \Re^m$

$U_2 = 1_m 1'_m - I_m \in sym(m)$

$$V_1 = \sum_{\substack{i,j=1 \\ i<j}}^{m} E_{iij}(e_i + e_i + e_j)' \in \Re^{\binom{m}{2}\times m},$$

$$v_2 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k=1 \\ k\notin\{i,j\}}}^{m} E_{iij} E'_k \in sym\left(\binom{m}{2}\right)$$

$$W_2 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k,l=1 \\ k<l}}^{m} E_{iij} E'_{kl} \in sym\left(\binom{m}{2}\right),$$
$$|\{i,j\} \cap \{k,l\}| = 1$$

$$W_3 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k,l=1 \\ k<l}}^{m} E_{iij} E'_{kl} \qquad \in sym\left(\binom{m}{2}\right).$$
$$\{i,j\} \cap \{k,l\} \neq 0$$

……………………………………………………………………………………………(14)

A matrix $C \in sym(s,H)$ can be uniquely represented as follows,

$$C=\begin{pmatrix} aI_m+bU_2 & cV_1+dV_2 \\ cV_1'+dV_2' & eI_{\binom{m}{2}}+fW_2+gW_3 \end{pmatrix}\text{...}(15)$$

with the coefficients $a,b,c,d,....., g \in \Re$. The terms that contain V_2, W_2 and W_3 only occur for $m \geq 3$ and for $m \geq 4$ respectively.

Proof

The block structure of the matrices in H allows for the partitioning of any symmetric matrix $C \in sym(s,H)$, that is,

$$C=\begin{pmatrix} C_{11} & C_{12} \\ C_{12}' & C_{22} \end{pmatrix}\text{..}(16)$$

with $C_{11} \in sym(m)$, $C_{21} \in \Re^{\binom{m}{2}\times m}$ and $C_{22} \in sym\left(\binom{m}{2}\right)$

$C_{11} \in span\{U_1,U_2\}$, $C_{21} \in span\{V_1,V_2\}$ and $C_{22} \in span\{W_1,W_2,W_3\}$.

In equation (16), a unique representation of this, follows from the linear independence of sets $\{U_1,U_2\}$, $\{V_1,V_2\}$ *and* $\{W_1,W_2,W_3\}$. The structure of $sym(s,H)$ is then turned , that is, the additional attribute that $sym(s,H)$ closes when matrix powers are formed. In equation (16), the block representation implied that, the powers of H-invariant symmetric matrices involve the products of U_i, V_j and W_k. Multiplication table for the matrices are presented by the following lemma.

Lemma 3.2

The results of multiplication of information matrices U_i, V_j and W_k are:

(i) Products in $span\{U_1, U_2\}$

$$U_1U_2 = U_2U_1 = U_2, \quad U_2^2 = (m-1)U_1 + (m-2)U_2.$$

$$V_1'V_1 = (m-1)U_1 + U_2, \quad V_2'V_2 = \binom{m-1}{2}U_1 + \binom{m-2}{2}U_2,$$
$$V_1'V_2 = V_2'V_1 = (m-2)U_2, \quad U_2^2 = (m-1)U_1 + (m-2)U_2.$$

$$U_1^2 = U_1$$

(ii) Products in $span\{V_1, V_2\}$

$$V_1'U_2 = V_1 + 2V_2, \quad V_2U_2 = (m-2)V_1 + (m-3)V_2,$$
$$W_2V_1 = (m-2)V_1 + 2V_2, \quad W_2V_2 = (m-2)V_1 + 2(m-3)V_2,$$
$$W_3V_1 = (m-3)V_2, \quad W_3V_2 = \binom{m-2}{2}V_1 + \binom{m-3}{2}V_2.$$

(iii) Products in $span\{W_1, W_2, W_3\}$

$$V_1V_1' = 2W_1 + W_2, \; V_2V_2' = (m-2)W_1 + (m-3)W_2 + (m-4)W_3,$$

$$V_1V_2' = V_2V_1' = W_2 + 2W_3, \; W_2^2 = 2(m-2)W_1 + (m-2)W_2 + 4W_3,$$

$$W_3^2 = \binom{m-2}{2}W_1 + \binom{m-3}{2}W_2 + \binom{m-4}{2}W_3,$$

$$W_2W_3 = W_3W_2 = (m-3)W_2 + 2(m-4)W_3$$

Proof

Verification of elementary calculations were done using the following identities;

$U_1 + U_2 = 1_m 1'_m$, $V_1 + V_2 = 1_{\binom{m}{2}} 1'_m$ and $W_1 + W_2 + W_3 = 1_{\binom{m}{2}} 1'_{\binom{m}{2}}$.

With lemma (3.1), by use of symbolic manipulation and multiplication of scalars, products of matrices in $sym(s,H)$ can be calculated . From this result, calculations that are involved in the design problem can be performed. Additionally, the multiplication table can be simply integrated into a computer algebra system, as a side result of lemma (3.1) and the $traceU_2 = traceW_2 = traceW_3 = 0$, the basis matrices;

$$B_1 = \begin{pmatrix} U_1 & 0 \\ 0 & 0 \end{pmatrix},\ B_2 = \begin{pmatrix} U_2 & 0 \\ 0 & 0 \end{pmatrix},\ B_3 = \begin{pmatrix} 0 & V_1 \\ V_1' & 0 \end{pmatrix},\ B_4 = \begin{pmatrix} 0 & V_2 \\ V_2' & 0 \end{pmatrix},$$

$$B_5 = \begin{pmatrix} 0 & 0 \\ 0 & W_1 \end{pmatrix},\ B_6 = \begin{pmatrix} 0 & 0 \\ 0 & W_2 \end{pmatrix} \text{and } B_7 = \begin{pmatrix} 0 & 0 \\ 0 & W_3 \end{pmatrix}$$

As given in lemma (3.2) form an orthogonal basis of $sym(s,H)$ in reverence to the Euclidean matrix scalar product $(A,B) \mapsto traceAB$ .With respect to lemma (3.2), results on Moore-Penrose inverses has the following implication, denoted by a superscript + sign and also on schur compliments:

Corollary 3.1

For all $m \geq 2$ factors, supposing that the matrix $C \in sym(s,H)$,is then partitioned with diagonal blocks C_{11}, C_{22} and off diagonal block C_{21} . Thus we have, $C_{11}^{+} \in span\{U_1, U_2\}$, $C_{11} - C_{21}^{'} C_{22}^{+} C_{21} \in span\{U_1, U_2\}$, $C_{22}^{+} \in span\{W_1, W_2, W_3\}$ and $C_{22} - C_2 C_{11}^{+} C_{21}^{'} \in span\{W_1, W_2, W_3\}$

Proof

The affirmations on C_{11}^{+} and C_{22}^{+} follow from $\begin{pmatrix} C_{11} & 0 \\ 0 & C_{22} \end{pmatrix} \in sym(s, H)$ and that quadratic sub-spaces are closed under Moore-Penrose inversion, (Rao, *et al.*1998, corollary 13.2.3). Together with lemma (3.2), the implication of these results claims on the schur complements of C_{11} and C_{22}.

3.1.3 Equivalence Theorem

The equivalence theorem thus provides the necessary and sufficient conditions for the existence of $\phi_P - optimal$ designs. As shown in Pukelsheim (1993), the design τ is called feasible for $K'\theta$ .Suppose $\eta(\alpha)$ satisfies the side condition C_k (M (τ)) $\in$ PD(s) and $C_j = C_k$ (M (η_j)) for j= (1, 2… m) and $p \in [-\infty, 1]$ .Then, $n(\alpha)$ is ϕ_p*-optimal* for $K'\theta$ in T if and only if,

$$trace C_j C_k(M(\eta(\alpha)))^{p-1} \begin{pmatrix} = trace C_k(M(\eta(\alpha)))^p \quad for \quad all \quad j \in \partial(\alpha) \\ \leq trace C_k(M(\eta(\alpha)))^p \quad otherwise \end{pmatrix} \ldots\ldots\ldots (17)$$

Equivalence theorem is mostly used in checking the optimality of given designs. To prove the equivalence theorem, sufficient conditions available from the following two theorems are applied:

Theorem 3.1

Let $\alpha \in T_m$ be a weight vector of the weighted centroid design $\eta(\alpha)$ and is feasible for $K'\theta$ and also, let $\partial(\alpha) = \{j = (1,2, \ldots m: \alpha_j > 0)\}$, be a set of active indices. Additionally, let $C = C_k(M(\eta(\alpha)))$ and $p \in (-\infty, 1)$ .Then $\eta(\alpha)$ is ϕ_p *-optimal* for $K'\theta$ in T if and only if,

$$traceC_j C_k^{p-1} \begin{cases} = trace^p & for \quad all \quad j \in \partial(\alpha) \\ < traceC^p & otherwise \end{cases}.$$

Proof

Kinyanjui (2007), gives the elaborate proof.

Theorem 3.2

Let $p \in (-\infty,1)$ and $\eta(\alpha)$ with $\alpha \in T_m$ be the weighted centroid design which is $\phi_p - optimal$ for $K'\theta$ in T. Then the following assertions hold:

If $\partial(\alpha) = \{1,2\}$, then there is no further design $\tau \in T$ that is $\phi_p - optimal$ for $K'\theta$ in T, that is, $\eta(\alpha)$ is unique.

If $\partial(\alpha) = \{1,2,3\}$, then there is no further exchangeable design $\bar{\tau} \in T$ that is $\phi_p - optimal$ for $K'\theta$ in T.

If there is a non-exchangeable design which is $\phi_p - optimal$ for $K'\theta$, then all its support points are centroids of depths 1, 2 or 3.

The proof of this Theorem is found in Kinyanjui, Koske, and Korir (2008) and Klein (2004). A consequence of this theorem to this study is that we restricted the work to the first two centroids η_1 and η_2, hence derived optimal weighted designs that are unique.

3.1.4 E-Optimal Weighted Centroid Design

The following theorems were made use in deriving the weighted centroid design for the smallest eigenvalue criterion, $\phi_{-\infty}$,that is E-optimality criteria. The three theorems in Pukelsheim (1993) were adopted, which specifically focuses on E-optimality.

Theorem 3.3

Assume the set M of competing moment matrices and convex, and intersects the feasibility cone $A(c)$. Then a competing moment matrix $M \in \mathrm{M}$ is optimal for $c'\theta$ in M if and only if M lies in the feasibility cone $A(c)$ and there exists a generalized inverse G of M such that $c'GAGc \leq c'M^{-}c \;\; for \;\; all \;\; A \in \mathrm{M}$.

Theorem 3.4

Let $\alpha \in T_m$, be a weight vector for the weighted centroid design $\eta(\alpha)$, and is feasible for $K'\theta$ and also, let $\partial(\alpha)$ be the set of active indices, ($\partial(\alpha) = \{ j = 1,...,m : \alpha_j > 0\}$).

Let $C = C_k(M(\eta(\alpha)))$ and $p \in (-\infty,1]$. Then the following assertions hold

The weighted centroid design $\eta(\alpha)$ is E-optimal for $K'\theta$ in T if and only if there is a matrix $E \in sym(s,H) \cap NND(s)$ satisfying

$$traceE = 1 \text{ and } traceC_j E \begin{cases} = \lambda_{\min}(C) & for \quad all \quad j \in \partial(\alpha) \\ < \lambda_{\min}(C) & otherwise \end{cases} \quad \text{……. (18)}$$

where $\lambda_{\min}(C)$, symbolizes the smallest eigenvalue of C.

Suppose $\eta(\alpha)$ is E-optimal for $K'\theta$ in T and E is a matrix satisfying the optimality condition for $\eta(\alpha)$ given in (i). Furthermore, let $\eta(\beta)$ be a further weighted design which is E-optimal for $K'\theta$ in T. then the information matrix

$\tilde{C} = C_k(M(\eta(\beta)))$, satisfies

$$\tilde{C}K = \lambda_{\min}(C)E$$

Then the following theorem dictates on the choice of the matrix E of theorem (3.4) above.

Theorem 3.5

Let $M \in M$ be a competing moment matrix which is feasible for $k'\theta$ and let $\pm z \in \Re^s$ be an eigenvector matching to the information matrix's $C_k(M)$ smallest eigenvalue. Then , M is $\phi_p - optimal$ for $k'\theta$ in M and the matrix $E = \frac{zz'}{\|z\|^2}$ satisfies the normality inequality of theorem (3.4) if and only if M is optimal for $z'k'\theta$ in M .

If the smallest eigenvalue of $C_k(M)$ has multiplicity 1, then M is $\phi_p - optimal$ for $k'\theta$ in M if and only if M is optimal for $z'k'\theta$ in M .

Proof

Normality inequality shows that $\phi_{-\infty} - optimality$ coincides with that theorem (3.3) for scalar optimality. With $E = \frac{zz'}{\|z\|^2}$,the normality inequality of theorem (3.4) reads,

$$z'k'G'AGKz \le \frac{\|z\|^2}{\lambda_{\min}(C_k(M))}, \text{ for all } A \in M .$$

The normality inequality of theorem (3.3) is $c'G'AGc \le c'M^{-}c$ for all $A \in M$

with $c = Kz$, The right hand side and left hand sides are identical because of

$$c'M^{-}c = z'K'M^{-}Kz = z'C^{-}z = \frac{\|z\|^{2}}{\lambda_{\min}(C_{k}(M))},$$

If the smallest eigenvalue of $C_{k}(M)$ has multiplicity 1, then the only choice for E is

$$E = \frac{zz'}{\|z\|^{2}}$$

Therefore, for the weighted centroid design, acquire the least eigenvalue and its corresponding eigenvector of the information matrix in order to obtain the best designs for the E-criterion. The information matrices used in our design can be uniquely partitioned as follows, based on equation (16).

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C'_{12} & C_{22} \end{pmatrix} \qquad (19)$$

for $\lambda \in \Re$

$$C = \begin{pmatrix} C_{11} - \lambda U_{1} & C'_{21} \\ C_{21} & C_{22} - \lambda W_{1} \end{pmatrix} \in sym(s, H) \qquad (20)$$

Consequently, the characteristic polynomial is denoted by,

$$\chi_{c}(\lambda) = \det(C - \lambda I_{s}) = \det(C_{11} - \lambda I_{s})\det\left[\left(C_{22} - \lambda W_{1}\right) - C_{21}\left(C_{11} - \lambda U_{1}\right)^{-1} C'_{21}\right]$$

where the matrix $\left[\left(C_{22}-\lambda W_{1}\right)-C_{21}\left(C_{11}-\lambda U_{1}\right)^{-1}C'_{21}\right]$ is the schur complement of $C_{11}-\lambda U_{1}$ and lies in the span $\{W_1 \quad W_2 \quad W_3\}$. The eigenvalues of the information matrix C make up the roots of this polynomial, which are computed as follows:

Lemma 3.3

Let a,….., g $\in \Re$ with d, f and g occurring only when $m \geq 3$ and for $m \geq 4$ respectively.

Moreover, define,

$$D_{1}=\left[a+(m-1)b-e-2(m-2)f-\binom{m-2}{2}g\right]^{2}+2(m-1)[2c+(m-2)d]^{2} \text{ ….. (21)}$$

$$D_{2}=[a-b-e-(m-4)f+(m-1)g]^{2}+4(m-2)(c-d)^{2} \text{ …………………….. (22)}$$

Then, in the case of $m \geq 4$,the matrix C has eigenvalues

$$\lambda_{1}-e-2f+g \text{ ……………………………………………………………… (23)}$$

$$\lambda_{2,3}=\frac{1}{2}\left[a+(m-1)b+e+2(m-3)f+\binom{m-2}{2}g \pm \sqrt{D_{1}}\right] \text{ …………………... (24)}$$

$$\lambda_{4,5}=\frac{1}{2}\left[a-b+e+(m-4)f-(m-3)g \pm \sqrt{D_{2}}\right] \text{…………………………..…. (25)}$$

with the multiplicities: $\frac{m(m-3)}{2}$, 1 and $(m-1)$ respectively.

In the case of m=2, only the eigenvalues $\lambda_2, \lambda_3, \lambda_4$,whereas for m=3 there are four eigenvalues $\lambda_2, \lambda_3, \lambda_4 and \lambda_5$.

The proof of this lemma is provided in Klein (2004).

3.2 Coefficient matrix

The coefficient matrix was computed using the parameter subsystem of interest. The Kronecker regression function's maximum parameter subsystem was chosen with the aid of the coefficient matrix. The Kronecker model's full parameter vector $\theta \in \Re^{m^3}$ is not estimable, it was made estimable through the study of a linear parameter subsystem of interest $K'\theta$, the focus was to estimate a system of linear function, $K'\theta$ of the parameter subsystem $\theta \in \Re^{m^3}$, where the coefficient matrix $K \in \Re^{m^3 \times \binom{m+1}{2}}$ was regarded as possessing full column rank.

Let $e_1, e_2 \ldots e_m$ denote the unit vectors in $\Re^m$ and E_{iij} denote the canonical unit vectors that are ordered lexicographically according to their indices $i, j \in \{1,2,\ldots m\}^3$ with $i < j$ and the unit vectors e_{iij} is for this study the Kronecker product of the unit vectors e_i, e_i and e_j ,that is, the set $e_{iij} = e_i \otimes e_i \otimes e_j$, for i<j, i, j= {1 2… m}.

The maximal coefficient matrix K which has a full column rank, which aided in the selection of the maximal parameter subsystem for the Kronecker regression function with a fixed number of factors, was then defined as;

$$K = (K_1; K_2) \in \Re^{m^3 \times \binom{m+1}{2}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (26)$$

where

$$K_1 = \sum_{i=1}^{m} e_{iii} e_i' K_2 = \frac{1}{6}\left\{\sum_{\substack{i,j=1 \\ i \neq j}}^{m} \left(e_{iij} + e_{iji} + e_{jii} + e_{jji} + e_{jij} + e_{ijj}\right)\right\} \ldots\ldots\ldots (27)$$

and

The matrix K is of full column rank. The parameter subsystem which was considered in this study was denoted by the following:

$$K'\theta = \begin{Bmatrix} (\theta_{iii})_{1\le i\le m} \\ \frac{1}{6}\left\{(\theta_{iij}+\theta_{iji}+\theta_{jii}+\theta_{jji}+\theta_{jij}+\theta_{ijj}),_{1\le i,j\le m}\right\} \end{Bmatrix} \in \Re^{\binom{m+1}{2}} \text{ For all } \theta \in \Re^{m^3} \text{....(28)}$$

where, $K = (K_1; K_2) \in \Re^{m^3\times\binom{m+1}{2}}$..(29)

The relevant subsystems are represented by the vectors on the right hand. In the full parameter model, the parameter subsystem of interest is a maximal parameter sub-system.

3.3 Optimal Moments and Information Matrix

Kronecker product was utilized to obtain the moments; R software was used to derive the numeral values. The moment matrix reflected well the statistical properties of the design τ . The moment matrix is given as,

$$M(\tau) = \int_\tau f(t)f(t)'d\tau \in NND(m^3) \text{..(30)}$$

where an entry of M (τ) is the sixth moments of a design τ, the regression function

f (t) is purely cubic and NND (m^3) is the cone of non-negative definite $m^3\times m^3$ matrices. A design τ is the experimental domain's probability measure with a set number of support points. The experimenter is instructed to take a percentage T ({t}) of all observations made under experimental condition F by the $S \in$ supp (τ) of each support point. In a simplex centroid design, the moment matrix can be partitioned into sub-moments in the following ways ,

$$m(n) = \alpha_1 m(n_1) + \alpha_2 m(n_2) + \ldots\ldots\ldots\ldots + \alpha_m m(n_m) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (31)$$

$C_k(M)$ is the information matrix for $K'\theta$ with $K \times S$ coefficient matrix K and full column S. K maximal coefficient matrix was defined in equation (26) as;

$$K = (K_1; K_2) \in \Re^{k \times s} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (32)$$

L was defined as; $L = (K'K)^{-1}K' \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (33)$

Where L is the coefficient matrix's left inverse, such that,

$$C_k(M(\tau)) = LM(\tau)L' \in \text{NND} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (34)$$

The entire parameter vector $\theta \in \Re^{m^3}$ of the Kronecker model was not estimable , the parameter subsystem $K'\theta$ was then considered to fit the model, where $K \in \Re^{k \times s}$. The information matrix then records the quantity of information a design τ has on $K'\theta$.

$C_k(M(\tau))=\min\left\{LM(\tau)L' : L \in \Re^{m^3 \times \binom{m+1}{2}}; LK = I_{\binom{m+1}{2}}\right\}$, is the information matrix for the j^th^ centroid. Where $I_{\binom{m+1}{2}}$ denotes the $\binom{m+1}{2} \times \binom{m+1}{2}$ identity matrix and L is the left inverse of K. With regard to Loewner ordering on the space $sym\left(\binom{m+1}{2}\right)$ of symmetric $\binom{m+1}{2} \times \binom{m+1}{2}$ matrices , the aforementioned minimum is understood.

The information matrix $C_k(M(\tau))$ is the precision matrix of the best linear unbiased estimator for $K'\theta$ under the design τ ,Pukelsheim (1993). The linear transformation of moment matrices yields the information matrices for $K'\theta$.

3.4 Optimal Weighted Centroid Designs

The set of competitors in a design problem, may be greatly diminished. In a mixture experiment with m factors, the jth elementary centroid design η_j , j$\in \{1, \ldots, m\}$, $m \geq 2$ is the uniform distribution on all points taking the form $\frac{1}{j}\sum_{i=1}^{j} e_k \in T_m$ with $1 \leq k1 < k2 < \cdots < kj \leq m$. There is m elementary centroid designs η_j for the m factors, placing equal weights $\frac{1}{\binom{m}{j}}$ on the points having j out of their m components equal to $\frac{1}{j}$ and zeros elsewhere.

The vertex design points η_1 and the overall centroid design η_2 was then used to construct weighted centroid designs as follows; for the weights $\alpha_1, \alpha_2 \geq 0$ with $\alpha_1 + \alpha_2 = 1$, the design $n(\alpha) = \alpha_1\eta_1 + \alpha_2\eta_2$ is a weighted centroid design.

The collection of weighted centroid designs in the third-degree mixture model with m factors, $n(\alpha) = \{\alpha_1\eta_1 + ... + \alpha_m\eta_m; (\alpha_1,..., \alpha_m)' \in \mathrm{T}\}$ is a convex and serves as the kiefer ordering's minimal complete class. Convex combination $\eta(\alpha) = \sum_{j=1}^{m} \alpha_j\eta_j$ with $\alpha = (\alpha_1,..., \alpha_m)' \in \mathrm{T}_m$ is called a weighted centroid design with a weight vector α and is limited by $\sum_{j=1}^{m} \alpha_j = 1$. Regarding the aim function of the design problem, the collection of weighted centroid designs represents a nearly complete class of designs.

In other words, there is a weighted centroid design $n \in T_m$ for each design $\tau \in$ T with $(\phi_p \circ C_k \circ M)(n) \geq (\phi_p \circ C_k \circ M)(\tau)$.

Hence, the design problem reduces to , maximize $(\phi_p \circ C_k \circ M \circ n)$ with $\alpha \in T_m$

subject to $C_k(M(n(\alpha))) \in PD(s)$

The necessary and sufficient conditions for the existence of $\phi_P - optimal$ designs are provided by the equivalence theorem. As shown in pukelsheim (1993), the design τ is called feasible for $K'\theta$ .Suppose $\eta(\alpha)$ satisfies the side condition C_k (M (τ))∈ PD(s) and $C_j = C_k$ (M (η_j)) for j= (1, 2… m) and $p \in [-\infty, 1]$.Then, $n(\alpha)$ is ϕ_p-*optimal* for $K'\theta$ in T if and only if,

$$traceC_j C_k(M(\eta(\alpha)))^{p^{-1}} \begin{pmatrix} = traceC_k(M(\eta(\alpha)))^p & for \quad all \quad j \in \partial(\alpha) \\ \leq traceC_k(M(\eta(\alpha)))^p & otherwise \end{pmatrix}.$$

With $\delta(\alpha) = \{j \setminus \alpha_j > 0\}$. The case $p = -\infty$, E-optimality, thus, has the same optimality criterion, Klein (2001). The aforementioned optimality criteria are difficult to solve in the absence of knowledge of the information matrices. But the invariance arguments will help to make the issue simpler. The general explanation of invariance strategies in experimental design was provided by Pukelsheim,(1993). Weighted centroid designs are interchangeable and invariant under permutation ingredients, Klein (2002).

3.5 Optimality Criteria

Due to the weighted centroid designs' completeness result, the optimal design problem was significantly diminished, results of theorem 3.2 of Draper, Heiligers and

Pukelsheim (2000). The optimality criteria are represented by a variety of functions that are specified on the set of the information matrices and have some statistical significance. Thus, if such a function reaches its maximum, designs are said to be at their best.

Moment matrices determine the properties of optimal designs as shown in Pukelsheim (1993). Polynomial fit model optimal designs are then computed. In the design of experiments, the optimal is sought among a collection of contending moment matrices. Prominently optimality criteria are: the average-variance criterion ϕ_{-1}, the determinant criterion ϕ_0 and the smallest eigenvalue criterion (E-criterion) and corresponds to parameter values -1, 0 and $-\infty$ respectively. These are particular cases of the matrix means ϕ_p with the parameter $p \in [-\infty; 1]$.

The D-optimality criterion, which looks for designs that maximize the determinant of the information matrix, is the most frequently used optimality criterion to choose the designs. D- optimality's objective is essentially a parameter estimation criterion.

The maximization of the information matrices' determinant is equivalent to the minimizing of the dispersion matrices' determinant. The D-optimality is then given by,

The determinant criterion, D-, $\phi_0(C) = (\det C)^{\frac{1}{s}}$, where $s = \binom{m+1}{2}$

The D-criterion has an important property in optimal designs because it minimizes the variances and also the covariance of the parameter estimates and for the smallest Eigen value criterion, it also, minimizes the largest Eigen value of the dispersion matrix and is given as follows, The smallest eigenvalue criterion, E-, $\phi_{-\infty}(C) = \lambda_{\min}(C)$.

The Eigen value criterion $\phi_{-\infty}$ is one extreme member of the matrix means ϕ_p corresponding to the parameter $P = -\infty$. And the average variance criterion minimizes the average variances and is given by,

The average variance criterion, A-, $\phi_{-1}(C) = \left(\frac{1}{s} traceC^{-1}\right)^{-1}$.

In this study, the information function matrix means ϕ_p was used, as expressed in Pukelsheim (1993).Kiefers ϕ_p -criteria provides an amount of information inherent to,C_K (M (τ)) $\in PD(s)$ with C_K (M (τ)) $\in PD\binom{m+1}{2}$, the set of $\binom{m+1}{2} \times \binom{m+1}{2}$ are positive definite matrices. Defined as follows,

$$\phi_p(C) = \begin{cases} \lambda_{\min}(C) & if \quad p = -\infty \\ \det(C)^{\frac{1}{\binom{m+1}{2}}} & if \quad p = 0 \\ \left[\frac{1}{\binom{m+1}{2}} traceC^P\right]^P & if \quad p \in [-\infty;1] \setminus \{0\} \end{cases},$$

For all C in $PD(s)$, the set of positive definite $s \times s$ matrices ,where $\lambda_{\min}(C)$ refers to the smallest eigenvalue of C.by definition, $\phi_p(C)$ is a scalar measure which is a function of the eigenvalues of C for all $p \in [-\infty,1]$, (Pukelsheim, 1993). And Kiefers ϕ_p-criteria provides an amount of information inherent to C_K (M (τ)) $\in PD(s)$.

3.6 Numerical Optimal Weighted Centroid Designs

The weighted centroid designs' optimal weights and values were then generated numerically using the R and Wxmaxima software. These were based on the general expressions for the weight vectors and the optimal values for each case of a design with m factors.

CHAPTER FOUR

RESULTS AND DISCUSSION

4.0 Introduction

Results and analysis of the study objectives as stated in the research methodology are presented in this chapter. This chapter contains optimal moments and information matrices and the derivations of A- , D- and E-optimal weighted centroid designs under study for $m=2$, $m=3$, $m=4$ and generalized to m factors.

4.1 Optimal Moments and Information Matrices

Coefficient matrix K was first defined, which was used in the identification of the parameter subsystem $K'\theta$ of interest. The moment matrices were then generated and information matrices C_k obtained. Starting with m=2, 3, 4 and generalized to m factors. The information matrices obtained was then used to obtain the optimality criteria.

4.1.1 Optimal Moments and Information Matrices For M=2 Factors.

Table 4.1: Simplex Centroid Design For M=2 Factors

Design points	t_1	t_2
1	1	0
2	0	1
3	$\frac{1}{2}$	$\frac{1}{2}$

with the elementary centroid designs given below,

$$\eta_1 = \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \text{ and } \eta_2 = \left\{ \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \right\}$$

Lemma 4.1,

The corresponding coefficient matrix K for the m=2 factors is as follows;

$$K = [K_1, K_2] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 1 & 0 \end{bmatrix}$$

Proof,

$$K_1 = \sum_{i=1}^{2} e_{iii} e_i' = e_{111} e_1' + e_{222} e_2' \text{ and}$$

$$K_2 = \frac{1}{6} \sum_{\substack{i,j=1 \\ i \neq j}}^{2} \left(e_{iij} + e_{iji} + e_{jii} \right) = \frac{1}{6} (e_{112} + e_{121} + e_{122} + e_{211} + e_{212} + e_{221}) .. (35)$$

and

The matrix K is of full column rank. The parameter subsystem which was considered in this study was denoted by the following:

$$K'\theta = \begin{Bmatrix} (\theta_{iii})_{1 \le i \le m} \\ \frac{1}{6} \left\{ (\theta_{iij} + \theta_{iji} + \theta_{jii} + \theta_{jji} + \theta_{jij} + \theta_{ijj}),_{1 \le i, j \le m} \right\} \end{Bmatrix} \in \Re^{\binom{m+1}{2}} \text{ For all } \theta \in \Re^{m^3}$$

where ,$K = (K_1; K_2) \in \Re^{m^3 \times \binom{m+1}{2}}$

The relevant subsystems are represented by the vectors on the right hand. In the full parameter model, the parameter subsystem of interest is a maximal parameter sub-system.

define $e_{iij} = e_i \otimes e_i \otimes e_j$, $e_{iji} = e_i \otimes e_j \otimes e_i$

and $e_{jii} = e_j \otimes e_i \otimes e_i$ i, j=1, 2, 3,

$$e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

hence $e_{111} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, $e_{222} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$,

$$e_{112} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

$$e_{121}=\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\1\\0\\0\\0\\0\\0\end{pmatrix},\qquad e_{122}=\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\1\\0\\0\\0\\0\end{pmatrix},$$

$$e_{211}=\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\1\\0\\0\\0\end{pmatrix},$$

$$e_{212}=\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\1\\0\\0\end{pmatrix}\text{ and }\quad e_{221}=\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\\1\\0\end{pmatrix}$$

hence,

$$e_{111}=\begin{pmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{112}=\begin{pmatrix}0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{121} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{122} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{211} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{212} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}',$$

$$e_{221} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}',$$

$$e_{222} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}',$$

substituting these in equation (35) gives,

$$K_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}, K_2 = \begin{pmatrix} 0 \\ \frac{1}{6} \\ \frac{1}{6} \\ \frac{1}{6} \\ \frac{1}{6} \\ \frac{1}{6} \\ \frac{1}{6} \\ 0 \end{pmatrix}.$$

hence, the coefficient matrix is given as,

$K = [K_1, K_2] =$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 1 & 0 \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (36)$$

Theorem 4.1

The information matrix $C_k(M(\eta(\alpha)))$ for a mixture design $\eta(\alpha)$ with m=2 factors is then given by,

$$C_k = C_k(M(n(\alpha))) = \begin{bmatrix} \frac{32\alpha_1 + \alpha_2}{64} & \frac{\alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{\alpha_2}{64} & \frac{32\alpha_1 + \alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{3\alpha_2}{32} & \frac{3\alpha_2}{32} & \frac{9\alpha_2}{16} \end{bmatrix}$$

Proof

Consider the moment matrix for m=2 factors which is given by,

$$M(\eta(\alpha)) = \begin{bmatrix} \mu_6 & \mu_{51} & \mu_{51} & \mu_{42} & \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} \\ \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} \\ \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} \\ \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} \\ \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} \\ \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} \\ \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} \\ \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} & \mu_{42} & \mu_{51} & \mu_{51} & \mu_6 \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots (37)$$

where the sixth moments are defined as,

$$\mu_6(\eta)=\int t_1{}^6 d\eta\ ,\ \ \mu_{51}(\eta)=\int t_1^5 t_2 d\eta,\ \ \mu_{42}(\eta)=\int t_1^4 t_2^2 d\eta,\ \ \mu_{33}(\eta)=\int t_1^3 t_2^3 d\eta\ .$$

there are m elementary centroid designs η_j , for m factors, placing equal weights $\frac{1}{\binom{m}{j}}$

on the points having j out of their m components equal to $\frac{1}{j}$ and zeros elsewhere.

A convex combination $\eta(\alpha)=\sum_{j=1}^{m}\alpha_j\eta_j$ with $\alpha=(\alpha_1,\alpha_2,...,\alpha_m)\in T_m$ is called a weighted centroid design with the weight vector α such that $\sum_{j=1}^{m}\alpha_j=1$.In a case of two factors the weighted centroid design is given as follows,

$$\eta(\alpha)=\sum_{j=1}^{2}\alpha_j\eta_j=\alpha_1\eta_1+\alpha_2\eta_2;\alpha=(\alpha_1,\alpha_2,0,0)\in T_2,\alpha_1+\alpha_2=1..........................(38)$$

with $\alpha=(\alpha_1,\alpha_2,0,0)\in T_2$ and $\alpha_1+\alpha_2=1$.

The sixth order moments are:

$\mu_6(\eta_j)=\frac{1}{j^5 m}$ and $\mu_{51}(\eta_j)=\mu_{42}(\eta_j)=\mu_{33}(\eta_j)=\frac{j-1}{j^5 m(m-1)}$ for j= (1, 2,…, m).

when m=2 factors, the moments are given as:

$\mu_6(\eta_1)=\frac{1}{2}$, $\mu_{51}(\eta_1)=\mu_{42}(\eta_1)=\mu_{33}(\eta_1)=0$, $\mu_6(\eta_2)=\frac{1}{64}$ and $\mu_{51}(\eta_2)=\mu_{42}(\eta_2)=\mu_{33}(\eta_2)=\frac{1}{64}$.

hence, the moment matrices for a given designs η_1 and η_2 are:

$$M(\eta_1) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \text{ and}$$

$$M(\eta_2) = \begin{bmatrix} \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} \end{bmatrix}. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (39)$$

the designs η_1 and η_2 information matrix is then obtained as follows,

$$L = (K'K)^{-1}K' = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(40)$$

the information matrix for the design η_1, is then given by,

$$C_1 = LM(n_1)L' = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} = C_k(M(n_1)) \text{..} (41)$$

And information matrix for the design η_2 is given by,

$$C_2 = LM(n_2)L' = \begin{bmatrix} \frac{1}{64} & \frac{1}{64} & \frac{3}{32} \\ \frac{1}{64} & \frac{1}{64} & \frac{3}{32} \\ \frac{3}{32} & \frac{3}{32} & \frac{9}{16} \end{bmatrix} = C_k(M(n_2)) \text{..................................} (42)$$

finally, for the design $\eta(\alpha)$, the information matrix is given as;

$$C_k(M(\eta(\alpha))) = \alpha_1 C_k(M(\eta_1)) + \alpha_2 C_k(M(\eta_2)).$$

replacing C_1 and C_2 yields,

$$C_k = C_k(M(n(\alpha))) = \begin{bmatrix} \frac{32\alpha_1+\alpha_2}{64} & \frac{\alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{\alpha_2}{64} & \frac{32\alpha_1+\alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{3\alpha_2}{32} & \frac{3\alpha_2}{32} & \frac{9\alpha_2}{16} \end{bmatrix} \text{..................................} (43)$$

Which is the desired information matrix for m=2 factors.

4.1.2 Optimal Moments And Information Matrices For M=3 Factors.

Table 4.2: Simplex Centroid Design For Three Factors

Design points	t_1	t_2	t_3
1	1	0	0

2	0	1	0
3	0	0	1
4	$\frac{1}{2}$	$\frac{1}{2}$	0
5	$\frac{1}{2}$	0	$\frac{1}{2}$
6	0	$\frac{1}{2}$	$\frac{1}{2}$
7	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$

with the elementary centroid designs given as,

$$\eta_1 = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}, \eta_2 = \left\{ \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \right\} \eta_3 = \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix}.$$

Lemma 4.2

The coefficient matrix K for m=3 factors is as follows;

$$K = [K_1, K_2]$$

$$= \frac{1}{6}\begin{bmatrix} 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}'$$

Proof,

$K_1 = \sum_{i=1}^{3} e_{iii} e_i' = e_{111} e_1' + e_{222} e_2' + e_{333} e_3'$, and

$$K_2 = \frac{1}{6}\left\{ \sum_{\substack{i,j=1 \\ i\neq j}}^{3} \left(e_{iij} + e_{iji} + e_{jii} + e_{jji} + e_{jij} + e_{ijj} \right) \right\} \quad \text{.........................} (44)$$

$$= \frac{1}{6}\begin{bmatrix} e_{112} & e_{121} & e_{211} & e_{221} & e_{212} & e_{122} \\ e_{113} & e_{131} & e_{311} & e_{331} & e_{313} & e_{133} \\ e_{223} & e_{232} & e_{322} & e_{332} & e_{323} & e_{233} \end{bmatrix}$$

and

The matrix K is of full column rank. The parameter subsystem which was considered in this study was denoted by the following:

$$K'\theta = \left\{ \begin{matrix} (\theta_{iii})_{1\le i\le m} \\ \frac{1}{6}\left\{ (\theta_{iij} + \theta_{iji} + \theta_{jii} + \theta_{jji} + \theta_{jij} + \theta_{ijj}),_{1\le i,j\le m} \right\} \end{matrix} \right\} \in \Re^{\binom{m+1}{2}} \quad \text{For all} \quad \theta \in \Re^{m^3}$$

where, $K = (K_1; K_2) \in \Re^{m^3 \times \binom{m+1}{2}}$

The relevant subsystems are represented by the vectors on the right hand. In the full parameter model, the parameter subsystem of interest is a maximal parameter sub-system.

define, $e_{iij} = e_i \otimes e_i \otimes e_j$ for i,j=1,2,3 , $e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

Thus,

$$e_{111} = \begin{pmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{112} = \begin{pmatrix}0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{113} = \begin{pmatrix}0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{121} = \begin{pmatrix}0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{122} = \begin{pmatrix}0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{123} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{131} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{132} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{133} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{211} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{212} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{213} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{221} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{222} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{223} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{231} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{232} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$e_{233} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{311} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{312} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{313} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{321} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{322} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{323} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0\end{pmatrix}',$$

$$e_{331} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\end{pmatrix}',$$

$$e_{332} = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0\end{pmatrix}',$$

$$e_{333} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}',$$

Substituting the above in equation 44 gives,

$$K_1 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}',$$

$$K_2 = \frac{1}{6}\begin{bmatrix} 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}',$$

therefore, the coefficient matrix K is given as ,

$$K = \left[K_1, K_2\right]$$

$$= \frac{1}{6}\begin{bmatrix} 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}'$$

……………………………………………………………………………………... (45)

Theorem 4.2

The information matrix $C_k(M(\eta(\alpha)))$ for a mixture design $\eta(\alpha)$ with m=3 factors is given by,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 \\ \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 & 0 \\ \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 \\ 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & 0 & \frac{3\alpha_2}{16} \end{pmatrix}$$

Proof,

Thus, consider the moment matrix for m=3 factors which is then given by,

$$M(\eta(\alpha)) = \begin{bmatrix} A & B & C \\ B & D & E \\ C & E & F \end{bmatrix} \text{...}(46)$$

where,

$$A = \begin{bmatrix} \mu_6 & \mu_{51} & \mu_{51} & \mu_{51} & \mu_{42} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} \\ \mu_{51} & \mu_{42} & \mu_{411} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} \\ \mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} \\ \mu_{51} & \mu_{42} & \mu_{411} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} \\ \mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} \\ \mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} \\ \mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} \\ \mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} \\ \mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} \end{bmatrix}$$

$$B=\begin{bmatrix}
\mu_{51} & \mu_{42} & \mu_{411} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321}\\
\mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222}\\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321}\\
\mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222}\\
\mu_{33} & \mu_{42} & \mu_{321} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{321}\\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321}\\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321}\\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321}\\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411}
\end{bmatrix}$$

$$C=\begin{bmatrix}
\mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33}\\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321}\\
\mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42}\\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321}\\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321}\\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411}\\
\mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42}\\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411}\\
\mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51}
\end{bmatrix}$$

$$D=\begin{bmatrix}
\mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222}\\
\mu_{33} & \mu_{42} & \mu_{321} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{321}\\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321}\\
\mu_{33} & \mu_{42} & \mu_{321} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{321}\\
\mu_{42} & \mu_{51} & \mu_{411} & \mu_{51} & \mu_{6} & \mu_{51} & \mu_{411} & \mu_{51} & \mu_{42}\\
\mu_{321} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{321} & \mu_{42} & \mu_{33}\\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321}\\
\mu_{321} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{321} & \mu_{42} & \mu_{33}\\
\mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42}
\end{bmatrix}$$

$$E = \begin{bmatrix} \mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} \\ \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} \\ \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411} \\ \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} \\ \mu_{321} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{321} & \mu_{42} & \mu_{33} \\ \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42} \\ \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411} \\ \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42} \\ \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{411} & \mu_{42} & \mu_{51} \end{bmatrix}$$

$$F = \begin{bmatrix} \mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} \\ \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411} \\ \mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51} \\ \mu_{321} & \mu_{222} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411} \\ \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{33} & \mu_{42} \\ \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{411} & \mu_{42} & \mu_{51} \\ \mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51} \\ \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{411} & \mu_{42} & \mu_{51} \\ \mu_{42} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} & \mu_{51} & \mu_{51} & \mu_{51} & \mu_{6} \end{bmatrix}$$

where the sixth moments are defined as follows,

$$\mu_6(\eta) = \int t_1{}^6 d\eta \quad , \quad \mu_{51}(\eta) = \int t_1^5 t_2 d\eta \quad , \quad \mu_{33}(\eta) = \int t_1^3 t_2^3 d\eta \quad , \quad \mu_{42}(\eta) = \int t_1^4 t_2^2 d\eta \quad ,$$

$$\mu_{411}(\eta) = \int t_1^4 t_2 t_3 d\eta \; , \; \mu_{321}(\eta) = \int t_1^3 t_2^2 t_3 d\eta \; , \; \mu_{222}(\eta) = \int t_1^2 t_2^2 t_3^2 d\eta$$

there are m elementary centroid designs η_j, for m factors, ,placing equal weights $\frac{1}{\binom{m}{j}}$

on the points having j out of their m components equal to $\frac{1}{j}$ and zeros elsewhere.

In a case of three factors, the weighted centroid design is given as,

$$\eta(\alpha)=\sum_{j=1}^{2}\alpha_j\eta_j=\alpha_1\eta_1+\alpha_2\eta_2;\alpha=(\alpha_1,\alpha_2,0,0)\in T_2,\alpha_1+\alpha_2=1 \qquad (47)$$

The sixth order moments are:

$$\mu_6(\eta_j)=\frac{1}{j^5m},$$

$$\mu_{51}(\eta_j)=\mu_{42}(\eta_j)=\mu_{33}(\eta_j)=\frac{j-1}{j^5m(m-1)},$$

$$\mu_{411}(\eta_j)=\mu_{321}(\eta_j)=\mu_{222}(\eta_j)=\frac{(j-1)(j-2)}{j^3m(m-1)(m-2)},$$ for j= (1, 2,…, m).

when m=3, the moments are:

$$\mu_6(\eta_1)=\frac{1}{3}, \quad \mu_{51}(\eta_1)=\mu_{42}(\eta_1)=\mu_{33}(\eta_1)=0, \quad \mu_{411}(\eta_1)=\mu_{321}(\eta_1)=\mu_{222}(\eta_1)=0,$$

$$\mu_6(\eta_2)=\frac{1}{96}, \mu_{51}(\eta_2)=\mu_{42}(\eta_2)=\mu_{33}(\eta_2)=\frac{1}{192} \text{ and } \mu_{411}(\eta_2)=\mu_{321}(\eta_2)=\mu_{222}(\eta_2)=0$$

for designs η_1 ,the moment matrices are given as,

$$M(n_1)=\begin{bmatrix} A_1 & B_1 & C_1 \\ B_1 & D_1 & E_1 \\ C_1 & E_1 & F_1 \end{bmatrix}$$

where,

$$A_1 = \frac{1}{3} e_{11} e_{11}' = \begin{bmatrix} \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$B_1 = 0_{9\times 9}$$

$$C_1 = 0_{9\times 9}$$

$$D_1 = \frac{1}{3} e_{22} e_{22}' = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$E_1 = 0_{9\times 9}$$

$$F_1 = \frac{1}{3} e_{33} e_{33}' = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \end{bmatrix}$$

for designs η_2,the moment matrices are given as,

$$M(n_2)=\begin{bmatrix} A_2 & B_2 & C_2 \\ B_2 & D_2 & E_2 \\ C_2 & E_2 & F_2 \end{bmatrix}$$

$$A_2=\begin{bmatrix} \frac{1}{96} & \frac{1}{192} & \frac{1}{192} & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} & 0 & 0 & 0 & 0 \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} & 0 & 0 & 0 & 0 \\ \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \end{bmatrix}$$

$$C_2=\begin{bmatrix} \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \end{bmatrix}$$

$$D_2 = \begin{bmatrix} \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} & 0 & 0 & 0 & 0 \\ \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} & 0 & 0 & 0 & 0 \\ \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{96} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \end{bmatrix}$$

$$E_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \end{bmatrix}$$

$$F_2 = \begin{bmatrix} \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & 0 & 0 & \frac{1}{192} & 0 & \frac{1}{192} \\ 0 & 0 & 0 & 0 & \frac{1}{192} & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} \\ \frac{1}{192} & 0 & \frac{1}{192} & 0 & \frac{1}{192} & \frac{1}{192} & \frac{1}{192} & \frac{1}{192} & \frac{1}{96} \end{bmatrix}$$

for the designs η_1 and η_2 ,the information matrix is obtained as follows,

$$L = (K'K)^{-1}K'$$

$$= \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1 \\ 0&1&0&1&1&0&0&0&0&1&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&1&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&1&0&0&0&0&1&1&0&1&0 \end{bmatrix}$$

…………………………….……………………….………………………………………... (48)

the information matrix for the design η_1 , is given by,

$$C_1 = LM(\eta_1)L' = \begin{bmatrix} \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} = C_K(M(n_1)) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (49)$$

while the information matrix for the design η_2 is given by,

$$C_2 = LM(n_2)L' = \begin{bmatrix} \frac{1}{96} & \frac{1}{192} & \frac{1}{192} & \frac{1}{32} & \frac{1}{32} & 0 \\ \frac{1}{192} & \frac{1}{96} & \frac{1}{192} & \frac{1}{32} & 0 & \frac{1}{32} \\ \frac{1}{192} & \frac{1}{192} & \frac{1}{96} & 0 & \frac{1}{32} & \frac{1}{32} \\ \frac{1}{32} & \frac{1}{32} & 0 & \frac{3}{16} & 0 & 0 \\ \frac{1}{32} & 0 & \frac{1}{32} & 0 & \frac{3}{16} & 0 \\ 0 & \frac{1}{32} & \frac{1}{32} & 0 & 0 & \frac{3}{16} \end{bmatrix} = C_k(M(n_2)) \ldots. (50)$$

finally, for the design $\eta(\alpha)$,the information matrix is then given as;

$$C_k(M(\eta(\alpha))) = \alpha_1 C_k(M(\eta_1)) + \alpha_2 C_k(M(\eta_2)).$$

replacing C_1 and C_2 yields,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 \\ \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 & 0 \\ \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 \\ 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & 0 & \frac{3\alpha_2}{16} \end{pmatrix}$$

……………………………………………………………………………………... (51)

This is the desired information matrix for three factors.

4.1.3 Optimal Moments And Information Matrices For M=4 Factors.

Table 4.3: Simplex Centroid Design For Four Factors

Design points	t_1	t_2	t_3	t_4
1	1	0	0	0
2	0	1	0	0
3	0	0	1	0
4	0	0	0	1
5	1/2	1/2	0	0
6	1/2	0	1/2	0
7	1/2	0	0	1/2

8	0	1/2	1/2	0
9	0	1/2	0	1/2
10	0	0	1/2	1/2
11	1/3	1/3	1/3	0
12	1/3	1/3	0	1/3
13	1/3	0	1/3	1/3
14	0	1/3	1/3	1/3
15	1/4	1/4	1/4	1/4

with the elementary centroid designs given as,

$$\eta_1 = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\} \quad , \quad \eta_2 = \left\{ \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \right\}$$

$$\eta_3 = \left\{ \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \\ 0 \end{pmatrix}, \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ 0 \\ \frac{1}{3} \end{pmatrix}, \begin{pmatrix} \frac{1}{3} \\ 0 \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix} \right\} \eta_4 = \left\{ \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} \right\}$$

Lemma 4.3

The coefficient matrix K, for m=4 factors is given as follows;

$K = (K_1, K_2)$

Proof,

for m=4

$K_1 = \sum_{i=1}^{4} e_{iii} e_i' = e_{111} e_1' + e_{222} e_2' + e_{333} e_3' + e_{444} e_4'$, and

$$K_2 = \frac{1}{6}\left\{ \sum_{\substack{i,j=1 \\ i \neq j}}^{4} \left(e_{iij} + e_{iji} + e_{jii} + e_{jji} + e_{jij} + e_{ijj} \right) \right\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (52)$$

$$= \frac{1}{6}\begin{Bmatrix} e_{112} + e_{121} + e_{211} + e_{212} + e_{122} + e_{221} \\ e_{113} + e_{131} + e_{311} + e_{331} + e_{313} + e_{133} \\ e_{114} + e_{141} + e_{411} + e_{441} + e_{414} + e_{144} \\ e_{223} + e_{232} + e_{322} + e_{332} + e_{323} + e_{233} \\ e_{224} + e_{242} + e_{422} + e_{442} + e_{424} + e_{244} \\ e_{334} + e_{343} + e_{433} + e_{443} + e_{434} + e_{344} \end{Bmatrix}$$ define, $e_{iij} = e_i \otimes e_i \otimes e_j$, i,j=1,2,3,4 ,

$e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, $e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, $e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ and $e_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Thus,

$$e_{111} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{112} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{113} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{114} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{121} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{122} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{123} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{124} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{131} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{132} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{133} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{134} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{141} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{142} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{143} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{144}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{211}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{212}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{213}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{214}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{221}=\begin{pmatrix}0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&&\end{pmatrix}',$$

$$e_{222}=\begin{pmatrix}0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&&\end{pmatrix}',$$

$$e_{223}=\begin{pmatrix}0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&&\end{pmatrix}',$$

$$e_{224}=\begin{pmatrix}0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&&\end{pmatrix}',$$

$$e_{231}=\begin{pmatrix}0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&&\end{pmatrix}',$$

$$e_{232} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{233} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{234} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{241} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{242} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{243} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{244} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{311} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{312} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{313} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{314}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{321}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{322}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{323}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{324}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{331} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{332} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{333} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{334} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{341} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{342} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{343} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{344} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{411} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{412} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{413} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{414} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{421} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{422} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{423} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & \end{pmatrix}',$$

$$e_{424} = \begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{431} = \begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{432} = \begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{433} = \begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&& \end{pmatrix}',$$

$$e_{434} = \begin{pmatrix} 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&& \end{pmatrix}',$$

$$e_{441} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{442} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}',$$

$$e_{443} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}',$$

$$e_{444} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}',$$

Therefore, substituting equation 52 gives the coefficient matrix as,

$$K = (K_1, K_2)$$

Theorem 4.3

For a mixture design $\eta(\alpha)$,the information matrix $C_k(M(\eta(\alpha)))$ with m=4 factors is given by,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 \\ \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 \\ \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} \\ \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & 0 & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} \\ \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 \\ 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 \\ 0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} \end{pmatrix}$$

Proof,

Consider the moment matrix for m=4 factors which is given by,

$$M(\eta(\alpha)) = \begin{bmatrix} P & Q & R & S \\ Q & T & U & V \\ R & U & W & X \\ S & V & X & Y \end{bmatrix} \qquad \text{..(53)}$$

$$Q=\begin{bmatrix}
\mu_{51} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} \\
\mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} \\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} \\
\mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} \\
\mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} \\
\mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} \\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} \\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} \\
\mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411}
\end{bmatrix}$$

where

$$P = \begin{bmatrix}
\mu_{6} & \mu_{51} & \mu_{51} & \mu_{51} & \mu_{51} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{42} \\
\mu_{51} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} \\
\mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} \\
\mu_{51} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{33} \\
\mu_{51} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} \\
\mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} \\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} \\
\mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} \\
\mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} \\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} \\
\mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} \\
\mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} \\
\mu_{51} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{33} \\
\mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{3111} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} \\
\mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} \\
\mu_{42} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{42}
\end{bmatrix}$$

$$R=\begin{pmatrix}
\mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} \\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} \\
\mu_{42} & \mu_{33} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} \\
\mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} \\
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} \\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} \\
\mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{2211} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} \\
\mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} \\
\mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} \\
\mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411}
\end{pmatrix}$$

$$S = \begin{bmatrix}
\mu_{51} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{33} \\
\mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} \\
\mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} \\
\mu_{42} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{42} \\
\mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} \\
\mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} \\
\mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} \\
\mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} \\
\mu_{42} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{42} \\
\mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} \\
\mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} \\
\mu_{33} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{51}
\end{bmatrix}$$

$$T = \begin{bmatrix}
\mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} \\
\mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} \\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} \\
\mu_{33} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} \\
\mu_{42} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{6} & \mu_{51} & \mu_{51} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} \\
\mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} \\
\mu_{321} & \mu_{411} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} & \mu_{2211} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} \\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} \\
\mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} \\
\mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} \\
\mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} \\
\mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} \\
\mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} \\
\mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42}
\end{bmatrix}$$

$$U = \begin{bmatrix}
\mu_{411} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} \\
\mu_{321} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{411} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} \\
\mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} \\
\mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} \\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} \\
\mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} \\
\mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411}
\end{bmatrix}$$

$$V=\begin{bmatrix}
\mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} \\
\mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} \\
\mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} \\
\mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} \\
\mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} \\
\mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} \\
\mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} \\
\mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} \\
\mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} \\
\mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51}
\end{bmatrix}$$

$$W = \begin{pmatrix}
\mu_{42} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} \\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} \\
\mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{42} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} \\
\mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} \\
\mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} \\
\mu_{222} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} \\
\mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} \\
\mu_{33} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{42} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} \\
\mu_{321} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} \\
\mu_{42} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{51} & \mu_{411} & \mu_{51} & \mu_{51} & \mu_{6} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{42} \\
\mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} \\
\mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} \\
\mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} \\
\mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42}
\end{pmatrix}$$

$$X = \begin{pmatrix}
\mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} \\
\mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} \\
\mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} \\
\mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} \\
\mu_{321} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} \\
\mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{222} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} \\
\mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} \\
\mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} \\
\mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} \\
\mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} \\
\mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} \\
\mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{51}
\end{pmatrix}$$

$$
Y = \begin{pmatrix}
\mu_{42} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{42} \\
\mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} \\
\mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} \\
\mu_{33} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{51} \\
\mu_{321} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} \\
\mu_{222} & \mu_{321} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{33} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} \\
\mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} \\
\mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51} \\
\mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} \\
\mu_{2211} & \mu_{2211} & \mu_{2211} & \mu_{3111} & \mu_{2211} & \mu_{321} & \mu_{222} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} \\
\mu_{222} & \mu_{2211} & \mu_{321} & \mu_{321} & \mu_{2211} & \mu_{222} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{33} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} \\
\mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{51} \\
\mu_{33} & \mu_{321} & \mu_{321} & \mu_{42} & \mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{51} \\
\mu_{321} & \mu_{321} & \mu_{3111} & \mu_{411} & \mu_{321} & \mu_{33} & \mu_{321} & \mu_{42} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51} \\
\mu_{321} & \mu_{3111} & \mu_{321} & \mu_{411} & \mu_{3111} & \mu_{321} & \mu_{321} & \mu_{411} & \mu_{321} & \mu_{321} & \mu_{33} & \mu_{42} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{51} \\
\mu_{42} & \mu_{411} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{42} & \mu_{411} & \mu_{51} & \mu_{411} & \mu_{411} & \mu_{42} & \mu_{51} & \mu_{51} & \mu_{51} & \mu_{51} & \mu_{6}
\end{pmatrix}
$$

where the sixth moments are defined as,

$$\mu_6(\eta)=\int t_1{}^6 d\eta \quad , \quad \mu_{33}(\eta)=\int t_1^3 t_2^3 d\eta \quad , \quad \mu_{42}(\eta)=\int t_1^4 t_2^2 d\eta \quad , \quad \mu_{411}(\eta)=\int t_1^4 t_2^1 t_3^1 d\eta,$$

$$\mu_{222}(\eta)=\int t_1^2 t_2^2 t_3^2 d\eta \quad , \quad \mu_{321}(\eta)=\int t_1^3 t_2^2 t_3^1 d\eta,\ \mu_{3111}(\eta)=\int t_1^2 t_2 t_3 t_{_2} d\eta,$$

$$\mu_{2211}(\eta)=\int t_1^2 t_2^2 t_3 t_{_2} d\eta.$$

there are m elementary centroid designs η_j for m factors ,placing equal weights $\frac{1}{\binom{m}{j}}$ on the points having j out of their m components equal to $\frac{1}{j}$ and zeros elsewhere.

for a case of four factors, the weighted centroid design is given as follows,

$$\eta(\alpha)=\sum_{j=1}^{2}\alpha_j\eta_j=\alpha_1\eta_1+\alpha_2\eta_2;\alpha=(\alpha_1,\alpha_2,0,0)\in T_2,\alpha_1+\alpha_2=1 \text{ .... } (54)$$

The sixth order moments are:

$$\mu_6(\eta_j)=\frac{1}{j^5 m}\ ,\mu_{51}(\eta_j)=\mu_{42}(\eta_j)=\mu_{33}(\eta_j)=\frac{j-1}{j^5 m(m-1)}\ ,$$

$$\mu_{411}(\eta_j)=\mu_{321}(\eta_j)=\mu_{222}(\eta_j)=\frac{(j-1)(j-2)}{j^5 m(m-1)(m-2)}$$

$$\mu_{2211}(\eta_j)=\mu_{3111}(\eta_j)=\frac{(j-1)(j-2)(j-3)}{j^5 m(m-1)(m-2)(m-3)}\text{, for j= (1, 2, …, m).}$$

for a case when m=4, these moments are given as:

for j=1

$\mu_6(\eta_1)=\frac{1}{4}$, $\mu_{51}(\eta_1)=\mu_{42}(\eta_1)=\mu_{33}(\eta_1)=0$, $\mu_{411}(\eta_1)=\mu_{321}(\eta_1)=\mu_{222}(\eta_1)=0$ and,

$\mu_{2211}(\eta_1)=\mu_{3111}(\eta_1)=0$

For j=2

$\mu_6(\eta_2)=\frac{1}{128}$, $\mu_{51}(\eta_2)=\mu_{42}(\eta_2)=\mu_{33}(\eta_2)=\frac{1}{384}$, $\mu_{411}(\eta_2)=\mu_{321}(\eta_2)=\mu_{222}(\eta_2)=0$

and,

$\mu_{2211}(\eta_2)=\mu_{3111}(\eta_2)=0$

For the designs η_1 and η_2 ,the moment matrices are:

$$M(\eta_1)=\begin{bmatrix} P' & Q' & R' & S' \\ Q' & T' & U' & V' \\ R' & U' & W' & X' \\ S' & V' & X' & Y' \end{bmatrix}$$

where, the entries are 16×16 block matrices

$P'=\frac{1}{4}e_{11}e'_{11}$, $Q'=0_{16\times16}$, $R'=0_{16\times16}$, $S'=0_{16\times16}$, $T'=\frac{1}{4}e_{22}e'_{22}$,

$U'=0_{16\times16}$, $V'=0_{16\times16}$, $W'=\frac{1}{4}e_{33}e'_{33}$, $X'=0_{16\times16}$, and $Y'=\frac{1}{4}e_{44}e'_{44}$

Similarly,

$$M(\eta_2)=\begin{bmatrix} P'' & Q'' & R'' & S'' \\ Q'' & T'' & U'' & V'' \\ R'' & U'' & W'' & X'' \\ S'' & V'' & X'' & Y'' \end{bmatrix}$$

where,

$$P'' = \begin{bmatrix}
\frac{1}{128} & \frac{1}{384} & \frac{1}{384} & \frac{1}{384} & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384} \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384} \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384}
\end{bmatrix}$$

$$Q' = \begin{bmatrix}
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

$$R'' = \begin{bmatrix}
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

$$S'' = \begin{bmatrix}
\frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384}
\end{bmatrix}$$

$$T'' = \begin{bmatrix}
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{128} & \frac{1}{384} & \frac{1}{384} & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384}
\end{bmatrix}$$

$$U'' = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

$$V'' = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384}
\end{bmatrix}$$

$$W'' = \begin{bmatrix}
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{384} & 0 & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & \frac{1}{384} & \frac{1}{384} & \frac{1}{128} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{384} & \frac{1}{384} & 0 & 0 & \frac{1}{384} & \frac{1}{384}
\end{bmatrix}$$

$$X''=\begin{bmatrix}
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{384}&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{384}&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{384}&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{384}&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}
\end{bmatrix}$$

$$Y''=\begin{bmatrix}
\frac{1}{384}&0&0&\frac{1}{384}&0&0&0&0&0&0&0&0&\frac{1}{384}&0&0&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
\frac{1}{384}&0&0&\frac{1}{384}&0&0&0&0&0&0&0&0&\frac{1}{384}&0&0&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&\frac{1}{384}&0&\frac{1}{384}&0&0&0&0&0&\frac{1}{384}&0&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&\frac{1}{384}&0&\frac{1}{384}&0&0&0&0&0&\frac{1}{384}&0&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{384}&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{384}&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}\\
\frac{1}{384}&0&0&\frac{1}{384}&0&0&0&0&0&0&0&0&\frac{1}{384}&0&0&\frac{1}{384}\\
0&0&0&0&0&\frac{1}{384}&0&\frac{1}{384}&0&0&0&0&0&\frac{1}{384}&0&\frac{1}{384}\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{384}&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}\\
\frac{1}{384}&0&0&\frac{1}{384}&0&\frac{1}{384}&0&\frac{1}{384}&0&0&\frac{1}{384}&\frac{1}{384}&\frac{1}{384}&\frac{1}{384}&\frac{1}{384}&\frac{1}{128}
\end{bmatrix}$$

for the designs η_1 and η_2, the information matrix is obtained as follows

$$L' = \left((K'K)K'\right)' = \left[A \quad B \quad C\right] \quad \text{..(55)}$$

the information matrix for the design η_1 is given by,

$$C_1 = LM(n_1)L' = \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} = C_k(M(n_1)) \text{...............(56)}$$

while the information matrix for the design η_2 is given by,

$$C_2 = C_k(M(\eta_2)) = LM(n_2)L' = \begin{pmatrix} \frac{1}{128} & \frac{1}{384} & \frac{1}{384} & \frac{1}{384} & \frac{1}{64} & \frac{1}{64} & \frac{1}{64} & 0 & 0 & 0 \\ \frac{}{384} & \frac{1}{128} & \frac{1}{384} & \frac{1}{384} & \frac{1}{64} & 0 & 0 & \frac{1}{64} & \frac{1}{64} & 0 \\ \frac{1}{384} & \frac{1}{384} & \frac{1}{128} & \frac{1}{384} & 0 & \frac{1}{64} & 0 & \frac{1}{64} & 0 & \frac{1}{64} \\ \frac{1}{384} & \frac{1}{384} & \frac{1}{384} & \frac{1}{128} & 0 & 0 & \frac{1}{64} & 0 & \frac{1}{64} & \frac{1}{64} \\ \frac{1}{64} & \frac{1}{64} & 0 & 0 & \frac{3}{32} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{64} & 0 & \frac{1}{64} & 0 & 0 & \frac{3}{32} & 0 & 0 & 0 & 0 \\ \frac{1}{64} & 0 & 0 & \frac{1}{64} & 0 & 0 & \frac{3}{32} & 0 & 0 & 0 \\ 0 & \frac{1}{64} & \frac{1}{64} & 0 & 0 & 0 & 0 & \frac{3}{32} & 0 & 0 \\ 0 & \frac{1}{64} & 0 & \frac{1}{64} & 0 & 0 & 0 & 0 & \frac{3}{32} & 0 \\ 0 & 0 & \frac{1}{64} & \frac{1}{64} & 0 & 0 & 0 & 0 & 0 & \frac{3}{32} \end{pmatrix}$$

……………………………………………………………………………… (57)

finally, for the design $\eta(\alpha)$, the information matrix is given as follows;

$$C_k(M(\eta(\alpha))) = \alpha_1 C_k(M(\eta_1)) + \alpha_2 C_k(M(\eta_2)).$$

replacing C_1 and C_2 yields,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix}
\frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 \\
\frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 \\
\frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} \\
\frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & 0 & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} \\
\frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 & 0 \\
\frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 \\
\frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 \\
0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 \\
0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 \\
0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32}
\end{pmatrix}$$

………………………………………………………………………………………. (58)

which is the desired information matrix for four factors.

4.1.4 Generalized Moments And Information Matrices For $m \geq 2$ Factors.

Theorem 4.4

For a mixture experiment, the information matrix for m factors is given by;

$$C_K = C(\alpha) = \alpha_1 C_1 + \alpha_2 C_2 = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{32m} U_1 + \frac{\alpha_2}{32m(m-1)} U_2 & \frac{3\alpha_2}{16m(m-1)} V \\ \frac{3\alpha_2}{16m(m-1)} V' & \frac{9\alpha_2}{8m(m-1)} I_{\binom{m}{2}} \end{pmatrix},$$

Proof,

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 + dV_2 \\ cV_1' + dV_2' & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \qquad (59)$$

With the coefficients $a, b, c, d, e, ..., g \in \Re$. The terms containing V_2, W_2, and W_3 only occur for $m \geq 3$ and also for $m \geq 4$, respectively.

For a given symmetric matrix $C \in sym(s)$, partitioning can be made according to the block structure of matrices , that is

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{12}' & C_{22} \end{pmatrix},$$

With $C_{11} \in sym(m)$, $C_{21} \in \Re^{\binom{m}{2} \times m}$ and $C_{22} \in sym\left(\binom{m}{2}\right)$.

and for j=1

$$C_{11,1} = \frac{1}{m} U_1 , \ C_{12,1} = 0 \text{ , and } C_{22,1} = 0$$

and for , U_1 ,U_2 and V_1 are as defined in lemma (3.1).

while for j=2

$$C_{11,2} = \frac{1}{32m} U_1 + \frac{1}{32m(m-1)} U_2 , \ C_{12,2} = \frac{3}{16m(m-1)} V \text{ and } C_{22,2} = \frac{9}{8m(m-1)} I_{\binom{m}{2}} ,$$

thus we have,

$$C_1 = \begin{pmatrix} \frac{1}{m} I_m & 0 \\ 0 & 0 \end{pmatrix} \qquad (60)$$

and,

$$C_2 = \begin{pmatrix} \frac{1}{32m} U_1 + \frac{1}{32m(m-1)} U_2 & \frac{3}{16m(m-1)} V \\ \frac{3}{16m(m-1)} V' & \frac{9}{8m(m-1)} I_{\binom{m}{2}} \end{pmatrix} \qquad (61)$$

finally, for the design $\eta(\alpha)$, the information matrix is then given as;

$$C_k(M(\eta(\alpha))) = \alpha_1 C_k(M(\eta_1)) + \alpha_2 C_k(M(\eta_2)) .$$

replacing C_1 and C_2 yields,

$$C_K = C(\alpha) = \alpha_1 C_1 + \alpha_2 C_2 = \begin{pmatrix} \frac{32\alpha_1 + \alpha_2}{32m} U_1 + \frac{\alpha_2}{32m(m-1)} U_2 & \frac{3\alpha_2}{16m(m-1)} V \\ \frac{3\alpha_2}{16m(m-1)} V' & \frac{9\alpha_2}{8m(m-1)} I_{\binom{m}{2}} \end{pmatrix} \ldots (62)$$

Which is the generalized information matrix C_k corresponding to the parameter subsystem of interest $K'\theta$. The information matrix C_k so obtained was used to generate unique optimal weighted centroid designs.

4.2 A-Optimal Weighted Centroid Design

For the average variance criterion, ϕ_{-1}, optimal weighted centroid designs was obtained. This criterion minimizes the average variances. The general equivalence theorem was adopted. The theorem provides the necessary and sufficient condition which is applicable to the specific problem.

4.2.1 A-Optimal Weighted Centroid Design For M=2 Factors.

Lemma 4.4

In third-degree Kronecker model for a mixture experiments with two factors, the unique A-optimal weighted centroid design for the $K'\theta$ is,

$$\eta\left(\alpha^{(A)}\right) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.603283327\eta_1 + 0.396716673\eta_2$$

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The maximum value of A-criterion for the $K'\theta$ in two factors is given by

$$V(\phi_{-1}) = 0.26558569S$$

Proof

The inverse of equation 43 is then given by;

$$C_k^{-1} = \begin{bmatrix} \frac{2}{\alpha_1} & 0 & \frac{-1}{3\alpha_1} \\ 0 & \frac{2}{\alpha_1} & \frac{-1}{3\alpha_1} \\ \frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} & \frac{16\alpha_1 + \alpha_2}{9\alpha_1\alpha_2} \end{bmatrix} \quad (63)$$

from $[C(M(\eta(\alpha)))]^{-2} = [C(m(\eta(\alpha)))^{-1}]^2 = [C(\alpha)]^{-2}$,

$$C_k^{-2} = \begin{bmatrix} \frac{37}{9\alpha_1^2} & \frac{1}{9\alpha_1^2} & -\frac{16\alpha_1 + 19\alpha_2}{27\alpha_1^2\alpha_2} \\ \frac{1}{9\alpha_1^2} & \frac{37}{9\alpha_1^2} & -\frac{16\alpha_1 + 19\alpha_2}{27\alpha_1^2\alpha_2} \\ -\frac{16\alpha_1 + 19\alpha_2}{27\alpha_1^2\alpha_2} & -\frac{16\alpha_1 + 19\alpha_2}{27\alpha_1^2\alpha_2} & \frac{256\alpha_1^2 + 32\alpha_1\alpha_2 + 19\alpha_2^2}{81\alpha_1^2\alpha_2^2} \end{bmatrix} \quad (64)$$

for j=1, the design is A-optimal if and only if,

$$traceC_1C_k(M(\eta(\alpha)))^{-2} = traceC_k(M(\eta(\alpha)))^{-1}$$

Thus,

$$C_1C_k^{-2} = \begin{bmatrix} \frac{37}{18\alpha_1^2} & \frac{1}{18\alpha_1^2} & -\frac{16\alpha_1+19\alpha_2}{54\alpha_1^2\alpha_2} \\ \frac{1}{18\alpha_1^2} & \frac{37}{18\alpha_1^2} & -\frac{16\alpha_1+19\alpha_2}{54\alpha_1^2\alpha_2} \\ 0 & 0 & 0 \end{bmatrix} \text{..}(65)$$

$$\text{trace}\, C_1C_k^{-2} = \frac{37}{18\alpha_1^2} + \frac{37}{18\alpha_1^2} + 0 = \frac{37}{9\alpha_1^2} \text{..}(66)$$

$$traceC_k^{-1} = \frac{2}{\alpha_1} + \frac{2}{\alpha_1} + \frac{16\alpha_1+\alpha_2}{9\alpha_1\alpha_2} = \frac{16\alpha_1+37\alpha_2}{9\alpha_1\alpha_2}$$

hence, $traceC_1C_k(M(\eta(\alpha)))^{-2} = traceC_k(M(\eta(\alpha)))^{-1}$

$$\Leftrightarrow \frac{37}{9\alpha_1^2} = \frac{16\alpha_1+37\alpha_2}{9\alpha_1\alpha_2},$$

which then reduces to,

$$21\alpha_1^2 - 74\alpha_1 + 37 = 0,$$

solving this polynomial with $\alpha_1 + \alpha_2 = 1$

yields $\alpha_1 = 0.603283327$ or $\alpha_1 = 2.920552619$6

take $\alpha_1 = 0.603283327$ since $\alpha_1 \in (0,1)$.

similarly, for j=2,

$$C_2C_k^{-2} = \begin{bmatrix} \frac{-1}{18\alpha_1\alpha_2} & \frac{-1}{18\alpha_1\alpha_2} & \frac{16\alpha_1+\alpha_2}{54\alpha_1\alpha_2} \\ \frac{-1}{18\alpha_1\alpha_2} & \frac{-1}{18\alpha_1\alpha_2} & \frac{16\alpha_1+\alpha_2}{54\alpha_1\alpha_2} \\ \frac{-1}{3\alpha_1\alpha_2} & \frac{-1}{3\alpha_1\alpha_2} & \frac{16\alpha_1+\alpha_2}{9\alpha_1\alpha_2^2} \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(67)$$

$$traceC_2C_k^{-2} = \frac{-1}{18\alpha_1\alpha_2} + \frac{-1}{18\alpha_1\alpha_2} + \frac{16\alpha_1+\alpha_2}{9\alpha_1\alpha_2^2} = \frac{16}{9\alpha_2^2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(68)$$

Therefore, $traceC_2C_k(M(\eta(\alpha)))^{-2} = traceC_k(M(\eta(\alpha)))^{-1}$

$\Leftrightarrow \frac{16}{9\alpha_2^2} = \frac{16\alpha_1+37\alpha_2}{9\alpha_1\alpha_2}$, and reduces to

$21\alpha_2^2 + 32\alpha_2 - 16 = 0$,

solving this polynomial with $\alpha_1 + \alpha_2 = 1$.

yields $\alpha_2 = 0.396716673 \text{ or } -1.92052619$

take $\alpha_2 = 0.396716673$ since $\alpha_2 \in (0,1)$.

therefore,

$\eta\left(\alpha^{(A)}\right) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.603283327\eta_1 + 0.396716673\eta_2$ is the unique A-optimal weighted centroid design for the $K'\theta$ in m=2 factors.

The average variance -criterion is then given by,

$v(\phi_{-1}) = \left(\frac{1}{s} * traceC(\alpha)^{-1}\right)^{-1}$, where's= $\binom{m+1}{2}$, s=3

for m=2,

$$\text{trace}\, C_k^{-1} = \frac{2}{\alpha_1} + \frac{2}{\alpha_1} + \frac{16\alpha_1 + \alpha_2}{9\alpha_1\alpha_2} = \frac{16\alpha_1 + 37\alpha_2}{9\alpha_1\alpha_2}$$

Thus, $v(\phi_{-1}) = \left(\frac{1}{3} * \frac{16\alpha_1 + 37\alpha_2}{9\alpha_1\alpha_2}\right)^{-1} = \left(\frac{11.29578892}{3}\right)^{-1} = 0.265585699$

The maximum value of the A-criterion for the $K'\theta$ in two factors is $V(\phi_{-1}) = 0.265585699$

4.2.2 A-Optimal Weighted Centroid Design For M=3 Factors

Lemma 4.5

In third-degree Kronecker model for the mixture experiments for the three factors, the unique A-optimal weighted centroid design for $K'\theta$ is,

$$n\left(\alpha^{(A)}\right) = \alpha_1 n_1 + \alpha_2 n_2 = 0.46502 n_1 + 0.53498 n_2$$

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The maximum value of the A-criterion for $K'\theta$ in three factors is

$V(\phi_{-1}) = 0.1192420$

Proof,

The inverse of equation 51 for m=3 factors is given as,

$$C_k^{-1} = \begin{bmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ c & c & d & e & d & d \\ c & d & c & d & e & d \\ d & c & c & d & d & e \end{bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(69)$$

where, $a = \frac{192}{64\alpha_1}$ $, b = \frac{-3\alpha_1}{\alpha_1(64\alpha_1 + \alpha_2)}$, $c = \frac{-32}{64\alpha_1 + \alpha_2}$ $, d = 0$ and

e= $\frac{16(64\alpha_1 + 3\alpha_2)}{3\alpha_2(64\alpha_1 + \alpha_2)}$

$[C(M(\eta(\alpha)))]^{-2} = [C(m(\eta(\alpha)))^{-1}]^2 = [C(\alpha)]^{-2}$, we get

$$C_k^{-2} = \begin{bmatrix} i & h & h & g & g & k \\ h & i & h & g & k & g \\ h & h & i & k & g & g \\ g & g & k & j & f & f \\ g & k & g & f & j & f \\ k & g & g & f & f & j \end{bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(70)$$

where;

$i = d^2 + 2c^2 + 2b^2 + a^2$, $h = 2cd + c^2 + b^2 + 2ab$

$g = ce + d^2 + cd + bd + bc + ac$

$k = de + 2cd + ad + 2bc$

$j = e^2 + 3d^2 + 2c^2$

$f = 2de + d^2 + 2cd + c^2$

the design is A-optimal, for j=1, if and only if

$trace C_1 C_k (M(\eta(\alpha)))^{-2} = trace C_k (M(\eta(\alpha)))^{-1}$.

Then,

$$C_1 C_k^{-2}$$

$$= \begin{bmatrix} i' & h' & h' & g' & g' & k' \\ h' & i' & h' & g' & k' & g' \\ h' & h' & i' & k' & g' & g' \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (71)$$

$$i' = \frac{d^2 + 2c^2 + 2b^2 + a^2}{3}, \quad h' = \frac{2cd + c^2 + b^2 + 2ab}{3},$$

$$g' = \frac{ce + d^2 + cd + bd + bc + ac}{3} \quad k' = \frac{de + 2cd + ad + 2bc}{3}$$

and trace $C_1 C_K^{-2}$

$$= (i' + i' + i' + 0 + 0 + 0) = \frac{a^2 + 2b^2 + 2c^2 + d^2}{3} + \frac{a^2 + 2b^2 + 2c^2 + d^2}{3} + \frac{a^2 + 2b^2 + 2c^2 + d^2}{3}$$

$$+ 0 + 0 + 0$$

$$= a^2 + 2b^2 + 2c^2 + d^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (72)$$

and $trace C_k^{-1} = a + a + a + e + e + e = 3(a + e)$

hence, $trace C_1 C_k (M(\eta(\alpha)))^{-2} = trace C_k (M(\eta(\alpha)))^{-1}$

$$\Leftrightarrow \left(\frac{192}{64\alpha_1}\right)^2 + 2\left(\frac{-3\alpha_2}{\alpha_1(64\alpha_1 + \alpha_2)}\right)^2 + 2\left(\frac{-32}{64\alpha_1 + \alpha_2}\right)^2 + 0 = 3\left(\frac{192}{64\alpha_1} + \frac{16(64\alpha_1 + 3\alpha_2)}{3\alpha_2(64\alpha_1 + \alpha_2)}\right)$$

which reduces to,

$$179928\alpha_1^5 + 544782\alpha_1^4 - 262890\alpha_1^3 - 13125\alpha^2{}_1 - 243\alpha_1 = 0$$

solving this polynomial with $\alpha_1 + \alpha_2 = 1$ for $\alpha_1 \in (0,1)$ yields

$$\alpha_1 = 0.46502 \text{ or } -3.44570$$

$$\alpha_1 = 0.46502$$

and also, for j=2,

$$C_2 C_k^{-2} = \begin{bmatrix} i'' & h'' & h'' & g'' & g'' & k'' \\ h'' & i'' & h'' & g'' & k'' & g'' \\ h'' & h'' & i'' & k'' & g'' & g'' \\ l'' & l'' & e'' & j'' & f'' & f'' \\ l'' & e'' & l'' & f'' & j'' & f'' \\ e'' & l'' & l'' & f'' & f'' & j'' \end{bmatrix} \qquad (73)$$

where,

$$i'' = \frac{1}{96}(a^2 + 3b^2 + 3c^2 + 2ab + 6ac + 6cb + 6ce + 7d^2 + 8cd + 6bd),$$

$$g'' = \frac{1}{192}\left(6e^2 + 27d^2 + 18c^2 + 12de + 17cd + ad + 5bc + 3ce + 3bd + 3ac\right),$$

$$k'' = \frac{1}{96}\left(15cb + ac + ec + 14de + 7d^2 + 15cd + 6c^2 + 3bc\right),$$

$$l'' = \frac{1}{32}\left(a^2 + 6ce + 7d^2 + 8cd + 6bd + 6bc + 8ac + 3c^2 + 3b^2\right),$$

$$j'' = \frac{1}{16}\left(3e^2 + 10d^2 + 6c^2 + ce + cd + bd + bc + ac\right)$$

$$e'' = \frac{1}{16}\left(3de + 8cd + 3ad + 6bc + c^2 + b^2 + 2ab\right)$$ and

$$f'' = \frac{1}{32}\left(12de + 7d^2 + 15cd + 6c^2 + ad + 3bc + ce + bd + ac\right)$$

$$traceC_k^{-1} = a + a + a + e + e + e = 3(a + e)$$

$$traceC_2C_k^{-2} = i'' + i'' + i'' + j'' + j'' + j'' = 3(i'' + j'')$$ or

$$\frac{1}{96}(a^2 + 3b^2 + 3c^2 + 2ab + 6ac + 6cb + 6ce + 7d^2 + 8cd + 6bd) +$$

$$\frac{1}{16}\left(3e^2 + 10d^2 + 6c^2 + ce + cd + bd + bc + ac\right))$$

$$traceC_2C_K^2 = \frac{1}{32}\left(a^2 + 18e^2 + 57d^2 + 40c^2 + 12ce + 14cd + 12bd + 12bc + 12ac + 3b^2 + 2ab\right)$$

therefore,

$$traceC_2C_k(M(\eta(\alpha)))^{-2} = traceC_k(M(\eta(\alpha)))^{-1}$$

$$\frac{1}{32}\left(a^2 + 18e^2 + 57d^2 + 40c^2 + 12ce + 14cd + 12bd + 12bc + 12ac + 3b^2 + 2ab\right) = 3(a + e)$$

$$\Leftrightarrow \left(\frac{192}{64\alpha_1}\right)^2 + 18\left(\frac{16(64\alpha_1 + 3\alpha_2)}{3\alpha_2(64\alpha_1 + \alpha_2)}\right)^2 + 57(0)^2 + 40\left(\frac{-32}{64\alpha_1 + \alpha_2}\right)^2 + 12\left(\frac{16(64\alpha_1 + 3\alpha_2)}{3\alpha_2(64\alpha_1 + \alpha_2)} * \left(\frac{-32}{64\alpha_1 + \alpha_2}\right)\right)$$

$$+12\left(\frac{192}{64\alpha_1} * 0\right) + 12\left(\frac{-32}{64\alpha_1 + \alpha_2} * \left(\frac{-3\alpha_2}{\alpha_1(64\alpha_1 + \alpha_2}\right)\right) + 12\left(\frac{192}{64\alpha_1} * \left(\frac{-32}{64\alpha_1 + \alpha_2}\right)\right) +$$

$$3\left(\frac{-3\alpha_2}{\alpha_1(64\alpha_1 + \alpha_2}\right)^2 +$$

$$2\left(\frac{192}{64\alpha_1} * \left(\frac{-3\alpha_2}{\alpha_1(64\alpha_1 + \alpha_2}\right)\right) = 32 * 3\left\{\frac{16(64\alpha_1 + 3\alpha_2}{3\alpha_2(64\alpha_1 + \alpha 2} + \frac{192}{64\alpha_1}\right\}$$

which reduces to,

$$-179928\alpha_2^5 + 1444422\alpha_2^4 - 3715518\alpha_2^3 + 4266177\alpha_2{}^2 - 2263605\alpha_2 + 448452 = 0$$

solving this polynomial with $\alpha_1 + \alpha_2 = 1$ yields

$$\alpha_2 = 0.53498 or 4.44570$$

$$\alpha_2 = 0.53498 \; \alpha_2 \in (0,1)$$

Therefore, $n\left(\alpha^{(A)}\right) = \alpha_1 n_1 + \alpha_2 n_2 = 0.46502 n_1 + 0.53498 n_2$

is the unique A-optimal weighted centroid design for the m=3 factors.

The average variance -criterion is then given by,

$v(\phi_{-1}) = \left(\frac{1}{s} * traceC(\alpha)^{-1}\right)^{-1}$, where $s = \binom{m+1}{2}$ and s=6

for m=3,

$$traceC_k^{-1} = \frac{9}{\alpha_1} + \frac{16(64\alpha_1 + 3\alpha_2)}{\alpha_2(64\alpha_1 + \alpha_2)}$$

implying that,

$$V(\phi_{-1}) = \left(\frac{1}{6} * \left(\frac{9}{0.46502} + \frac{16(64 * 0.46502 + 3 * 0.53498)}{0.53498(64 * 0.46502 + 0.53498)}\right)\right)^{-1} \quad = \quad \left(\frac{1}{6} * (50.31788)\right)^{-1}$$

=0.1192420. Therefore, the maximum value of the A-criterion for $K'\theta$ in m=3 factors is,

$V(\phi_{-1}) =$ 0.1192420.

4.2.3 A-Optimal Weighted Centroid Design For The M=4 Factors.

Lemma 4.6

In third-degree Kronecker model for the mixture experiments with four factors, unique A-optimal weighted centroid design for the $K'\theta$ is,

$$\eta\left(\alpha^{(A)}\right) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.44372\eta_1 + 0.55628\eta_2$$

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

maximum value of the A-criterion for $K'\theta$ in four factors is

$V(\phi_{-1}) = 0.06491356.$

Proof,

The inverse of equation 58 is given as,

$$C_k^{-1} = C_k(M(n(\alpha)))^{-1} = \begin{bmatrix} a'' & b'' & b'' & b'' & c'' & c'' & c'' & d'' & d'' & d'' \\ b'' & a'' & b'' & b'' & c'' & d'' & d'' & c'' & c'' & d'' \\ b'' & b'' & a'' & b'' & d'' & c'' & d'' & c'' & d'' & c'' \\ b'' & b'' & b'' & a'' & d'' & d'' & c'' & d'' & c'' & c'' \\ c'' & c'' & d'' & d'' & e'' & d'' & d'' & d'' & d'' & d'' \\ c'' & d'' & c'' & d'' & d'' & e'' & d'' & d'' & d'' & d'' \\ c'' & d'' & d'' & c'' & d'' & d'' & e'' & d'' & d'' & d'' \\ d'' & c'' & c'' & d'' & d'' & d'' & d'' & e'' & d'' & d'' \\ d'' & c'' & d'' & c'' & d'' & d'' & d'' & d'' & e'' & d'' \\ d'' & d'' & c'' & c'' & d'' & d'' & d'' & d'' & d'' & e'' \end{bmatrix}$$

…………………………………………………………………………………... (74)

where $a'' = \dfrac{4}{\alpha_1}$, $b'' = \dfrac{-4\alpha_2}{\alpha_1(48\alpha_1 + \alpha_2)}$, $c'' = \dfrac{-32}{48\alpha_1 + \alpha_2}$, $e'' = \dfrac{64(24\alpha_1 + \alpha_2)}{3\alpha_2(48\alpha_1 + \alpha_2)}$

and $d'' = 0$,from $[C(M(\eta(\alpha)))]^{-2} = [C(m(\eta(\alpha)))^{-1}]^2 = [C(\alpha)]^{-2}$, we get

$$C_k(M(n(\alpha)))^{-2} = \begin{bmatrix} i & h & h & h & g & g & g & k & k & k \\ h & i & h & h & g & k & k & g & g & k \\ h & h & i & h & k & g & k & g & k & g \\ h & h & h & i & k & k & g & k & g & g \\ g & g & k & k & j & l & l & l & l & m \\ g & k & g & k & l & j & l & l & m & l \\ g & k & k & g & l & l & j & m & l & l \\ k & g & g & k & l & l & m & j & l & l \\ k & g & k & g & l & m & l & l & j & l \\ k & k & g & g & m & l & l & l & l & j \end{bmatrix}$$ ………… (75)

where;

$i = 3d''^2 + 3c''^2 + 3b''^2 + a''^2$, j$= e''^2 + 7d''^2 + 2c^2$,

h$= d''^2 + 4cd + c''^2 + 2b''^2 + 2ab$, g$= c''e'' + 3d''^2 + 2c''d'' + 2b''d'' + b''c'' + a''c''$,

k= $d''e'' + 2d''^2 + 3c''d'' + b''d'' + a''d'' + 2b''c''$, l= $2de + 5d^2 + 2cd + c^2$,

$m = 2d''e'' + 4d''^2 + 4cd$

the design is A-optimal, for j=1, if and only if,

$traceC_1C_k(M(\eta(\alpha)))^{-2} = traceC_k(M(\eta(\alpha)))^{-1}$.

$$C_1C_k^{-2} = \begin{bmatrix} i' & h' & h' & h' & g' & g' & g' & k' & k' & k' \\ h' & i' & h' & h' & g' & k' & k' & g' & g' & k' \\ h' & h' & i' & h' & k' & g' & k' & g' & k' & g' \\ h' & h' & h' & i' & k' & k' & g' & k' & g' & g' \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad \text{.....................................(76)}$$

where,

$$i' = \frac{3d''^2 + 3c''^2 + 3b''^2 + a''^2}{4},\ h' = \frac{d''^2 + 4c''d'' + c''^2 + 2b''^2 + 2a''b''}{4},$$

$$g = \frac{c''e'' + 3d''^2 + 2c''d'' + 2b''d'' + b''c'' + a''c''}{4}$$

and $k' = \dfrac{d''e'' + 2d''^2 + 3c''d'' + b''d'' + a''d'' + 2b''c''}{4}$

$$traceC_1C_k^{-2} = 4\left(\frac{a''^2 + 3b''^2 + 3c''^2 + 3d''^2}{4}\right) = a''^2 + 3b''^2 + 3c''^2 + 3d''^2$$

$$= \left(\frac{4}{\alpha_1}\right)^2 + 3\left(\frac{-4\alpha_2}{\alpha_1(48\alpha_1 + \alpha_2)}\right) + 3\left(\frac{-32}{48\alpha_1 + \alpha_2}\right) + 3(0)^2$$

$$= \frac{48\alpha_2^2}{\alpha_1^2(48\alpha_1+\alpha_2)} + \frac{3072}{(48\alpha_1+\alpha_2)^2} + \frac{16}{\alpha_1^2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (77)$$

$$traceC_k^{-1} = 4a'' + 6e'' = 4\left(\frac{4}{\alpha_1}\right) + 6\left(\frac{64(24\alpha_1+\alpha_2)}{3\alpha_2(48\alpha_1+\alpha_2)}\right)$$

$$= \frac{128(\alpha_2+24\alpha_1)}{\alpha_2(\alpha_2+48\alpha_1)} + \frac{16}{\alpha_1}.$$

Therefore, $traceC_1C_k(M(\eta(\alpha)))^{-2} = traceC_k(M(\eta(\alpha)))^{-1}$

$$\Leftrightarrow \frac{48\alpha_2^2}{\alpha_1^2(48\alpha_1+\alpha_2)} + \frac{3072}{(48\alpha_1+\alpha_2)^2} + \frac{16}{\alpha_1^2} = \frac{128(\alpha_2+24\alpha_2)}{\alpha_2(\alpha_2+48\alpha_1)} + \frac{16}{\alpha_1}$$

this reduces to,

$$436160\alpha_1^5 + 2304640\alpha_1^4 - 1094592\alpha_1^3 - 976\alpha_1^2 - 2304\alpha_1 = 0$$

solving this equation with $\alpha_1 + \alpha_2 = 1$ yields

$$\alpha_1 = 0.44372 or 0 or -5.72245$$

$$\alpha_1 = 0.44372 \text{ for } \alpha_1 \in (0,1)$$

Similarly, for j=2

$$C_2 C_k^{-2} = \begin{bmatrix} i'' & h'' & h'' & h'' & g'' & g'' & g'' & k'' & k'' & k'' \\ h'' & i'' & h'' & h'' & g'' & k'' & k'' & g'' & g'' & k'' \\ h'' & h'' & i'' & h'' & k'' & g'' & k'' & g'' & k'' & g'' \\ h'' & h'' & h'' & i'' & k'' & k'' & g'' & k'' & g'' & g'' \\ n'' & n'' & p'' & p'' & j'' & l'' & l'' & l'' & l'' & m'' \\ n'' & p'' & n'' & p'' & l'' & j'' & l'' & l'' & m'' & l'' \\ n'' & p'' & p'' & n'' & l'' & l'' & j'' & m'' & l'' & l'' \\ p'' & n'' & n'' & p'' & l'' & l'' & m'' & j'' & l'' & l'' \\ p'' & n'' & p'' & n'' & l'' & m'' & l'' & l'' & j'' & l'' \\ p'' & p'' & n'' & n'' & m'' & l'' & l'' & l'' & l'' & j'' \end{bmatrix} \text{..............................(78)}$$

where,

$$i'' = \frac{1}{384}(66d''^2 + 10c''^2 + 11b''^2 + 3a''^2 + 40c''d'' + 2a''b'' + 18c''e'' + 36b''d'' + 18b''c'' + 18a''c''),$$

$$j'' = \frac{1}{32}\left(22d''^2 + 4c''d'' + 7c''^2 + 2b''^2 + 2a''b'' + 3e''^2\right),$$

$$h'' = \frac{1}{384}\left(a''^2 + 50d''^2 + 64c''d'' + 7c''^2 + 11b''^2 + 8a''b'' + 6c''e'' + 18b''d'' + 30b''c'' + 6a''c'' + 12d''e'' + 6a''d''\right),$$

$$g'' = \frac{1}{192}(2c''e'' + 44d'' + 13c''d'' + 5b''d'' + 4b''c'' + 2a''c'' + 2d''e'' + a''d'' + 3e''^2 + 9c''^2),$$

$$k'' = \frac{1}{192}\left(20d''e'' + 49d''^2 + 32c''d'' + 4b''d'' + 2a''d'' + 5b''c'' + c''e'' + a''c'' + 6c''^2\right),$$

$$n'' = \frac{1}{64}(a''^2 + 22d''^2 + 4c''^2 + 5b''^2 + 16c''d'' + 2a''b'' + 6c''e'' + 12b''d'' + 6b''c'' + 6a''c''),$$

$$p'' = \frac{1}{32}\left(7d''^2 + 13c''d'' + c''^2 + 2b''^2 + 2a''b'' + 3d''e'' + 3b''d'' + 3a''d'' + 6b''c''\right),$$

and

$$m'' = \frac{1}{64}\left(14d''e'' + 28d''^2 + 30c''d'' + 2b''d'' + a''d'' + 4b''c''\right)$$

$$traceC_2C_k^{-2} = 4i'' + 6j''$$

$$4(\frac{1}{384}(66d''^2 + 10c''^2 + 11b''^2 + 3a''^2 + 40c''d'' + 2a''b'' + 18c''e'' + 36b''d'' + 18b''c'' + 18a''c'')) +$$

$$6(\frac{1}{32}\left(22d''^2 + 4c''d'' + 7c''^2 + 2b''^2 + 2a''b'' + 3e''^2\right)),$$

$$= \frac{1}{16}\left\{\begin{array}{l}\frac{1067}{16}(d'')^2 + \frac{2026}{96}(c'')^2 + \frac{587}{96}(b'')^2 + \frac{1192}{96}(c''d'') + \frac{578}{96}(a''b'') + 6e''^2 + \frac{18}{96}(c''e'') + \frac{36}{96}(b''d'') \\ + \frac{18}{96}(b''c'') + \frac{18}{96}(a''c'')\end{array}\right\}$$

……………………………………………………………………………………… (79)

Therefore,

$$traceC_2C_k(M(\eta(\alpha)))^{-2} = traceC_k(M(\eta(\alpha)))^{-1}$$

$$\frac{1}{16}\left\{\begin{array}{l}\frac{1067}{16}(0)^2 + \frac{2026}{96}\left(\frac{-32}{48\alpha_1+\alpha_2}\right)^2 + \frac{587}{96}\left(\frac{-4\alpha_2}{\alpha_1(48\alpha_1+\alpha_2)}\right)^2 + \frac{1192}{96}\left(\frac{-32}{48\alpha_1+\alpha_2}*0\right) + \\ \frac{578}{96}\left(\frac{4}{\alpha_1}*\frac{-4\alpha_2}{\alpha_1(48\alpha_1+\alpha_2)}\right) + 6\left(\frac{64(24\alpha_1+\alpha_2)}{3\alpha_2(48\alpha_1+\alpha_2)}\right)^2 + \frac{18}{96}\left(\frac{-32}{48\alpha_1+\alpha_2}*\frac{64(24\alpha_1+\alpha_2)}{3\alpha_2(48\alpha_1+\alpha_2)}\right) + \\ \frac{36}{96}\left(\frac{-4\alpha_2}{\alpha_1(48\alpha_1+\alpha_2)}*0\right) + \frac{18}{96}\left(\frac{-4\alpha_2}{\alpha_1(48\alpha_1+\alpha_2)}*\frac{-32}{48\alpha_1+\alpha_2}\right) + \frac{18}{96}\left(\frac{4}{\alpha_1}*\frac{-32}{48\alpha_1+\alpha_2}\right)\end{array}\right\}$$

$$= \left\{4\left(\frac{4}{\alpha_1}\right) + 6\left(\frac{64(24\alpha_1+\alpha_2)}{3\alpha_2(48\alpha_1+\alpha_2)}\right)\right\}$$

which reduces to,

$$-436160\alpha_2^5 + 4485440\alpha_2^4 - 12485568\alpha_2^3 - 14904688\alpha_2^2 - 8111328\alpha_2 + 1642928 = 0,$$

solving this equation with $\alpha_1 + \alpha_2 = 1$ yields

$$\alpha_2 = 0.55628 or 1 or 6.72245$$

$\alpha_2 = 0.55628$ for $\alpha_2 \in (0,1)$.

Therefore, $\eta(\alpha^{(A)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.44372n_1 + 0.55628n_2$ is the A-optimal weighted centroid design that is unique for $K'\theta$ in m=4 factors.

The average variance -criterion is then given by,

$$v(\phi_{-1}) = \left(\frac{1}{s} * traceC(\alpha)^{-1}\right)^{-1}, \text{ where } s = \binom{m+1}{2}, \text{ s=10}$$

and $traceC_k^{-1} = 4a'' + 6e'' = 4\left(\frac{4}{\alpha_1}\right) + 6\left(\frac{64(24\alpha_1 + \alpha_2)}{3\alpha_2(48\alpha_1 + \alpha_2)}\right)$

$$= \frac{128(\alpha_2 + 24\alpha_1)}{\alpha_2(\alpha_2 + 48\alpha_1)} + \frac{16}{\alpha_1}.$$

Implying that, $V(\phi_{-1}) = \left(\frac{1}{10} * \left(\frac{128(0.55628 + 24*0.44372)}{0.55628(0.55628 + 48*0.44372} + \frac{16}{0.44372}\right)\right)^{-1}$ =

$$\left(\frac{1}{10} * (154.051)\right)^{-1}$$

$$= (15.4051)^{-1}$$

=0.06491356

Therefore, for the A-criterion ,the maximum value for the $K'\theta$ in m=4 factors is

$V(\phi_{-1}) = 0.0649136.$

4.2.4 Generalized A-Optimal Weighted Centroid Design For $m \geq 2$ Factors

Theorem 4.6

In third-degree Kronecker model for the mixture experiments with $m \geq 2$ factors, unique A-optimal design for the $K'\theta$ is given by;

$\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2$.

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid* ,with α_1 the solution of $a\alpha_1^4 + b\alpha_1^3 + c\alpha_1^2 + d\alpha_1 + e = 0$ and α_2 the solution of $a'\alpha_2^5 + b'\alpha_2^4 + c'\alpha_2^3 + d'\alpha_2{}^2 + e'\alpha_2 + f' = 0$, so that $\alpha_1 + \alpha_2 = 1$ and $\alpha_1, \alpha_2 \in (0,1)$

The A-criterion maximum value for $K'\theta$ in m factors is,

$$v(\phi_{-1}) = \left(\frac{1}{s} traceC(\alpha)^{-1}\right)^{-1}$$

$$= \left\{ \frac{2}{m(m+1)} \left(\frac{32m^2(m-1)\alpha_1 + m^2(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} + \frac{(8m^4 - 16m^3 + 8m^2)(32(m-1)\alpha_1 + m\alpha_2)}{18\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} \right) \right\}^{-1}.$$

Proof

Supposing that ,$\eta(\alpha)$ is A-optimal for $K'\theta$ in T,also, let $\alpha = (\alpha_1, \alpha_2, 0, ..., 0)' \in T_m$ be a weight vector with $\partial(\alpha) = \{1,2\}$ .and let $C(\alpha) = C_k(M(\eta(\alpha)))$.The weighted centroid design $\eta(\alpha)$ is A-optimal for $K'\theta$ if and only if,

$$trace(C_j C(\alpha)^{-2}) \begin{cases} = trace(C(\alpha)^{-1}) & for \quad j \in \{1,2\}, \\ < trace(C(\alpha)^{-1}) & otherwise \end{cases} \qquad \text{.....................................(80)}$$

A unique representation of a matrix $C \in sym(s, H)$ is given as,

$$C=\begin{pmatrix} aI_m+bU_2 & cV_1+dV_2 \\ cV_1'+dV_2' & eI_{\binom{m}{2}}+fW_2+gW_3 \end{pmatrix} \qquad (81)$$

with the coefficients $a,b,c........,g\in\Re$. The terms that contain V_2, W_2 and W_3 only occur for $m\geq 3$ and for $m\geq 4$, respectively.

$trace\left(I_{\binom{m}{2}}\right)=\frac{m(m-1)}{2}$ and trace (W_2)=0, $trace(I_m)=m$, Also $trace(I_s)=\frac{m(m+1)}{2}$

The cubic property of $C(\alpha)\in Sym(s,H)$ allows us to determine $C(\alpha)^{-1}$ through solving the system of linear equation $C(\alpha)X=I_{\binom{m+1}{2}}$. This result in

$$C(\alpha)^{-1}=\begin{pmatrix} \frac{32m(m-1)\alpha_1+m(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1+(m-2)\alpha_2]}U_1- \\ \frac{(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1+(m-2)\alpha_2]}U_2 & -\frac{16m(m-1)}{3(32(m-1)\alpha_{11}+(m-2)\alpha_2}V \\ -\frac{16m(m-1)}{3(32(m-1)\alpha+(m-2)\alpha_2)}V' & \frac{(8m^2-8m)(32(m-1)\alpha_1+m\alpha_2)}{9\alpha_2(32m(m-1)\alpha_1+(m-2)\alpha_2)}I_{\binom{m}{2}} \end{pmatrix}$$

………………………………………………………………………………(82)

now obtain $C(\alpha)^{-2}$ as follows,

$$C(\alpha)^{-2}=[C(\alpha)^{-1}]^2=\begin{pmatrix} jI_m+kU_2 & lV \\ lV' & nI_{\binom{m}{2}} \end{pmatrix} \qquad (83)$$

where,

$$j=\frac{9472m^2(m^2-2m+1)\alpha_1^2+576m^2(m^2-3m+2)\alpha_1\alpha_2+9m^3(m^2-4m+4)\alpha_2^2}{9\alpha_1^2[32(m-1)\alpha_1+(m-2)\alpha_2]^2},$$

$$k = \frac{128m^2(m^2-2m+1)\alpha_1^2 + 576m^2(m^2-3m+2)\alpha_1\alpha_2 + 9m^3(m^2-4m+4)\alpha_2^2}{9\alpha_1^2[32(m-1)\alpha_1 + (m-2)\alpha_2]^2},$$

$$l = -\frac{256m^2(37m^2-74m+1)\alpha_1^2 + 576m^2(m^2-3m+2)\alpha_1\alpha_2 + 9m^2(m^3-4m^2+4m-8)\alpha_2^2}{9\alpha_1^2\left[32(m-1)\alpha_1 + (m-2)\alpha_2\right]^2}$$

and

$$n = \frac{1024m^2(m^4-2m^3+5m^2-4m+1)\alpha_1^2 + 64m^3(m^3-3m^2+3m-1)\alpha_1\alpha_2 + m^2(37m^2-72m+36+2m^3)\alpha_2^2}{81\alpha_2^2[32(m-1)\alpha_1 + (m-2)\alpha_2]^2}.$$

now compute $\alpha_1, \alpha_2 \in [0,1]$ as follows.

for $j = 1$, $traceC_1C(\alpha)^{-2} = traceC(\alpha)^{-1}$.

now from equations (60) and (83) we get

$$C_1C(\alpha)^{-2} = \begin{pmatrix} \frac{j}{m}U_1 + \frac{k}{m}U_2 & \frac{l}{m}V \\ 0 & 0 \end{pmatrix} \quad \text{.. (84)}$$

j, k and l are as in equation (83).

hence,

$traceC_1C(\alpha)^{-2} = trace\left(\frac{j}{m}U_1 + \frac{k}{m}U_2\right) = trace\left(\frac{j}{m}U_1\right) + trace\left(\frac{k}{m}U_2\right) = trace\left(\frac{j}{m}U_1\right)$, but $trace\left(\frac{j}{m}U_2\right) = 0$ and $trace(U_2) = 0$ gives,

$$traceC_1C(\alpha)^{-2} = \frac{9472m^2(m^2-2m+1)\alpha_1^2 + 576m^2(m^2-3m+2)\alpha_1\alpha_2 + 9m^3(m^2-4m+4)\alpha_2^2}{9\alpha_1^2[32(m-1)\alpha_1 + (m-2)\alpha_2]^2},$$

.... (85)

from equation (82)

$$traceC(\alpha)^{-1} = trace\left(\frac{32m(m-1)\alpha_1 + m(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}U_1 - \frac{(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}U_2 + \frac{(8m^2-8m)(32(m-1)\alpha_1 + m\alpha_2)}{9\alpha_2(32m(m-1)\alpha_1 + (m-2)\alpha_2)}\frac{V'V}{m}\right)$$

$$= \left(\frac{32m^2(m-1)\alpha_1 + m^2(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} + \frac{(8m^2-8m)(32(m-1)\alpha_1 + m\alpha_2)}{9\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} * \left(\frac{m(m-1)}{2}\right)\right)$$

……..……………………………………………………………………….…… (86)

but $trace(U_2) = 0$.Therefore, $traceC_1C(\alpha)^{-2} = traceC(\alpha)^{-1}$,

$$\Leftrightarrow \frac{9472m^2(m^2-2m+1)\alpha_1^2 + 576m^2(m^2-3m+2)\alpha_1\alpha_2 + 9m^3(m^2-4m+4)\alpha_2^2}{9\alpha_1^2[32(m-1)\alpha_1 + (m-2)\alpha_2]^2}$$

$$trace\left(I_{\binom{m}{2}}\right) = \frac{m(m-1)}{2}$$

$$= \left(\frac{32m^2(m-1)\alpha_1 + m^2(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} + \frac{(8m^2-8m)(32(m-1)\alpha_1 + m\alpha_2)}{9\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} I_{\binom{m}{2}}\right),$$

upon inserting the simplex restriction $\alpha_1 + \alpha_2 = 1$, it reduces to

$$a\alpha_1^4 + b\alpha_1^3 + c\alpha_1^2 + d\alpha_1 + e = 0 \text{..} (87)$$

where,

$$a = (-186m^4 + 7930m^3 + 436m^2 - 7680m),$$

$$b = (9m^5 + 16418m^4 - 31793m^3 + 8076m^2 - 512m),$$

$$c = (-27m^5 - 7689m^4 + 15620m^3 - 6140m^2),$$

$d = (27m^5 + 9m^4 + 27m^3 - 1116m^2 - 3701m)$, and

$e = (-9m^5 + 36m^4 - 36m^3)$

when polynomial (87) is solved, it yields values of α_1 where we pick α_1 in that $\alpha_1 \in (0,1)$ .Also, for j=2, equation (61) and (83) gives the following,

$$C_2C(\alpha)^{-2} = \begin{pmatrix} j'I_m + k'U_2 & l'V \\ l'V' & n'I_{\binom{m}{2}} \end{pmatrix} \text{..}(88)$$

where, $j' = \left(\frac{j}{32m} + \frac{(m-1)k}{32m(m-1)} + \frac{3l}{16m(m-1)} \right)$,

$k' = \left(\frac{k}{32m} + \frac{j}{32m(m-1)} + \frac{(m-2)k}{32m(m-1)} + \frac{3l}{16m(m-1)} \right)$,

$l' = \left(\frac{l}{32m} + \frac{(m-1)l}{32m(m-1)} + \frac{3n}{16m(m-1)} \right)$ and $n' = \left(\frac{3ml}{16m(m-1)} + \frac{9n}{8} \right)$,

$j, k,$ and l are as in equation (83).but,

$trace(U_2) = 0$

$$traceC_2C(\alpha)^{-2} = trace\left(j'U_1 + k'U_2\right) + trace\left(n'\frac{V'V}{m}\right) = trace\left(j'U_1\right) + trace\left(n'I_{\binom{m}{2}}\right)$$

$$traceC_2C(\alpha)^{-2} = m\left(\frac{j}{32m} + \frac{(m-1)k}{32m(m-1)} + \frac{3l}{16m(m-1)} \right) + \left(\frac{m(m-1)}{2} \right)\left(\frac{3ml}{16m(m-1)} + \frac{9n}{8} \right)$$

$$= \frac{9472m^2(m^2-2m+1)\alpha_1^2 + 576m^2(m^2-3m+2)\alpha_1\alpha_2 + 9m^3(m^2-4m+4)\alpha_2^2}{32 \times 9\alpha_1^2[32(m-1)\alpha_1 + (m-2)\alpha_2]^2}$$

$$+ \frac{1}{32} \times \frac{128m^2(m^2-2m+1)\alpha_1^2 + 576m^2(m^2-3m+2)\alpha_1\alpha_2 + 9m^3(m^2-4m+4)\alpha_2^2}{9\alpha_1^2[32(m-1)\alpha_1 + (m-2)\alpha_2]^2},$$

$$-\frac{768m^2(37m^2-74m+1)\alpha_1^2+1728m^2(m^2-3m+2)\alpha_1\alpha_2+27m^2(m^3-4m^2+4m-8)\alpha_2^2}{9\times16\alpha_1^2\left[32(m-1)\alpha_1+(m-2)\alpha_2\right]^2}$$

$$+\frac{9}{16}\times\frac{1024m^2(m^4-2m^3+5m^2-4m+1)\alpha_1^2+64m^3(m^3-3m^2+3m-1)\alpha_1\alpha_2+m^2(37m^2-72m+36+2m^3)\alpha_2^2}{81\alpha_2^2[32(m-1)\alpha_1+(m-2)\alpha_2]^2}.$$

$$-\frac{3}{16}\times\frac{256m^2(37m^2-74m+1)\alpha_1^2+576m^2(m^2-3m+2)\alpha_1\alpha_2+9m^2(m^3-4m^2+4m-8)\alpha_2^2}{9\alpha_1^2\left[32(m-1)\alpha_1+(m-2)\alpha_2\right]^2}$$

………………………………………………………………………………… (89)

therefore,

$$traceC_2C(\alpha)^{-2}=traceC(\alpha)^{-1}$$

$$\frac{9472m^2(m^2-2m+1)\alpha_1^2+576m^2(m^2-3m+2)\alpha_1\alpha_2+9m^3(m^2-4m+4)\alpha_2^2}{32\times9\alpha_1^2[32(m-1)\alpha_1+(m-2)\alpha_2]^2}$$

$$+\frac{1}{32}\times\frac{128m^2(m^2-2m+1)\alpha_1^2+576m^2(m^2-3m+2)\alpha_1\alpha_2+9m^3(m^2-4m+4)\alpha_2^2}{9\alpha_1^2[32(m-1)\alpha_1+(m-2)\alpha_2]^2}$$

$$-\frac{768m^2(37m^2-74m+1)\alpha_1^2+1728m^2(m^2-3m+2)\alpha_1\alpha_2+27m^2(m^3-4m^2+4m-8)\alpha_2^2}{9\times16\alpha_1^2\left[32(m-1)\alpha_1+(m-2)\alpha_2\right]^2}$$

$$-\frac{3}{16}\times\frac{256m^2(37m^2-74m+1)\alpha_1^2+576m^2(m^2-3m+2)\alpha_1\alpha_2+9m^2(m^3-4m^2+4m-8)\alpha_2^2}{9\alpha_1^2\left[32(m-1)\alpha_1+(m-2)\alpha_2\right]^2}$$

$$+\frac{9}{16}\times\frac{1024m^2(m^4-2m^3+5m^2-4m+1)\alpha_1^2+64m^3(m^3-3m^2+3m-1)\alpha_1\alpha_2+m^2(37m^2-72m+36+2m^3)\alpha_2^2}{81\alpha_2^2[32(m-1)\alpha_1+(m-2)\alpha_2]^2}.$$

$$=\left(\frac{32m^2(m-1)\alpha_1+m^2(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1+(m-2)\alpha_2]}+\frac{(8m^2-8m)(32(m-1)\alpha_1+m\alpha_2)}{9\alpha_2(32(m-1)\alpha_1+(m-2)\alpha_2)}*\frac{m(m-1)}{2}\right)$$

upon inserting the simplex restriction $\alpha_1+\alpha_2=1$, it reduces to,

$$a'\alpha_2^5 + b'\alpha_2^4 + c'\alpha_2^3 + d'\alpha_2^{\;2} + e'\alpha_2 + f' = 0 \qquad (90)$$

where, $a' = (186m^4 - 7930m^3 - 436m^2 + 7680m)$,

$b' = (9m^5 + 15488m^4 + 7851m^3 + 10256m^2 - 38912m)$,

$c' = (-9m^5 - 56123m^4 + 32252m^3 - 30524m^2 + 78848m)$,

$d' = (73590m^4 - 64571m^3 + 33280m^2 - 83572m)$,

$e' = (-41729m^4 + 40644m^3 - 13832m^2 + 47848m)$ and

$f' = (8588m^4 - 8252m^3 + 1256m^2 - 11892m)$

Hence, solving the polynomial (90) gives values of α_2 from where we choose α_2 so that, $\alpha_2 \in (0,1)$. Which is the unique solution in (0, 1) for the *m* factors, as weight vector. The two equations in conditions (86) and (89) is satisfied through the construction of the weight vector $\alpha^{(A)} = (\alpha_1^{(A)}, \alpha_2^{(A)}, 0, \ldots, 0)'$.

hence, $\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2$ is the A-optimal for the $K'\theta$ in T.

Therefore adopt the definition of Average-variance criterion $v(\phi_{-1}) = \left(\frac{1}{s} traceC(\alpha)^{-1}\right)^{-1}$, where $s = \binom{m+1}{2}$ to obtain the optimal value for m factors, as provided in Pukelsheim (1993). Since trace (W_2) =0 , $trace(I_m) = m$,

$trace(I_s) = \frac{m(m+1)}{2}$, Hence, $v(\phi_{-1}) = \left(\frac{1}{\binom{m+1}{2}} traceC(\alpha)^{-1}\right)^{-1}$ for *m*-factors, from equation (86),

$$traceC(\alpha)^{-1} = \left(\frac{32m^2(m-1)\alpha_1 + m^2(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} + \quad \frac{(8m^2 - 8m)(32(m-1)\alpha_1 + m\alpha_2)}{9\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} I_{\binom{m}{2}} \right)$$

$$trace\left(I_{\binom{m}{2}} \right) = \frac{m(m-1)}{2}, trace(I_m) = m,$$

implying,

$$v(\phi_{-1}) = \left(\frac{1}{s} traceC(\alpha)^{-1} \right)^{-1}$$

$$= \left\{ \frac{2}{m(m+1)} \left(\frac{32m^2(m-1)\alpha_1 + m^2(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} + \frac{(8m^4 - 16m^3 + 8m^2)(32(m-1)\alpha_1 + m\alpha_2)}{18\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} \right) \right\}^{-1}.$$

The actual value is then obtained by substituting the values of α_1 and α_2 from the solutions of equations (87) and (90).

4.3 D-optimal Weighted Centroid Designs

For the determinant criterion ϕ_0, optimal weighted centroid designs is derived, that is the , D-optimality criteria. The D- criterion has an important property in optimal designs because it minimizes the variance and the covariance of the parameters estimates.

4.3.1 D-Optimal Weighted Centroid Design For M=2 Factors

Lemma 4.7

In third-degree Kronecker model for the mixture experiments with the two factors, the unique D-optimal design for the $K'\theta$ is,

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2.$$

Where, n_1 $is\ the\ vertex\ design\ point\ \ and\ n_2\ is\ the\ overall\ centroid$

The D-criterion maximum value for the $K'\theta$ in two factors is, $v(\phi_0) = 0.275160602$

Proof,

For $p=0$, $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if the $traceC_j C(\alpha)^{-1} = traceC(\alpha)^0 = traceI \ for\ all\ j \in \{1,2\}$.

$$C_1 C_k^{-1} = \begin{pmatrix} \frac{1}{\alpha_1} & 0 & \frac{-1}{6\alpha_1} \\ 0 & \frac{1}{\alpha_1} & \frac{-1}{6\alpha_1} \\ 0 & 0 & 0 \end{pmatrix} \quad \text{..........} \quad (91)$$

with,

$$traceC_1 C(\alpha)^{-1} = \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + 0 = \frac{2}{\alpha_1} \quad \text{..........} \quad (92)$$

and $traceC_k^0 = traceI_3 = 3$,

$traceC_1 C(\alpha)^{-1} = traceI_3 \Leftrightarrow \frac{2}{\alpha_1} = 3 \Rightarrow \alpha_1 = \frac{2}{3}$ .and

$$C_2C_k^{-1} = \begin{pmatrix} 0 & 0 & \frac{1}{6\alpha_2} \\ 0 & 0 & \frac{1}{6\alpha_2} \\ 0 & 0 & \frac{1}{\alpha_2} \end{pmatrix} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(93)$$

$$traceC_2C(\alpha)^{-1} = 0 + 0 + \frac{1}{\alpha_2} = \frac{1}{\alpha_2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(94)$$

$$traceC_2C(\alpha)^{-1} = traceI_3 \Leftrightarrow \frac{1}{\alpha_2} = 3 \Rightarrow \alpha_2 = \frac{1}{3}.$$

Therefore, D-optimal weighted centroid design is the unique for the $K'\theta$ in two factors is $\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{2}{3}\eta_1 + \frac{1}{3}\eta_2$

the D-criterion maximum value is then obtained as,

$v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{s}}$, and , $s = \begin{pmatrix} m+1 \\ 2 \end{pmatrix}$,given that $m = 2$, then, $v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{3}}$.

for the design with two factors, the information matrix is given as below,

$$C_k = C_k(M(n(\alpha))) = \begin{bmatrix} \frac{32\alpha_1 + \alpha_2}{64} & \frac{\alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{\alpha_2}{64} & \frac{32\alpha_1 + \alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{3\alpha_2}{32} & \frac{3\alpha_2}{32} & \frac{9\alpha_2}{16} \end{bmatrix}.$$

by substituting for the values of α_1 and α_2,

$$C(\alpha) = \begin{pmatrix} 0.338541666 & 0.005208333 & 0.031250000 \\ 0.005208333 & 0.338541666 & 0.031250000 \\ 0.031250000 & 0.031250000 & 0.187500000 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ (95)$$

$Det[C_k] = 0.020833333$.

Hence, the optimal value for $K'\theta$ in two factors is $v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{3}} = \left(0.020833333\right)^{\frac{1}{3}} = 0.275160602$.

4.3.2 D-Optimal Weighted Centroid Design For M=3 Factors.

Lemma 4.8

In the third-degree Kronecker model for the mixture experiments with three factors ,D-optimal design is unique for $K'\theta$ is,

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 .$$

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The D-criterion maximum value for the $K'\theta$ in three factors is

$$v(\phi_0) = 0.125$$

Proof,

For $p = 0$, $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if

$$traceC_j C(\alpha)^{-1} = traceC(\alpha)^0 = traceI \ \ for\ all\ \ j \in \{1,2\} .$$

Thus,

$$C_1C_k^{-1} = \begin{pmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ c & c & d & e & d & d \\ c & d & c & d & e & d \\ d & c & c & d & d & e \end{pmatrix} \qquad (96)$$

where:

$$a = \frac{1}{\alpha_1}, \quad b = \frac{-\alpha_2}{\alpha_1(64\alpha_1+\alpha_2)}, \quad c = \frac{-32}{3(64\alpha_1+\alpha_2)}, \text{ d=0 , e=0}$$

$$traceC_1C(\alpha)^{-1} = \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + 0 + 0 + 0 = \frac{3}{\alpha_1}$$

and $traceC_k^0 = traceI_6 = 6$.

Thus, $traceC_1C(\alpha)^{-1} = traceI_4 \Leftrightarrow \frac{3}{\alpha_1} = 6, \ \alpha_1 = \frac{1}{2}$ ……………………………(97)

similarly,

$$C_2C_k^{-1} = \begin{pmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ e & e & f & g & h & h \\ e & f & e & h & g & h \\ f & e & e & h & h & g \end{pmatrix} \qquad (98)$$

where,

$$a = 0, b = \frac{-\alpha_2}{32\alpha_1(64\alpha_1+\alpha_2)}, c = \frac{32\alpha_1}{3\alpha_2(64\alpha_1+\alpha_2)}, d = \frac{-1}{3(64\alpha_1+\alpha_2)}, e = 0,$$

$$f = \frac{-3\alpha_2}{16\alpha_1(64\alpha_1+\alpha_2)}, g = \frac{1}{\alpha_2}, h = \frac{-1}{64\alpha_1+\alpha_2}$$

Thus,

$$trace C_2 C(\alpha)^{-1} = 0+0+0+\frac{1}{\alpha_2}+\frac{1}{\alpha_2}+\frac{1}{\alpha_2}=\frac{3}{\alpha_2}$$

$$trace C_2 C(\alpha)^{-1} = trace I_6 = 6 \quad ,$$

$$\frac{3}{\alpha_2} = 6$$

$$\alpha_2 = \frac{1}{2} \quad \text{...(99)}$$

Therefore, D-optimal weighted centroid design is unique for $K'\theta$ in m=3 factors is $\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{1}{2}\eta_1 + \frac{1}{2}\eta_2$ as required.

the D-criterion maximum value is then obtained as follows,

$v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{s}}$, where $s = \binom{m+1}{2}$.

For $m=3$, $v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{6}}$.

for a design with three factors, the information matrix is given as below,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 \\ \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 & 0 \\ \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 \\ 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & 0 & \frac{3\alpha_2}{16} \end{pmatrix}$$

…………………………………………………………………………………… (100)

substituting for the values of α_1 and α_2 we get

$$C_\alpha = \begin{bmatrix} 0.34375 & 0.00260 & 0.00260 & 0.01563 & 0.01563 & 0 \\ 0.00260 & 0.34375 & 0.002604167 & 0.015625000 & 0 & 0.015625000 \\ 0.002604167 & 0.002604167 & 0.34375 & 0 & 0.01525000 & 0.015625000 \\ 0.015625000 & 0.015625000 & 0 & 0.10938 & 0 & 0 \\ 0.015625000 & 0 & 0.015625000 & 0 & 0.10938 & 0 \\ 0 & 0.015625000 & 0.015625000 & 0 & 0 & 0.10938 \end{bmatrix}$$

…………………………………………………………………………………… (101)

and,

$$Det[C_k] = 0.0000038147$$

hence the optimal value of the D-criterion for $K'\theta$ in three factors is given as,

$$v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{6}} = \left(0.0000038147\right)^{\frac{1}{6}} = 0.125$$

4.3.3 D-Optimal Weighted Centroid Design For M=4 Factors.

Lemma 4.9

In the third-degree Kronecker model for the mixture experiments with four factors,

unique D-optimal design for $K'\theta$ is,

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2,$$

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The D-criterion maximum value for the $K'\theta$ in four factors is

$$v(\phi_0) = 0.07080$$

Proof,

For $p = 0$, $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if

$$trace C_j C(\alpha)^{-1} = trace C(\alpha)^0 = trace I \ \ for\ all\ \ j \in \{1,2\}.$$

Thus,

$$C_1 C_k^{-1} = \begin{pmatrix} a & b & b & b & c & c & c & d & d & d \\ b & a & b & b & c & d & d & c & c & d \\ b & b & a & b & d & c & d & c & d & c \\ b & b & b & a & d & d & c & d & c & c \\ c & c & d & d & e & d & d & d & d & d \\ c & d & c & d & d & e & d & d & d & d \\ c & d & d & c & d & d & e & d & d & d \\ d & c & c & d & d & d & d & e & d & d \\ d & c & d & c & d & d & d & d & e & d \\ d & d & c & c & d & d & d & d & d & e \end{pmatrix} \text{...(102)}$$

where,

$$a = \frac{1}{\alpha_1}, b = \frac{-\alpha_2}{\alpha_1(48\alpha_1 + \alpha_2)}, c = \frac{-8}{48\alpha_1 + \alpha_2}, d = 0, e = 0$$

$$traceC_1C(\alpha)^{-1} = \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + 0 + 0 + 0 + 0 + 0 + 0$$

$$= \frac{4}{\alpha_1} \text{..(103)}$$

And $traceC_k^0 = traceI_{10} = 10$.

Thus , $traceC_1C(\alpha)^{-1} = traceI_{10} \Leftrightarrow \frac{4}{\alpha_1} = 10$

$$\alpha_1 = \frac{2}{5}$$

$$C_2C_k^{-1} = \begin{pmatrix} a & b & b & b & c & c & c & d & d & d \\ b & a & b & b & c & d & d & c & c & d \\ b & b & a & b & d & c & d & c & d & c \\ b & b & b & a & d & d & c & d & c & c \\ f & f & g & g & e & g & g & g & g & g \\ f & g & f & g & g & e & g & g & g & g \\ f & g & g & f & g & g & e & g & g & g \\ g & f & f & g & g & g & g & e & g & g \\ g & f & g & f & g & g & g & g & e & g \\ g & g & f & f & g & g & g & g & g & e \end{pmatrix} \text{...(104)}$$

where,

$$a = 0, b = \frac{-\alpha_2}{32\alpha_1(48\alpha_1 + \alpha_2)}, c = \frac{8\alpha_1}{\alpha_2(48\alpha_1 + \alpha_2)}, d = \frac{-1}{6(48\alpha_1 + \alpha_2)}, e = \frac{1}{\alpha_2},$$

$$f = 0, g = \frac{-\alpha_2}{8\alpha_1(48\alpha_1 + \alpha_2)}$$

with $traceC_2C(\alpha)^{-1} = 0 + 0 + 0 + 0 + \frac{1}{\alpha_2} + \frac{1}{\alpha_2} + \frac{1}{\alpha_2} + \frac{1}{\alpha_2} + \frac{1}{\alpha_2} + \frac{1}{\alpha_2}$.

$$= \frac{6}{\alpha_2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (105)$$

Thus , $trace C_2 C(\alpha)^{-1} = trace I_{10} \Leftrightarrow \frac{6}{\alpha_2} = 10$

$\alpha_2 = \frac{3}{5}$

Therefore, the unique D-optimal weighted centroid design for $K'\theta$ in m=4 factors is expressed as $\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{2}{5}\eta_1 + \frac{3}{5}\eta_2$ as required.

The maximum value of the D-criterion is obtained as follows,

$v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{s}}$, and $s = \binom{m+1}{2}$.

for $m = 4$,then, $v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{10}}$.

for the design with four factors, the information matrix is given by,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 \\ \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 \\ \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} \\ \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & 0 & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} \\ \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 \\ 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 \\ 0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} \end{pmatrix}$$

substituting for the values of α_1 and α_2 gives the following,

$$= \begin{bmatrix} 0.2578125 & 0.0015625 & 0.0015625 & 0.0015625 & 0.0093750 & 0.0093750 & 0.0093750 & 0 & 0 & 0 \\ 0.0015625 & 0.2578125 & 0.0015625 & 0.0015625 & 0.0093750 & 0 & 0 & 0.0093750 & 0.0093750 & 0 \\ 0.0015625 & 0.0015625 & 0.2578125 & 0.0015625 & 0 & 0.0093750 & 0 & 0.0093750 & 0 & 0.0093750 \\ 0.0015625 & 0.0015625 & 0.0015625 & 0.2578125 & 0 & 0.0093750 & 0 & 0.0093750 & 0.0093750 \\ 0.0093750 & 0.0093750 & 0 & 0 & 0.1125 & 0 & 0 & 0 & 0 & 0 \\ 0.0093750 & 0 & 0.0093750 & 0 & 0 & 0.1125 & 0 & 0 & 0 & 0 \\ 0.0093750 & 0 & 0 & 0.0093750 & 0 & 0 & 0.1125 & 0 & 0 & 0 \\ 0 & 0.0093750 & 0.0093750 & 0 & 0 & 0 & 0 & 0.1125 & 0 & 0 \\ 0 & 0.0093750 & 0 & 0.0093750 & 0 & 0 & 0 & 0 & 0.1125 & 0 \\ 0 & 0 & 0.0093750 & 0.0093750 & 0 & 0 & 0 & 0 & 0 & 0.1125 \end{bmatrix}$$

……………………………………………………………………………………(106)

$$Det[C_k] = 0.0000000000316764$$

Hence the maximum value for $K'\theta$ in m=4 factors is given as,

$$v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{10}} = \left(0.0000000000038147\right)^{\frac{1}{10}} = 0.07080$$

4.3.4 Generalized D-Optimal Weighted Centroid Design For $m \geq 2$ Factors

Theorem 4.7

In the third -degree Kronecker model for the mixture experiments with $m \geq 2$ factors, unique D-optimal design for $K'\theta$ is,

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 .$$

where,

$$\alpha_1 = \frac{(m^2 - 63m + 58) + \sqrt{(m^4 + 122m^3 + 3597m^2 - 7564m + 3844)}}{2(31m^2 + m - 30)}$$

$$\alpha_2 = \frac{(-63m^2 + 61m + 2) - \sqrt{(12033m^4 - 31622m^3 + 26893m^2 - 7052m - 252)}}{2(31m^2 + m - 30)}$$

and, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The optimal value of D-criterion for the $K'\theta$ in $m \geq 2$ factors is given by,

$$v(\phi_0) = (\det C(\alpha))^{\frac{1}{s}} = \left\{\left(\frac{9}{8m(m+1)}\right)\left(\frac{2}{m(m+1)}\right)^m\right\}^{\frac{1}{\binom{m+1}{2}}}$$

Proof

Let $\alpha = (\alpha_1, \alpha_2, 0, ..., 0)' \in T_m$ be a weight vector with $\partial(\alpha) = \{1,2\}$ and supposing that $\eta(\alpha)$ is D-optimal for the $K'\theta$ in T.

Let $C(\alpha) = C_k(M(\eta(\alpha)))$.Equation (14) implies that for p=0,

$$trace(C_j C^{-1}) \begin{cases} = trace(C(\alpha)^0) & for\ j \in \{1,2\} \\ < trace(C(\alpha)^0) & otherwise \end{cases} \qquad \text{……..……………………......... (107)}$$

from equation (24) a unique representation for any matrix $C \in Sym(s)$, is given as follows,

$$C = \begin{pmatrix} aI_m + bU_2 & cV \\ cV' & dI_{\binom{m}{2}} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(108)}$$

with the coefficients $a, b, c, d \in \Re$.

again, partitioning of any given symmetric matrix $C \in Sym(s)$, can be done in accordance to the block structure of the matrices in H, as shown below,

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C'_{12} & C_{22} \end{pmatrix},$$

with $C_{11} \in sym(m)$, $C_{12} \in \Re^{m*1}$ and $C_{22} \in \Re^{1}$,Klein (2004).

and for $j = 1$, $\quad traceC_1C_k(\alpha)^{-1} = traceC(\alpha)^0 = trace(I)$

From equations (60) and (83), we get

$$C_1C_k(\alpha)^{-1} = \begin{pmatrix} \frac{a}{m}U_1 + \frac{b}{m}U_2 & \frac{c}{m}V \\ 0 & 0 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(109)}$$

where, $a = \dfrac{32m(m-1)\alpha_1 + m(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}$, $b = \dfrac{-m(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}$,and

$$c = \frac{-16m(m-1)}{3(32(m-1)\alpha_1 + (m-2)\alpha_2)}$$

resulting in,

$$trace(C_1C_k(\alpha)^{-1}) = trace\left(\frac{a}{m}U_1 + \frac{b}{m}U_2\right) + 0 = trace\frac{a}{m}U_1, \text{ since } trace(U_2) = 0$$

Therefore,

$$trace(C_1C_k(\alpha)^{-1}) = \left\{ m\frac{32m(m-1)\alpha_1 + m(m-2)\alpha_2}{m\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} \right\}$$

$$= \frac{32m(m-1)\alpha_1 + m(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} \quad \text{..(110)}$$

also for m factors, $trace(I_s) = \binom{m+1}{2}$, where $s = \binom{m+1}{2}$.

hence, $traceC_1C_k(\alpha)^{-1} = traceC(\alpha)^0 = trace(I)$,

$$\Leftrightarrow \frac{32m(m-1)\alpha_1 + m(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} = \binom{m+1}{2} = \left(\frac{m(m+1)}{2}\right).$$

this reduces to

$$(31m^2 + m - 30)\alpha_1^2 + (m^2 - 63m + 58)\alpha_1 - 2(m-2) = 0$$

solving this polynomial together with $\alpha_1 + \alpha_2 = 1$ yields

$$\alpha_1 = \frac{(m^2 - 63m + 58) + \sqrt{(m^4 + 122m^3 + 3597m^2 - 7564m + 3844)}}{2(31m^2 + m - 30)} \quad \alpha_1 \in (0,1).$$

again, from equations (61) and (83), we obtain

$$C_2C_k(\alpha)^{-1} = \begin{pmatrix} a'''U_1 + b'''U_2 & c'''V \\ c'''V' & d'''I_{\binom{m}{2}} \end{pmatrix} \quad \text{..(111)}$$

where, $a''' = \dfrac{32(m-1)\alpha_1}{32\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}$, $b''' = \dfrac{-(m-2)\alpha_2}{32\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}$,

$c''' = \dfrac{32(m-1)\alpha_1}{6\alpha_2[32(m-1)\alpha_1 + (m-2)\alpha_2]}$ and $d''' = \dfrac{32(m-1)\alpha_1}{\alpha_2[32(m-1)\alpha_1 + (m-2)\alpha_2]}$

hence,

$$trace(C_2 C_k(\alpha)^{-1}) = \left\{ m\left(\frac{32(m-2)\alpha_1}{32\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} \right) + \frac{32(m-1)\alpha_1}{\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} I_{\binom{m}{2}} \right\}$$

$$= \left\{ \left(\frac{32m(m-2)\alpha_1}{32\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} \right) + \frac{32(m-1)\alpha_1}{\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} * \left(\frac{m(m-1)}{2} \right) \right\}$$

…………………………………………………………………………………..(112)

Therefore,

$$traceC_2 C_k(\alpha)^{-1} = trace(I) = traceC(\alpha)^0,$$

$$\Leftrightarrow \left\{ \left(\frac{32m(m-2)\alpha_1}{32\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} \right) + \frac{32(m-1)\alpha_1}{\alpha_2(32(m-1)\alpha_1 + (m-2)\alpha_2)} * \left(\frac{m(m-1)}{2} \right) \right\} = \binom{m+1}{2}$$
$$= \left(\frac{m(m+1)}{2} \right)$$

which reduces to,

$$(31m^2 + m - 30)\alpha_2^2 + (-63m^2 + 61m + 2)\alpha_2 + (32m^2 - 64m + 32) = 0$$

solving this polynomial together with $\alpha_1 + \alpha_2 = 1$ yields

$$\alpha_2 = \frac{(-63m^2 + 61m + 2) - \sqrt{(12033m^4 - 31622m^3 + 26893m^2 - 7052m - 252)}}{2(31m^2 + m - 30)}$$

$\alpha_2 \in (0,1)$.

From equation (62), for a design with *m* factors, the information matrix is given by,

$$C_k(\alpha) = \alpha_1 C_1 + \alpha_2 C_2 = \begin{pmatrix} \frac{32\alpha_1 + \alpha_2}{32m} I_m + \frac{\alpha_2}{32m(m-1)} U_2 & \frac{3\alpha_2}{16m(m-1)} V \\ \frac{3\alpha_2}{16m(m-1)} V' & \frac{9\alpha_2}{8m(m-1)} I_{\binom{m}{2}} \end{pmatrix}$$

Thus the optimal value of the D-criterion for the $K'\theta$ in $m \geq 2$ factors is given as,

$$v(\phi_0) = (\det C(\alpha))^{\frac{1}{s}} = \left\{ \left(\frac{9}{8m(m+1)} \right) \left(\frac{2}{m(m+1)} \right)^m \right\}^{\frac{1}{\binom{m+1}{2}}}$$

………..…………………………………………………………………………… (113)

where,

$$\alpha_1 = \frac{(m^2 - 63m + 58) + \sqrt{(m^4 + 122m^3 + 3597m^2 - 7564m + 3844)}}{2(31m^2 + m - 30)}$$

$$\alpha_2 = \frac{(-63m^2 + 61m + 2) - \sqrt{(12033m^4 - 31622m^3 + 26893m^2 - 7052m - 252)}}{2(31m^2 + m - 30)}$$

and $s = \binom{m+1}{2}$.

lemma 4.7, 4.8 and 4.9 given earlier serves as particular examples for m=2, m=3, and m=4 factors.

4.4 E-Optimal Weighted Centroid Designs

The optimal weighted centroid designs for the smallest eigenvalue criterion are calculated.

4.4.1 E-Optimal Weighted Centroid Design For M=2 Factors

Lemma 4.11

In the third-degree kronecker model with two factors, the weighted centroid design

$n\left(\alpha^{(E)}\right) = \alpha_1 n_1 + \alpha_2 n_2 = 0.53488 n_1 + 0.46511 n_2$ is the E-optimal for $K'\theta$ in T.

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid* .The maximum value of E-criterion for the $K'\theta$ in m=2 factors is

$$v\left(\phi_{-\infty}\right) = \lambda_{\min}\left(C\right) = 0.209302$$

Proof

The information matrix for m=2 factors is given as:

$$C_k = C_k\left(M\left(n(\alpha)\right)\right) = \begin{bmatrix} \frac{32\alpha_1 + \alpha_2}{64} & \frac{\alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{\alpha_2}{64} & \frac{32\alpha_1 + \alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{3\alpha_2}{32} & \frac{3\alpha_2}{32} & \frac{9\alpha_2}{16} \end{bmatrix}$$

………………………………………...……………………………………. (114)

A unique representation of any matrix C $\in sym(s, H)$ is of the form given below,

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 + dV_2 \\ cV_1' + dV_2' & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \quad (115)$$

the information matrix $C_k(M(n(\alpha)))$ for m=2 factors, is given as

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 \\ cV_1' & eW_1 \end{pmatrix}$$

with the coefficients; a, b, c, e $\in \Re$, as the terms that contain V_2, W_2 and W_3 only occurs for $m > 2$ factors.

from lemma (3.1), we have,

$$U_1 = I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, U_2 = I_2 I_2' - I_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \text{ and}$$

$$V = \sum_{i=1}^{2}(e_i) \in \Re^{2\times 1} = (e_1 + e_2) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and } W_1 = I_{\binom{2}{2}} = 1 \quad (116)$$

Hence, the information matrix is given by,

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 \\ cV_1' & eW_1 \end{pmatrix} = \begin{bmatrix} a\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & c\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ c(1 \quad 1) & e(1) \end{bmatrix} = \begin{pmatrix} a & b & c \\ b & a & c \\ c & c & e \end{pmatrix} \quad (117)$$

from lemma 3.3, the eigenvalue for two factors is computed as follows,

$$D_1 = [a + b - d]^2 + 2[2c]^2 =$$
$$\left[\frac{32\alpha_1 + \alpha_2}{64} + \frac{\alpha_2}{64} + \frac{9\alpha_2}{16}\right]^2 + 2\left[\frac{2\times 3\alpha_2}{32}\right] = \frac{1161\alpha_1^2 - 1266\alpha_1 + 361}{32^2}$$

the eigenvalues are;

$$\lambda_{2,3} = \frac{1}{2}\left[a + (2-1)b + d \pm \sqrt{D_1}\right] = \frac{1}{2}\left[\frac{32\alpha_1 + \alpha_2}{64} + \frac{\alpha_2}{64} + \frac{9\alpha_2}{16} \pm \sqrt{\left(\frac{1161\alpha_1^2 - 1266\alpha_1 + 361}{32^2}\right)}\right]$$
$$= \frac{1}{64}\left[19 - 3\alpha_1 \pm \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right]$$

with multiplicity 1.

$$\lambda_{4,5} = \frac{1}{2}\left[a - b + d \pm \sqrt{D_2}\right] = \left[\frac{32\alpha_1 + \alpha_2}{64} - \frac{\alpha_2}{64} + \frac{9\alpha_2}{16} \pm \sqrt{\left(\frac{289\alpha_1^2 - 306\alpha_1 + 81}{16^2}\right)^2}\right]$$
$$= \frac{\alpha_1}{2}$$

with multiplicity m-1, The eigenvalues that occur for m=2 are,

$$\lambda_2 = \frac{1}{64}\left[19 - 3\alpha_1 + \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right]$$

$$\lambda_3 = \frac{1}{64}\left[19 - 3\alpha_1 - \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right]$$

$$\lambda_4 = \frac{\alpha_1}{2}$$

The choice for the matrix E is $E = \frac{zz'}{\|z\|^2}, z \in \Re^s$, if the smallest eigenvalue of $C_k(M)$ has multiplicity 1, where $z \in \Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$.The smallest eigenvalue is

$$\lambda_3 = \frac{1}{64}\left[19 - 3\alpha_1 - \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right]$$

now let $\lambda_{\min} = \frac{1}{64}\left[19 - 3\alpha_1 - \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right]$

Then, $\lambda_{\min}$ is the eigenvalue of C and corresponds to eigenvector, say $\bar{z}$,then,

$(C - \lambda I)\bar{z} = \bar{0}$ or $C\bar{z} = \lambda\bar{z}$ with $\bar{z} \neq \bar{0}$

Let $\bar{z} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$,be the eigenvector of C which corresponds to λ

Then, $(C - \lambda_{\min} I)\vec{z} = \vec{0}$ Implies that,

$$\begin{bmatrix} \frac{32\alpha_1 - 18 + \sqrt{(1161\alpha_1^2 - 1266\alpha_1 + 361)}}{64} & \frac{\alpha_2}{64} & \frac{3\alpha_2}{32} \\ \frac{\alpha_2}{64} & \frac{32\alpha_1 - 18 + \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}}{64} & \frac{3\alpha_2}{32} \\ \frac{3\alpha_2}{32} & \frac{3\alpha_2}{32} & \frac{17 - 33\alpha_1 + \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}}{64} \end{bmatrix}$$

Let, $p = 34\alpha_1 - 18 + \sqrt{(1161\alpha_1^2 - 1266\alpha_1 + 361)}, q = \alpha_2$ and

$r = 17 - 33\alpha_1 + \sqrt{(1161\alpha_1^2 - 1266\alpha_1 + 361)}$

$$\Leftrightarrow \begin{bmatrix} p & q & 6q \\ q & p & 6q \\ 6q & 6q & r \end{bmatrix}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

giving the following equations,

$pz_1 + pz_2 + 6qz_3 = 0$

$$qz_1 + pz_2 + 6qz_3 = 0$$

$$6qz_1 + 6qz_2 + rz_3 = 0$$

Solving these equations we get eigenvector corresponding to $\lambda_{\min}$ as,

$$\bar{z} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \frac{-12q}{r} \end{pmatrix}$$

hence,

$$\overline{zz'} = \begin{pmatrix} 1 & 1 & \frac{-12q}{r} \\ 1 & 1 & \frac{-12q}{r} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} \end{pmatrix}, \text{ and } \|z\|^2 = \frac{2r^2 + 144q^2}{r^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(118)}$$

and the matrix E is given as,

$$E = \frac{\overline{zz}}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{2r^2+144q^2} & \frac{r^2}{2r^2+144q^2} & \frac{-12qr}{2r^2+144q^2} \\ \frac{r^2}{2r^2+144q^2} & \frac{r^2}{2r^2+144q^2} & \frac{-12qr}{2r^2+144q^2} \\ \frac{-12qr}{2r^2+144q^2} & \frac{-12qr}{2r^2+144q^2} & \frac{144q^2}{2r^2+144q^2} \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(119)}$$

and from equation (41)

$$C_1E = \begin{pmatrix} \frac{r^2}{2(2r^2+144q^2)} & \frac{r^2}{2(2r^2+144q^2)} & \frac{-12qr}{2(2r^2+144q^2)} \\ \frac{r^2}{2(2r^2+144q^2)} & \frac{r^2}{2(2r^2+144q^2)} & \frac{-12qr}{2(2r^2+144q^2)} \\ 0 & 0 & 0 \end{pmatrix} \text{……………..} \quad (120)$$

$$C_1E = \left(\frac{r^2}{2(2r^2+144q^2)} + \frac{r^2}{2(2r^2+144q^2)} + \frac{r^2}{2(2r^2+144q^2)} = \frac{r^2}{2r^2+144q^2} \right)$$

Hence,

$$traceC_1E = \lambda_{\min}(C)$$
$$\Leftrightarrow \frac{r^2}{2r^2+144q^2} = \frac{1}{64}\left[19 - 3\alpha_1 - \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right] \text{……………………..} \quad (121)$$

Substituting the values

$p = 34\alpha_1 - 18 + \sqrt{(1161\alpha_1^2 - 1266\alpha_1 + 361)}, q = \alpha_2$ and

$r = 17 - 33\alpha_1 + \sqrt{(1161\alpha_1^2 - 1266\alpha_1 + 361)}$

Reduces the equation (121) to

$$2674944\alpha_1^6 - 13616640\alpha_1^5 + 28512000\alpha_1^4 - 31380480\alpha_1^3 + 19111680\alpha_1^2 - 6096384\alpha_1 + 794880 = 0$$

Solving this polynomial yields the roots;

$\alpha_1 = 0.999719815 or 0.555555556 or 0.534883721$ as the possible values of α_1

$\alpha_1 \in (0,1)$ and $\alpha_2 = 1 - \alpha_1$

Substituting $\lambda_{\min}$ we get,

$\alpha_1 = 0.555555556$

$$\lambda_{\min} = \frac{1}{64}\left[19 - 3\alpha_1 - \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right] = 0.208333333$$

$\alpha_1 = 0.999719815$

$$\lambda_{\min} = \frac{1}{64}\left[19 - 3\alpha_1 - \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right] = 0.000157601$$

$\alpha_1 = 0.534883721$

$$\lambda_{\min} = \frac{1}{64}\left[19 - 3\alpha_1 - \sqrt{1161\alpha_1^2 - 1266\alpha_1 + 361}\right] = 0.209302325$$

Therefore, $\lambda_{\min}$ is maximum when $\alpha_1 = 0.534883721$ and $\alpha_2 = 0.465116279$

For m=2 factors. The optimal E-criterion is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.209302325$$

4.4.2 E-Optimal Weighted Centroid Design For M=3 Factors

Lemma 4.12

In third-degree kronecker model with m=3 factors, the weighted centroid design

$n(\alpha^{(E)}) = \alpha_1 n_1 + \alpha_2 n_2 = 0.59208 n_1 + 0.40792 n_2$ is the E-optimal for the $K'\theta$ in T.

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The maximum value of the E-criterion for the $K'\theta$ for m=3 factors is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.07164$$

for third-degree kronecker model with m=3 factors, the information matrix $C_k\left(M\left(n(\alpha)\right)\right)$ is given as,

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 + dV_2 \\ cV_1' + dV_2' & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \text{...(122)}$$

where $a = \frac{32\alpha_1 + \alpha_2}{96}, b = \frac{\alpha_2}{192}, c = \frac{\alpha_2}{32}, d = 0, e = \frac{3\alpha_2}{16}$ *and* $f = 0$

from lemma (3.1),with matrices; $U_1, U_2, V_1, V_2, W_1, W_2$ and W_3 well defined

Proof

for m=3 factors, the information matrix is then given as:

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 \\ \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} \\ \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 & 0 \\ \frac{\alpha_2}{32} & 0 & \frac{\alpha_2}{32} & 0 & \frac{3\alpha_2}{16} & 0 \\ 0 & \frac{\alpha_2}{32} & \frac{\alpha_2}{32} & 0 & 0 & \frac{3\alpha_2}{16} \end{pmatrix}$$

A unique representation for any matrix C$\in sym(s,H)$ is of the form

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 + dV_2 \\ cV_1' + dV_2' & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \text{...(123)}$$

With the coefficients; a,…, g$\in\Re$, with the terms that contain V_2, W_2 and W_3 only occurring for $m > 3$ and for $m > 4$ respectively.

The information matrix $C_k\left(M\left(n(\alpha)\right)\right)$, for the case m=3 factors is written as follows,

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 + dV_2 \\ cV_1' + dV_2' & eI_{\binom{m}{2}} + fw_2 \end{pmatrix}$$

from lemma (3.1),

$$U_1 = I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, U_2 = I_3 I_3' - I_3 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$V_1 = E_{12}(e_1 + e_2)' + E_{13}(e_1 + e_3)' + E_{23}(e_2 + e_3)' = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$V_2 = E_{12}e_3' + E_{13}e_2' + E_{23}e_1' = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$W_2 = E_{12}E_{13}' + E_{12}E_{23}' + E_{13}E_{12}' + E_{13}E_{23}' + E_{23}E_{12}' + E_{23}E_{13}' = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Thus the information matrix

$$C = \begin{bmatrix} a\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}+b\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix} & c\begin{pmatrix}1&1&0\\1&0&1\\0&1&1\end{pmatrix}+d\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix} \\ c\begin{pmatrix}1&1&0\\1&0&1\\0&1&1\end{pmatrix}+d\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix} & e\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}+f\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix} \end{bmatrix}$$

$$\begin{bmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ c & c & d & e & f & f \\ c & d & c & f & e & f \\ d & c & c & f & f & e \end{bmatrix} \qquad \ldots\ldots\ldots (124)$$

$a = \dfrac{32\alpha_1 + \alpha_2}{96}, b = \dfrac{\alpha_2}{192}, c = \dfrac{\alpha_2}{32}, d = 0, e = \dfrac{3\alpha_2}{16}$ *and*
$f = 0$

From lemma 3.3, for the above matrix, the eigenvalues are computed as follows

$$D_1 = [a + 2b - e]^2 + 4[2c - d]^2 = \frac{153\alpha_1^2 - 114\alpha_1 + 25}{576}$$

$$D_2 = [a - b - e]^2 + 4[c - d]^2 = \frac{13401\alpha_1^2 - 14130\alpha_1 + 4825}{36864}$$

The eigenvalues are

$$\lambda_{2,3} = \frac{1}{2}\left[a + 2b + e \pm \sqrt{D_1}\right] = \frac{1}{48}\left[3\alpha_1 + 5 \pm \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right]$$

$$\lambda_{4,5} = \frac{1}{2}\left[a - b + e \pm \sqrt{D_2}\right] = \frac{1}{384}\left[25\alpha_1 + 37 \pm \sqrt{13401\alpha_1^2 - 14130\alpha_1 + 4825}\right]$$

The eigenvalues $\lambda_2, \lambda_3, \lambda_4, \lambda_5$ that occur for m=3 are,

$$\lambda_2 = \frac{1}{48}\left[3\alpha_1 + 5 + \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right]$$, with multiplicity 1

$$\lambda_3 = \frac{1}{48}\left[3\alpha_1 + 5 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right]$$, with multiplicity 1

$$\lambda_4 = \frac{1}{384}\left[25\alpha_1 + 37 + \sqrt{13401\alpha_1^2 - 14130\alpha_1 + 4825}\right]$$, with multiplicity 2 and

$$\lambda_5 = \frac{1}{384}\left[25\alpha_1 + 37 - \sqrt{13401\alpha_1^2 - 14130\alpha_1 + 4825}\right]$$, with multiplicity 2

The smallest eigenvalue is

$$\lambda_3 = \frac{1}{48}\left[3\alpha_1 + 5 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right]$$, with multiplicity 1

get an eigenvector z that corresponds to the smallest eigenvalue of the matrix $C_k(M)$.

$\lambda \in \Re$, is the eigenvalue of a matrix C if,

$(C - \lambda I)\bar{z} = \bar{0}$ or $C\bar{z} = \lambda\bar{z}$ with $\bar{z} \neq \bar{0}$

where $\bar{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix}$,be the eigenvector of C that corresponds to λ

Hence, as given in equation (124)

$\left(C - \lambda_{\min} I\right)\vec{z} = \vec{0}$ suggests that,

$$\begin{pmatrix} p & q & q & 6q & 6q & 0 \\ q & p & q & 6q & 0 & 6q \\ q & q & p & 0 & 6q & 6q \\ 6q & 6q & o & r & 0 & 0 \\ 6q & 0 & 6q & 0 & r & 0 \\ 0 & 6q & 6q & 0 & 0 & r \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

where $p = 25\alpha_1 - 9 + \sqrt{(153\alpha_1^2 - 114\alpha_1 + 25)}, q = 1 - \alpha_1$ and $r = -3\alpha_1 + 1 + \sqrt{(153\alpha_1^2 - 114\alpha_1 + 25)}$

giving the following equations,

$$py_1 + qy_2 + qy_3 + 6qy_4 + 6qy_5 = 0$$

$$py_1 + py_2 + qy_3 + 6qy_4 + qy_6 = 0$$

$$qy_1 + qy_2 + py_3 + 6qy_5 + 6qy_6 = 0$$

$$6qy_1 + 6qy_2 + ry_4 = 0$$

$$6qy_1 + 6qy_3 + ry_5 = 0$$

$$6qy_2 + 6qy_3 + ry_6 = 0$$

by solving these equations, the eigenvector corresponding to $\lambda_{\min}$ is written as,

$$\vec{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \frac{-12q}{r} \\ \frac{-12q}{r} \\ \frac{-12q}{r} \end{pmatrix}$$

hence,

$$zz' = \begin{pmatrix} 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \end{pmatrix}, \|z\|^2 = \frac{3r^2 + 432q^2}{r^2}$$

and the matrix E is given as follows,

$$zz' = \begin{pmatrix} \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} \\ \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} \\ \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} \\ \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} \\ \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} \\ \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} \end{pmatrix}$$

a weighted centroid design $n(\alpha)$ is E-optimal for $K'\theta$ in T if and only if

$$traceC_j E = \lambda_{\min}(C)$$

$$C_1 E = \begin{bmatrix} a & a & a & b & b & b \\ a & a & a & b & b & b \\ a & a & a & b & b & b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad \ldots\ldots (125)$$

Where $a = \dfrac{r^2}{3(3r^2 + 432q^2)}$, $b = \dfrac{-12qr}{3(3r^2 + 432q^2)}$

$$traceC_1 E = \left(\frac{r^2}{3(3r^2 + 432q^2)} + \frac{r^2}{3(3r^2 + 432q^2)} + \frac{r^2}{3(3r^2 + 432q^2)} + 0 = \frac{r^2}{3r^2 + 432q^2} \right)$$

$traceC_j E = \lambda_{\min}(C)$, implies

$$\frac{r^2}{3r^2 + 432q^2} = \frac{1}{48}\left[3\alpha_1 + 5 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] \ldots\ldots (126)$$

This simplifies to

$$88128\alpha_1^6 - 330048\alpha_1^5 + 547344\alpha_1^4 - 505584\alpha_1^3 + 260064\alpha_1^2 - 65280\alpha_1 + 5376 = 0$$

$$\ldots\ldots (127)$$

substituting values of q and r and solving this polynomial yields the roots;

$\alpha_1 = 0.14880 or 0.59208 or 0.71178$ as the possible values of α_1

$\alpha_1 \in (0,1)$ and $\alpha_2 = 1 - \alpha_1$

substituting $\lambda_{\min}$,

$$\alpha_1 = 0.14880$$

$$\lambda_{\min} = \frac{1}{48}\left[3\alpha_1 + 5 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.04302$$

when $\alpha_1 = 0.59208$

$$\lambda_{\min} = \frac{1}{48}\left[3\alpha_1 + 5 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.07164$$

$$\alpha_1 = 0.71178$$

$$\lambda_{\min} = \frac{1}{48}\left[3\alpha_1 + 5 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.05234$$

Therefore, $\lambda_{\min}$ is maximum when $\alpha_1 = 0.59208$ and $\alpha_2 = 0.40792$

as given in Pukelsheim (1993), the smallest eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$

$$\lambda_{\min} = \frac{1}{48}\left[3\alpha_1 + 5 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.07164$$

The optimal value for m=3 factors E-criterion is given as,

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.07164$$

4.4.3 E-Optimal Weighted Centroid Design For M=4 Factors

Lemma 4.13

In third-degree kronecker model for m=4 factors, the weighted centroid design

$n\left(\alpha^{(E)}\right) = \alpha_1 n_1 + \alpha_2 n_2 = 0.638661 n_1 + 0.361339 n_2$ is the E-Optimal for the $K'\theta$ in T. Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The maximum value of the E-criterion for $K'\theta$ for m=4 factors is given by,

$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.069741$

Proof

The information matrix for m=4 factors is as follows:

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 \\ \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 \\ \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & \frac{\alpha_2}{384} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} \\ \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{\alpha_2}{384} & \frac{32\alpha_1+\alpha_2}{128} & 0 & 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} \\ \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{64} & 0 & 0 & \frac{\alpha_2}{64} & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 & 0 \\ 0 & \frac{\alpha_2}{64} & 0 & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} & 0 \\ 0 & 0 & \frac{\alpha_2}{64} & \frac{\alpha_2}{64} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{32} \end{pmatrix}$$

where $a = \frac{32\alpha_1 + \alpha_2}{128}$, $b = \frac{\alpha_2}{384}$, $c = \frac{\alpha_2}{64}$, d=0, $e = \frac{3\alpha_2}{32}$,f=0 and g=0…………......(128)

a unique representation for any matrix C $\in sym(s,H)$ is of the form,

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 + dV_2 \\ cV_1' + dV_2' & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \quad \text{...(129)}$$

With the coefficients; a,…….,g $\in \Re$,with the terms that contain V_2, W_2 and W_3 only occurring for $m > 3$ and for $m > 4$ respectively.

The information matrix $C_k(M(n(\alpha)))$, for m=4 factors, is given as follows,

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 + dV_2 \\ cV_1' + dV_2' & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \quad \text{...(130)}$$

from lemma (3.1),

$$U_1 = I_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} ,$$

$$U_2 = I_4 I_4' - I_4 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

$$V = \sum_{\substack{i,j=1 \\ i<j}}^{4} (e_i) \in \Re^{4\times 1} = (e_1 + e_2 + e_3 + e_4) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

Thus the information matrix,

$$C=\begin{pmatrix} aU_1+bU_2 & cV \\ cV' & d\dfrac{V'V}{m}\end{pmatrix}=\left[a\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}+b\begin{pmatrix}0&1&1&1\\1&0&1&1\\1&1&0&1\\1&1&1&0\end{pmatrix} \quad c\begin{pmatrix}1\\1\\1\\1\end{pmatrix} \atop c\begin{pmatrix}1&1&1&1\end{pmatrix} \qquad d(1)\right]$$

Where $a=\dfrac{32\alpha_1+\alpha_2}{128}$, $b=\dfrac{\alpha_2}{384}$, $c=\dfrac{\alpha_2}{64}$, d=0, $e=\dfrac{3\alpha_2}{32}$,f=0 and g=0

from lemma (3.3),

$$D_1=[a+3b-e-4f-g]^2+6[2c-2d]^2=\left[\frac{3\alpha_1+\alpha_2}{128}+3\left[\frac{\alpha_2}{384}\right]-\frac{3\alpha_2}{32}\right]^2+6\left[\frac{\alpha_2}{64}\right]^2$$
$$=\frac{456\alpha_1^2-258\alpha_1+49}{4096}$$

$$D_2=[a-b-e+f]^2+4(4-2)[c]^2=\left[\frac{32\alpha_1+\alpha_2}{128}-\frac{\alpha_2}{384}-\frac{3\alpha_2}{32}\right]^2+4(2)\left[\frac{\alpha_2}{64}\right]^2$$
$$=\frac{6025\alpha_1^2-5810\alpha_1+2089}{36864}$$

the eigenvalues are,

$$\lambda_{2,3}=\frac{1}{2}\left[a+2b+e\pm\sqrt{D_1}\right]=\frac{1}{128}\left[9\alpha_1+7\pm\sqrt{\frac{(456\alpha_1^2-258\alpha_1+49)}{4096}}\right]$$

$$\lambda_{4,5}=\frac{1}{2}\left[a-b+e\pm\sqrt{D_2}\right]=\frac{1}{384}\left[29\alpha_1+19\pm\sqrt{\frac{(6025\alpha_1^2-5810\alpha_1+2089)}{36864}}\right]$$

The eigenvalues $\lambda_1,\lambda_2,\lambda_3,\lambda_4,\lambda_5$ that occur for m=4 are,

$\lambda_1=e-2f+g=\dfrac{3\alpha_2}{32}=\dfrac{3-3\alpha_1}{32}$, with the multiplicity 2

$$\lambda_2 = \frac{1}{128}\left[9\alpha_1 + 7 + \sqrt{\frac{\left(456\alpha_1^2 - 258\alpha_1 + 49\right)}{4096}}\right] \text{ with multiplicity 1}$$

$$\lambda_3 = \frac{1}{128}\left[9\alpha_1 + 7 - \sqrt{\frac{\left(456\alpha_1^2 - 258\alpha_1 + 49\right)}{4096}}\right] \text{ with multiplicity 1}$$

$$\lambda_4 = \frac{1}{384}\left[29\alpha_1 + 19 + \sqrt{\frac{\left(6025\alpha_1^2 - 5810\alpha_1 + 2089\right)}{36864}}\right] \text{ with multiplicity 3}$$

$$\lambda_5 = \frac{1}{384}\left[29\alpha_1 + 19 - \sqrt{\frac{\left(6025\alpha_1^2 - 5810\alpha_1 + 2089\right)}{36864}}\right] \text{ with multiplicity 3}$$

The smallest eigenvalue is,

$$\lambda_3 = \frac{1}{128}\left[9\alpha_1 + 7 - \sqrt{\frac{\left(456\alpha_1^2 - 258\alpha_1 + 49\right)}{4096}}\right] \text{ with multiplicity 1}$$

Then, an eigenvector z, corresponding to the smallest eigenvalue of the matrix $C_k(M)$

. $\lambda \in \Re$, is an eigenvalue of a matrix C if

$\left(C - \lambda I\right)\bar{z} = \bar{0}$ or $C\bar{z} = \lambda\bar{z}$ with $\bar{z} \neq \bar{0}$

where $\bar{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \end{pmatrix}$, be the eigenvector of C corresponding to λ

Thus from equation (128)

$\left(C - \lambda_{\min} I\right)\vec{z} = \vec{0}$ suggests that,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} P & q & q & q & 6q & 6q & 6q & 0 & 0 & 0 \\ q & p & q & q & 6q & 0 & 0 & 6q & 6q & 0 \\ q & q & p & q & 0 & 6q & 0 & 6q & 0 & 6q \\ q & q & q & p & 0 & 0 & 6q & 0 & 6q & 6q \\ 6q & 6q & 0 & 0 & r & 0 & 0 & 0 & 0 & 0 \\ 6q & 0 & 6q & 0 & 0 & r & 0 & 0 & 0 & 0 \\ 6q & 0 & 0 & 6q & 0 & 0 & r & 0 & 0 & 0 \\ 0 & 6q & 6q & 0 & 0 & 0 & 0 & r & 0 & 0 \\ 0 & 6q & 0 & 6q & 0 & 0 & 0 & 0 & r & 0 \\ 0 & 0 & 6q & 6q & 0 & 0 & 0 & 0 & 0 & r \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

where $p = 11\alpha_1 - 3 + \sqrt{(153\alpha_1^2 - 114\alpha_1 + 25)}, q = 1 - \alpha_1$ and

$r = -21\alpha_1 + 5 + \sqrt{(153\alpha_1^2 - 114\alpha_1 + 25)}$

giving the following equations,

$$py_1 + qy_2 + qy_3 + qy_4 + 6qy_5 + 6qy_6 + 6qy_7 = 0$$

$$py_1 + py_2 + qy_3 + qy_4 + 6qy_5 + 6qy_8 + 6qy_9 = 0$$

$$qy_1 + qy_2 + py_3 + qy_4 + 6qy_6 + 6qy_8 + 6qy_{10} = 0$$

$$qy_1 + qy_2 + qy_3 + py_4 + 6qy_7 + 6qy_9 + 6qy_{10} = 0$$

$$6qy_1 + 6qy_2 + ry_5 = 0$$

$$6qy_1 + 6qy_3 + ry_6 = 0$$

$$6qy_1 + 6qy_4 + ry_7 = 0$$

$$6qy_2 + 6qy_3 + ry_8 = 0$$

$$6qy_2 + 6qy_4 + ry_9 = 0$$

$$6qy_3 + 6qy_4 + ry_{10} = 0,$$

by solving these equations gives the eigenvector that corresponds to $\lambda_{\min}$ as,

$$\bar{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \frac{-12q}{r} \\ \frac{-12q}{r} \\ \frac{-12q}{r} \\ \frac{-12q}{r} \\ \frac{-12q}{r} \\ \frac{-12q}{r} \end{pmatrix},$$

hence,

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} 1 & 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ 1 & 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ 1 & 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ 1 & 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \end{pmatrix}$$

$$, \|z\|^2 = \frac{4r^2 + 864q^2}{r^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (131)$$

and the matrix E is given as,

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \end{pmatrix}$$

Where $a = \frac{r^2}{4r^2 + 864q^2}$ $, b = \frac{-3qr}{r^2 + 216q^2}$ $, c = \frac{36q^2}{r^2 + 216q^2}$

…………………………………………………………………………....… (132)

a weighted centroid design $n(\alpha)$ is E-optimal for $K'\theta$ in T if and only if $traceC_j E = \lambda_{\min}(C)$,

$$C_1 E = \begin{pmatrix} a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \text{…………………… (133)}$$

where $a = \frac{r^2}{4(4r^2 + 864q^2)}, b = \frac{-3qr}{4(r^2 + 216q^2)}, c = \frac{36q^2}{4(r^2 + 216q^2)}$

$$traceC_1E = \left(\frac{r^2}{4(4r^2+864q^2)} + \frac{r^2}{4(4r^2+864q^2)} + \frac{r^2}{4(4r^2+864q^2)} + \frac{r^2}{4(4r^2+864q^2)} = \frac{r^2}{4r^2+864q^2} \right)$$

$traceC_jE = \lambda_{\min}(C)$, implies that,

$$\frac{r^2}{4r^2+864q^2} = \frac{1}{128}\left[9\alpha_1 + 7 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] \text{……..………………….... (134)}$$

This simplifies to,

$$193194\alpha_1^6 - 863136\alpha_1^5 + 2231280\alpha_1^4 - 3129792\alpha_1^3 + 2025264\alpha_1^2 - 552096\alpha_1 + 46224 = 0$$

……………………………………………………….…………………..… (135)

substituting values of q and r and Solving this polynomial yields the roots;

$\alpha_1 = 0.638661 or 0.172892 or 0.369951$ as the possible values of α_1

$\alpha_1 \in (0,1)$ and $\alpha_2 = 1 - \alpha_1$

substituting $\lambda_{\min}$ when,

$\alpha_1 = 0.638661$

$$\lambda_{\min} = \frac{1}{128}\left[9\alpha_1 + 7 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.069741$$

when $\alpha_1 = 0.172892$

$$\lambda_{\min} = \frac{1}{128}\left[9\alpha_1 + 7 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.04230$$

when $\alpha_1 = 0.369951$

$$\lambda_{\min} = \frac{1}{128}\left[9\alpha_1 + 7 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.06553$$

Therefore, $\lambda_{\min}$ is maximum when $\alpha_1 = 0.638661$ and $\alpha_2 = 0.361349$

According to Pukelsheim (1993), the smallest eigenvalue criterion is given as $v(\phi_{-\infty}) = \lambda_{\min}(C)$

$$\lambda_{\min} = \frac{1}{128}\left[9\alpha_1 + 7 - \sqrt{153\alpha_1^2 - 114\alpha_1 + 25}\right] = 0.069741$$

The optimal value for m=4 factors E-criterion is given as,

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.069741$$

4.4.4 Generalized E-Optimal Weighted Centroid Design For $m \geq 2$ Factors

Theorem 4.14

In third degree kronecker model with m factors, the weighted centroid design is given as,

$$n\left(\alpha^{(E)}\right) = \alpha_1 n_1 + \alpha_2 n_2$$

Where, n_1 *is the vertex design point and* n_2 *is the overall centroid*

The E-criterion maximum value for the $K'\theta$ with m factors is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{32m(m-1)}\left[(15m-33)\alpha_1 + (m+17) - \sqrt{D}\right]$$

where $D = \left(256m^2 + 162m - 63\right)\alpha_1^2 - \left(30m^2 - 708m + 30\right)\alpha_1 + \left(m^2 + 34m + 289\right)$

Proof,

From lemma 3.1 ,a unique representation for any matrix $C \in sym(s, H)$ is of the form

$$C = \begin{pmatrix} aU_1 + bU_2 & cV \\ cV' & d\dfrac{V'V}{m} \end{pmatrix}$$

the information matrix $C(M(n(\alpha)))$ for m factors, can be written as follows,

$$C = \begin{pmatrix} aU_1 + bU_2 & cV \\ cV' & d\dfrac{V'V}{m} \end{pmatrix}$$

with the coefficients $a, b, c, d \in \Re$

from lemma (3.1),

$$U_1 = I_m = \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & . \\ 0 & . & . & . & . & 1 \end{pmatrix}$$

$$U_2 = I_m I'_m - I_m = \begin{pmatrix} 1 & . & . & . & . & 1 \\ . & . & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & . \\ 1 & . & . & . & . & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & . \\ 0 & . & . & . & . & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & . & . & . & 1 \\ 1 & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & . \\ 1 & . & . & . & . & 0 \end{pmatrix}$$

and

$$V = \sum_{i=1}^{m} (e_i) \in \Re^{m\times 1} = (e_1 + e_2 + ... + e_m) = \begin{pmatrix} 1 \\ . \\ . \\ . \\ . \\ 1 \end{pmatrix}$$

The information matrix $C(M(n(\alpha)))$ is then given by ,

$$C_K(M(n(\alpha))) = \begin{pmatrix} aU_1 + bU_2 & cV \\ cV' & d\frac{V'V}{m} \end{pmatrix} = \left[\begin{matrix} a\begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & \\ . & & . & & & \\ . & & & . & & \\ . & & & & . & \\ 0 & . & . & . & . & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 & . & . & . & 1 \\ 1 & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & . \\ 1 & . & . & . & . & 0 \end{pmatrix} & c\begin{pmatrix} 1 \\ . \\ . \\ . \\ . \\ 1 \end{pmatrix} \\ c(1 \quad . \quad . \quad . \quad . \quad 1) & d(1) \end{matrix}\right]$$

$$\begin{pmatrix} \frac{32\alpha_1 + \alpha_2}{32m} U_1 + \frac{3\alpha_2}{32m(m-1)} U_2 & \frac{3\alpha_2}{16m(m-1)} V \\ \frac{3\alpha_2}{16m(m-1)} V' & \frac{9\alpha_2}{8m(m-1)} \frac{V'V}{m} \end{pmatrix} \qquad (136)$$

from lemma (3.3) for m factors,

$$D_1 = [a + (m-1)b - d]^2 + 2(m-1)[2c]^2 \qquad (137)$$

$$= \left[\frac{32\alpha_1 + \alpha_2}{32m} + \frac{(m-1)\alpha_2}{32m(m-1)} - \frac{9\alpha_2}{8m(m-1)}\right]^2 + 2(m-1)\left[\frac{2\times 3\alpha_2}{16m(m-1)}\right]^2$$

$$= \frac{\left(\left(225m^2 + 162m - 63\right)\alpha_1^2 + \left(30m^2 - 708m + 30\right)\alpha_1 + \left(m^2 + 34m + 289\right)\right)}{256m^2(m-1)}$$

$$D_2 = [a - b - d]^2 + 4(m-2)[2c]^2 \qquad (138)$$

$$= \left[\frac{32\alpha_1 + \alpha_2}{32m} - \frac{\alpha_2}{32m(m-1)} - \frac{9\alpha_2}{8m(m-1)} \right]^2 + 4(m-2)\left[\frac{2\times 3\alpha_2}{16m(m-1)} \right]^2$$

$$= \frac{\left(\left(961m^2 + 516m - 252\right)\alpha_1^2 + \left(62m^2 - 2632m + 120\right)\alpha_1 + \left(m^2 + 68m + 1156\right)\right)}{1024m^2\left(m-1\right)^2}$$

The eigenvalues are:

$$\lambda_{2,3} = \frac{1}{2}\left[a + \left(m-1\right)b + d \pm \sqrt{D}\right]$$

$$= \frac{1}{2}\left[\frac{32\alpha_1 + \alpha_2}{32m} + \frac{\left(m-1\right)\alpha_2}{32m(m-1)} + \frac{9\alpha_2}{8m(m-1)} \pm \sqrt{D} \right] \qquad \text{..............................} (139)$$

$$= \frac{1}{32m\ \left(m-1\right)}\left[\left(15m - 33\right)\alpha_1 + \left(m+17\right) + \sqrt{D}\right]$$

$$D = \left(256m^2 + 162m - 63\right)\alpha_1^2 - \left(30m^2 - 708m + 30\right)\alpha_1 + \left(m^2 + 34m + 289\right)$$

$$\lambda_{4,5} = \frac{1}{2}\left[a - b + d \pm \sqrt{D_2}\right]$$

$$= \frac{1}{2}\left[\frac{32\alpha_1 + \alpha_2}{32m} - \frac{\alpha_2}{32m(m-1)} + \frac{9\alpha_2}{8m(m-1)} \pm \sqrt{D_2} \right] \qquad \text{..............................} (140)$$

$$= \frac{1}{64m\ \left(m-1\right)}\left[\left(31m - 66\right)\alpha_1 + \left(m+34\right) + \sqrt{D_2}\right]$$

hence the smallest eigenvalue is

$$\lambda_3 = \frac{1}{32m\ \left(m-1\right)}\left[\left(15m - 33\right)\alpha_1 + \left(m+17\right) - \sqrt{D}\right]$$, let

$$\lambda_{\min} = \frac{1}{32m\ \left(m-1\right)}\left[\left(15m - 33\right)\alpha_1 + \left(m+17\right) - \sqrt{D}\right]$$

where $D=\left(256m^{2}+162m-63\right)\alpha_{1}^{2}-\left(30m^{2}-708m+30\right)\alpha_{1}+\left(m^{2}+34m+289\right)$

$\lambda_{\min}$ is the eigenvalue for C that corresponds to the eigenvector, $\bar{z}$,then,

$(C-\lambda I)\bar{z}=\bar{0}$ or $C\bar{z}=\lambda\bar{z}$ with $\bar{z}\neq\bar{0}$

let , $\bar{z}=\begin{pmatrix} z_1 \\ . \\ . \\ . \\ . \\ z_{m+1} \end{pmatrix}$, represent the eigenvector of C that corresponds to λ

Hence, $(C-\lambda I)$ is given as ,

$$\begin{pmatrix} \frac{(16m+2)\alpha_1-18+\sqrt{D}}{32m(m-1)}U_1+\frac{\alpha_2}{32m(m-1)}U_2 & \frac{3\alpha_2}{16m(m-1)}V \\ \frac{3\alpha_2}{16m(m-1)}V' & \frac{(-15m-3)\alpha_1+\left(-m+19+\sqrt{D}\right)}{32m(m-1)}\frac{V'V}{m} \end{pmatrix}$$

Let, $p=(16m+2m)\alpha_1-18+\sqrt{D}, q=\alpha_2=1-\alpha_1$ and

$r=(-15m-3)\alpha_1+(-m+19)+\sqrt{D}$

and $D=\left(256m^{2}+162m-63\right)\alpha_{1}^{2}-\left(30m^{2}-708m+30\right)\alpha_{1}+\left(m^{2}+34m+289\right)$

Thus, $(C-\lambda I)\bar{z}=\bar{0}$

$$\Leftrightarrow \frac{1}{32m(m-1)}\begin{pmatrix} pU_1+qU_2 & 6qV \\ 6qV' & r\frac{V'V}{m} \end{pmatrix}\begin{pmatrix} z \\ . \\ . \\ z_{m+1} \end{pmatrix}=\begin{pmatrix} 0 \\ . \\ . \\ 0 \end{pmatrix}$$

solving these equations for z_1,

$$\bar{z} = \begin{pmatrix} z_1 \\ . \\ . \\ . \\ . \\ z_{m+1} \end{pmatrix} = \begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \\ \frac{-cmq}{r} \end{pmatrix}$$

Where c=3 represents the even number for factors and c varies for the odd numbers of factors as the eigenvector corresponds to $\lambda_{\min}$

Hence,

$$\overline{zz'} = \begin{pmatrix} U_1 + U_2 & \frac{-cmq}{r}V \\ \frac{-cmq}{r}V', & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix}, \|z\|^2 = \frac{mr^2 + c^2m^2q^2}{r^2} \text{.........................…. (141)}$$

$$E = \frac{\overline{zz}}{\|z\|^2} = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} U_1 + U_2 & \frac{-cmq}{r}V \\ \frac{-cmq}{r}V', & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix} \text{............................. (142)}$$

and from equation (60)

$$C_1E = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} \frac{1}{m}U_1 + \frac{1}{m}U_2 & -cqV \\ 0 & 0 \end{pmatrix}$$

from theorem (3.4) a weighted centroid design $n(\alpha)$ is E-optimal for $K'\theta$ in T if and only if $traceC_jE = \lambda_{\min}(C)$

For $j=1, traceC_1E = \frac{r^2}{m(mr^2+c^2m^2q^2)} + ... + \frac{r^2}{m(mr^2+c^2m^2q^2)} = \frac{r^2}{(mr^2+c^2m^2q^2)}$

hence $traceC_jE = \lambda_{\min}(C)$

$$\Leftrightarrow \frac{r^2}{(mr^2+c^2m^2q^2)} = \frac{1}{32m(m-1)}\left[(15m-33)\alpha_1 + (m+17) - \sqrt{D}\right]$$

putting $q=\alpha_2 = 1-\alpha_1$ and $r = (-15m-3)\alpha_1 + (-m+19) + \sqrt{D}$

and $D = (256m^2 + 162m - 63)\alpha_1^2 - (30m^2 - 708m + 30)\alpha_1 + (m^2 + 34m + 289)$

Solving the polynomial using Wxmaxima software, the value of α_1

is then chosen such that $\alpha_1 \in (0,1)$; now substitute the value to $\lambda_{\min}$ and get the values

that maximizes the $\lambda_{\min}$,thus , the optimal E-criterion is,

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{32m(m-1)}\left[(15m-33)\alpha_1 + (m+17) - \sqrt{D}\right]$$

Table 4.4: Summary of $\phi_p - optimal$ weights for $K'\theta$, $m=2,3,4$

m	p	$\alpha_1^{(p)}$	$\alpha_2^{(p)}$	v_p
2	$-\infty$	0.534882	0.465110	0.209302
	-1	0.603283	0.396716	0.265585
	0	0.66666667	0.33333333	0.275160
3	$-\infty$	0.592080	0.407921	0.071642
	-1	0.465023	0.534982	0.1192420

	0	0.50000000	0.50000000	0.125000
4	$-\infty$	0.638661	0.361339	0.06974
	-1	0.443721	0.556281	0.064913
	0	0.40000000	0.60000000	0.070800

A numerical example using fruit blending experiment of three components mixture experiment

The D optimal design for three factors can now be applied to three factor numerical example .Three fruits (Mangoes, passion, and banana) were involved in the experiment. The response on a scale 1-7 was taken as the average score . The twenty one data values are from seven support points for the weighted centroid design each replicated three times. The points comprised the three pure blends, three binary blends, and the three fruits together in the mixture.

Consider the following simplex centroid design for three factors as the initial design

Design points	t_1	t_2	t_3	Average score
1	1	0	0	12.3

2	0	1	0	10.5
3	0	0	1	8.9
4	$\frac{1}{2}$	$\frac{1}{2}$	0	13.5
5	$\frac{1}{2}$	0	$\frac{1}{2}$	12.6
6	0	$\frac{1}{2}$	$\frac{1}{2}$	12.8
7	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	11.8

Where t1=passion,t2=passion and t3=Bananas

From equation 97, $\alpha_1 = \frac{1}{2}$

And from equation 99 $\alpha_2 = \frac{1}{2}$

The unique D-optimal weighted centroid design for $K'\theta$ in m=3 factors is $\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{1}{2}\eta_1 + \frac{1}{2}\eta_2$

Therefore, the corresponding A-optimal for the above designs is as follows,

Design points	t_1	t_2	t_3
1	$\frac{1}{2}$	0	0
2	0	$\frac{1}{2}$	0
3	0	0	$\frac{1}{2}$

4	$\frac{1}{4}$	$\frac{1}{4}$	0
5	$\frac{1}{4}$	0	$\frac{1}{4}$
6	0	$\frac{1}{4}$	$\frac{1}{4}$
7	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$

CHAPTER FIVE

CONCLUSION AND RECOMMENDATION

5.0 Introduction

This chapter presents conclusions, recommendation and recommendations for further research work for this study.

5.1 Conclusion

The study was done based on the selection of the optimality criteria. Kiefer-Wolfowitz equivalence theorem was then applied to each design. All considerations were limited to the weighted centroid designs due to the completeness result. The coefficient matrix K was obtained by use of unit vectors and characterization of feasible weighted centroid designs. Depending on the coefficient matrix $K'\theta$ of interest selected, the optimal moments and information matrices were then obtained. Consequently, unique A- , D- and E-optimal weighted centroid designs were obtained for the third degree Kronecker model with $m \geq 2$ factors. From the results obtained, the unique A- , D- and E-optimal weighted centroid designs for the $K'\theta$ exists, for third-degree model with $m \geq 2$ factors for the selection of the coefficient matrix unique to this study. The weights $\alpha_1^{(p)}$, $\alpha_2^{(p)}$ and the appropriate optimum value $v_p = (\phi_p \circ C_k \circ M \circ \eta)(\alpha^{(p)})$ for respective factors were obtained numerically for selected values of $p \in [-\infty,1]$ .The results obtained indicated that: Coefficient matrix K obtained had a full column rank and helped in identification of the linear parameter subsystem; the optimal moments obtained reflected the statistical properties of designs and was useful in finding the information matrix; The average-variance criterion (A- criterion) and the optimality criteria were both dependent on the information matrix, as the number of m factors increases, $\alpha_1^{(p)}$ decreases while $\alpha_2^{(p)}$ increases and the value of the maximum criterion decreases. For the determinant criterion (D-criterion), as the number of m factors increases, $\alpha_1^{(p)}$ decreases while $\alpha_2^{(p)}$ increases and the value of the maximum criterion decreases. For the smallest eigenvalue criterion (E-criterion) as the number of m factors increases, $\alpha_1^{(p)}$ increases while $\alpha_2^{(p)}$ decreases and the value of the maximum criterion decreases. This indicates that the maximal parameter design reflects well the statistical properties due to increasing symmetry as the number of factor's increases unlike the other designs. In conclusion, results based on maximal parameter subsystem, third degree mixture model with two, three, four, and generalized to m factors for D-, A- and E-optimal weighted centroid designs for the parameter subsystem exist and thus the goal for this specific study was achieved. The study brought in improvement in D-, A- and E-optimal designs as the study improved from second degree Kronecker model maximal parameter subsystem to third degree Kronecker model maximal parameter subsystem in which the information matrix obtained carries more information . The D-optimality criterion, which looks for designs that maximize the determinant of the information matrix, is the most frequently used optimality criterion to choose the designs. The D-optimality criterion has a very important property in optimal designs ,it minimizes the variance and the covariance of the parameter estimates.

5.2 Recommendation

In this study, the third degree mixture Kronecker model was considered adequate and reliable for use in estimation and prediction in mixture experiments to yield optimal results. The Kronecker model is useful in situations where decisions are made on the amounts of the various components have to be decided to give desired properties of the mixture. Therefore, the study recommends use of designs obtained by experimenters in designing of experiments to yield optimal results in technological fields.

5.3 Recommendations for Further Research Work

This study concentrated on optimal weighted centroid designs for maximal parameter subsystem for third degree Kronecker model mixture experiments. The study recommends that the third degree Kronecker model can be extended to fourth degree Kronecker model mixture experiments. The fourth degree will develop more improved designs, since the symmetric matrix will be larger than second and the third degree carrying more information and more optimal values.

REFERENCES

Abd El-Sattar, H., Sultan, H. M., Kamel, S., Khurshaid, T., & Rahmann, C. (2021). Optimal design of stand-alone hybrid PV/wind/biomass/battery energy storage system in Abu-Monqar, Egypt. *Journal of Energy Storage*, *44*, 103336.

Atkinson, A.C and Donev, A.N (1992). *Optimum Experimental Designs.* Oxford: Clarendon Press.

Bai, Z. Z., & Wu, W. T. (2021). On greedy randomized augmented Kaczmarz method for solving large sparse inconsistent linear systems. *SIAM Journal on Scientific Computing*, *43*(6), A3892-A3911.

Bu, X., Majumdar, D., & Yang, J. (2020). D-optimal designs for multinomial logistic models.

Buedo-Fernández, S., & Nieto, J. J. (2020). Basic control theory for linear fractional differential equations with constant coefficients. *Frontiers in Physics*, *8*, 377.

Chen, Y. (2021). *Autonomous Navigation and Planning Technology for Quad-rotors Unmanned Aerial Vehicle (UAV) System* (Doctoral dissertation, University of Technology Sydney (Australia)).

Cheng, C. S. (1995). Complete class results for the moment matrices of designs over permutation-invariant sets. Annals of statistics, Vol. 23: 41-54.

Chernoff, H. (1953). Locally optimal designs for estimating parameters. *Annals of mathematical Statistics*, 24(4), 586–602.

Cheruiyot, W.K. (2017). Optimal designs for third degree kronecker model mixture experiments with application in blending of chemicals for the control of mites in strawberries. *Ph.D. Thesis Moi University*.

Cherutich, M. (2012). Information matrices non-maximal parameter subsystem for Second-degree mixture experiments, *American journal of mathematics and Mathematical sciences,* (*Open access journal*).

Cornell, J. A. (1990). *Designing experiments with mixtures*. Willy New York.

Cornell, J. A. (2002). Experiments with Mixtures, Third Edition. John Wiley, New York.

Draper, N. R. and Pukelsheim, F. (1998). Mixture models based on homogeneous Polynomials. *Journal of statistical planning and inference,* **71**, 303-311.

Draper, N. R., Heiligers, B. and Pukelsheim, F. (1996). Optimal third order rotatable designs. In: *Annals of the Institute of statistical Mathematics,* Vol. **48:**395-402.

Draper, N. R., Heiligers, B. and Pukelsheim, F. (1998). Kiefer ordering of simplex designs for second-degree mixture models with four or more ingredients. *Annals of statistics.*

Draper, N. R., Heiligers, B. and Pukelsheim, F. (1999). Kiefer ordering of simplex designs for second-degree mixture models with four or more ingredients. *Annals of statistics*. Vol. **79(2)**: 325-348.

Draper, N. R., Heiligers, B. and Pukelsheim, F. (2000). Kiefer ordering of simplex designs for mixture models with four or more ingredients. *Annals of statistics*, **28**, 578-590.

Ehrenfeld, E. (1955). On the efficiency of experimental design. *Annals Mathematical Statistics*, 26(2), 247–255.

Elfving, G. (1952). Optimum allocation in linear regression theory. *The Annals of Mathematical Statistics*, *23*(2), 255-262.

Gaffke, N., (1987). Further characterizations of design optimality and admissibility for partial parameter estimation in linear regression. *Annals of Statistics,* Vol. **15,** 942-957.

Gaffke, N.and Heiligers. (1996). Approximate designs for polynomial regression: invariance admissibility, and optimality, in design and analysis of Experiments. *Handbook of Statistics, Vol. 13(Ghosh, S. and Rao, C. R., Eds),* Vol. **13:**1149-1199. North-Holland, Amsterdam.

Galil, Z. and Kiefer, J. C. (1977). Comparison of simplex designs for quadratic mixture models. *Technometrics*, **19**, 445-453.

Gichuki, K. T., Joseph, K., & John, M. (2020). The D-, A-, E-and T-optimal values of a second order rotatable design in four dimension constructed using balanced incomplete block designs. *American Journal of Applied Mathematics*, *8*(3), 83-88.

Gou, J., Sun, L., Du, L., Ma, H., Xiong, T., Ou, W., & Zhan, Y. (2022). A representation coefficient-based k-nearest centroid neighbor classifier. *Expert Systems with Applications*, *194*, 116529.

Gregory K., Joseph K., Mike R., Korir B., Benard R., Kinyanyui J., Kungu P.(2014). D-Optimal Designs for Third-Degree Kronecker Model Mixture Experiments with an Application to Artificial Sweetener Experiment,IOSR Journal of Mathematics, Vol.10,32-41.

Hajibabaei, H., Seydi, V., & Koochari, A. (2023). Community detection in weighted networks using probabilistic generative model. *Journal of Intelligent Information Systems*, *60*(1), 119-136.

Hsissou, R., Seghiri, R., Benzekri, Z., Hilali, M., Rafik, M., & Elharfi, A. (2021). Polymer composite materials: A comprehensive review. *Composite structures*, *262*, 113640.

Husain, B., & Hafeez, A. (2023). D-and A-optimal orthogonally blocked mixture component-amount designs via projections. *Statistics, Optimization & Information Computing*, *11*(3), 655-669.

Janczura, M., Sip, S., & Cielecka-Piontek, J. (2022). The development of innovative dosage forms of the fixed-dose combination of active pharmaceutical ingredients. *Pharmaceutics, 14*(4), 834.

Karatina, K. (2021). A-Optimal Slope Design for Second Degree Kronecker Model Mixture Experiment With Four Ingredients With Application in Selected Fruits Blending. *International Journal of Statistics and Probability, 10*(2).

Kerich, G.K. (2012). Optimal designs for third degree Kronecker model mixture experiments. *Ph.D. Thesis Moi University.*

Kiefer, J. C. (1959). Optimum experimental designs. *J. Roy. Statist. Sec ser.* Vol. **B. 21**:272-304.

Kiefer, J. C. (1975). Optimal design: variation in structure and performance under change of criterion. *Biometrika,* **62**, 277-288.

Kiefer, J. C. (1978). Asymptotic approach to families of design problems. Comm.*Statist. Theory methods,* **A7**, 1347-1362.

Kiefer, J., & Wolfowitz, J. (1959). Optimum designs in regression problems. *The Annals of Mathematical Statistics*, 271-294.

Kinyanjui, J. K. (2007). "Some optimal designs for second-degree Kronecker model mixture experiments." *Ph.D. Thesis Moi University.*

Kinyanjui, J. K., Koske, J. K. and Korir, B. C. (2008). Optimal Kiefer ordering of Simplex designs for second-degree mixture models with three ingredients: An application to the Blending Chemicals pesticides for control of Termites. *Journal of Agriculture, Pure and Applied Science and Technology 2, 45-63.*

Kinyanyui, J., Kungu, P., Ronoh, B., Korir, B., Koske, J., & Kerich, G. (2014). D-Optimal Designs for Third-Degree Kronecker Model Mixture Experiments with an Application to Artificial Sweetener Experiment.

Kiplagat, k. (2014). Optimal design for second-degree Kronecker model mixture experiments for Maximal parameter subsystem. *M.Sc. Thesis University of Eldoret.*

Klein, T. (2001). Optimal designs for second-degree kroneker model mixture experiments. *Journal of statistical planning and inference,* Vol.**123:**117-131.

Klein, T. (2002). Optimal designs for second-degree Kronecker model mixture experiments. *Journal of statistical planning and inference.*

Klein, T. (2004). Invariant symmetric block matrices for the design of mixture experiments. *Linear Algebra and its Applications,* Vol.**388:**261-278.

Korir, B.C. (2008). Kiefer ordering of simplex designs for third –degree mixture Models.*Ph.D. Thesis Moi University.*

Kung'u, N. P., Koske, J. A., & Kinyanjui, J. K. (2020). D-Optimal Slope Design for Second Degree Kronecker Model Mixture Experiment With Three Ingredients. *International Journal of Statistics and Probability*, *9*(2), 1-30.

LaMotte, L. R., (1977). A canonical form for the general linear model. *Annals of Statistics,* Vol.**5:**787-789.

London, Griffin. Scheffe', H. (1958). Experiments with mixtures. J. *Roy. Statist. Soc. Ser.B**20**,*344-360.

Lu, M., Hydock, J., Radlińska, A., & Guler, S. I. (2022). Reliability analysis of a bridge deck utilizing generalized gamma distribution. *Journal of Bridge Engineering*, *27*(4), 04022006.

Lyche, T. (2020). *Numerical linear algebra and matrix factorizations* (Vol. 22). Springer Nature.

Mandal, S. (2000). Construction of optimizing distributions with applications in estimation and optimal design. *Ph.D. Thesis, University of Glasgow*.

Mannarswamy, A. K. (2018). *Engineering Applications of D-Optimal Designs*. New Mexico State University.

Marks, J., Andalman, B., Beardsley, P. A., Freeman, W., Gibson, S., Hodgins, J., ... & Shieber, S. (2023). Design galleries: A general approach to setting parameters for computer graphics and animation. In *Seminal Graphics Papers: Pushing the Boundaries, Volume 2* (pp. 73-84).

Muriungi R.G., Koske J.K. & J.M. Mutiso. (2017). Applying the polynomial model in simplex-centroid design to formulate the optimum dairy feed International Journal of Sciences: Basic and applied science, ISSN 2307-4531PP.101-117.

Ngigi, P. K. (2009). "Optimality criteria for second-degree Kronecker model mixture experiments with two, three, and four ingredients. *Phil. Thesis Moi University.*

Özbek, N. S., & Eker, I. (2020). Design of an optimal fractional fuzzy gain-scheduled Smith Predictor for a time-delay process with experimental application. *ISA transactions*, *97*, 14-35.

Pázman, A. (1986). *Foundations of optimum experimental design* (Vol. 14). Springer.

Piepel G. F and Cornell J.A. (1994). Mixture experiment approaches: examples, discussion, and recommendation. *Journal of Quality Technology, Vol 26,177-196.*

Prescott, P.; Dean, A.M.; Draper, N.R., Lewis, S.M., (2002). Mixture experiments; III Conditioning and Quadratic Model Specification. *Technometrices,* **44**: 260-268.

Pukelsheim, F. (1993)." Optimal design of experiments". Wiley, New York.

Qi, R., Tao, G., & Jiang, B. (2019). Fuzzy system identification and adaptive control.

Quenouille M. H., (1953), "The Design and Analysis of Experiment",

Rao, C.R.and Rao, M.B. (1998). Matrix Algebra and its Application to Statistics and Economics, *World Scientific*, Singapore.

Scheffe`, H. (1958). Experiments with mixtures. *J. Roy. Statist. Soc. Ser*. Vol. **B 20**: 344-360.

Scheffe', H. (1963). The simplex-centroid design for experiments with mixtures.*J. Roy. Statist. Soc. Ser*. **B 25**, 235-257.

Schennach, S. M., & Starck, V. (2022). *Optimally-transported generalized method of moments*. Cemmap, Centre for Microdata Methods and Practice, The Institute for Fiscal Studies, Department of Economics, UCL.

Searle, S. R., & Khuri, A. I. (2017). *Matrix algebra useful for statistics*. John Wiley & Sons.

Shah, S. B., Zhe, C., Yin, F., Khan, I. U., Begum, S., Faheem, M., & Khan, F. A. (2018). 3D weighted centroid algorithm & RSSI ranging model strategy for node localization in WSN based on smart devices. *Sustainable cities and society*, *39*, 298-308.

Shahmohammadi, A., & McAuley, K. B. (2018). Sequential model-based a-optimal design of experiments when the fisher information matrix is noninvertible. *Industrial & Engineering Chemistry Research*, *58*(3), 1244-1261.

Sitienei, C. (2019). *An Application Of Mixture Experiments In Formulation Of Poultry Feed For Modelling Chick Weight* (Doctoral Dissertation, University Of Eldoret).

Sitienei, C. M., Okango, A. A., & Otieno, A. R. (2019). Application of Mixture Experiments in Poultry Feed Formulation. *African Journal of Education, Science and Technology*, *5*(3), 15-28.

Smith, K. (1918). On the Standard Deviations of Adjusted and Interpolated Values of an Observed Polynomial Function and Its Constant and the Guidance, they give towards a proper choice of the distribution of the observation. *Biometrika* 12,1-85.

Wald, A. (1943). On the efficient design of statistical investigations. *The annals mathematical statistics*, *14*(2), 134-140.

Wambui, N. E., Joseph, K., & John, M. (2021). I-Optimal Axial Designs for Four Ingredient Concrete Experiment. *American Journal of Theoretical and Applied Statistics*, *10*(1), 32-37.

Wang, C., Fan, H., & Qiang, X. (2023). A Review of Uncertainty-Based Multidisciplinary Design Optimization Methods Based on Intelligent Strategies. *Symmetry*, *15*(10), 1875.

Yang, M. (2008). A-optimal designs for generalized linear models with two parameters. *Journal of Statistical Planning and Inference*, *138*(3), 624-641.

Zhu, J. X., Zhu, Z., & Au, S. K. (2023). Accelerating computations in two-stage Bayesian system identification with Fisher information matrix and eigenvalue sensitivity. *Mechanical Systems and Signal Processing*, *186*, 109843.