E-OPTIMAL DESIGNS FOR SECOND-DEGREE KRONECKER MODEL MIXTURE EXPERIMENTS

BY

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DECLARATION

Declaration by the student

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DEDICATION

To my beloved parents and future family.

ABSTRACT

Many products are formed by mixing together two or more ingredients. For example, in building construction, concrete is formed by mixing sand, water and cement. Many practical problems are associated with investigation of mixtures of m ingredients, assumed to influence the response through the proportions in which they are blended together. Second degree Kronecker model put forward by Draper and Pukelsheim isapplied in the study.This study investigate E-optimal designs in the second degree Kronecker model for maximal and non-maximal parameter subsystem for $m \geq 2$ ingredients, where Kiefer's function serves as optimality criteria. The consideration is restricted to weighted centroid design for completeness of results. By employing the Kronecker model approach, coefficient matrices and a set of feasible weighted centroid designs for maximal and non-maximal subsystem of parameters is obtained. Once the coefficient matrix is developed, information matrices associated to the parameter subsystem of interest for two, three, four and generalization to m ingredients is obtained. E-optimal weighted centroid designs based on maximal and non-maximal parameter subsystem for the corresponding two, three, four and m ingredients is derived. A general formula also for the computation of smallest eigenvalues is obtained. In addition optimal, weights and values for the weighted centroid designs are numerically obtained using Matlab software. Results based on non-maximal and maximal parameter subsystem, second degree mixture model with $m \geq 2$ ingredient for E-optimal weighted centroid design for $K'\theta$ hence exist.

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CHAPTER ONE

INTRODUCTION

1.1 Background information

A mixture experiment involves mixing of different proportions of two or more components to make different compositions of an end product. Consequently, many practical problems are associated with the investigation of mixture ingredients which are assumed to influence the response through the proportions in which they are blended together. The definitive text, Cornell (1990) lists numerous examples and provides a thorough discussion of both theories and practices. Early seminal work was done by Scheffe' (1958, 1963) in which he suggested and analyzed canonical models when the regression function for the expected response is a polynomial of degree one, two, or three, Cherutich (2012).

The m component proportions, $t_1,\ldots,t_m$ form the column vector of experimental conditions, $t_i=(t_1,\ldots,t_m)'$ with $t_i \geq 0$ and further subject to the simplex restriction,

$$\sum_{i=1}^{m} t_i = 1 \qquad (1.1)$$

Let $1_m = (1,\ldots,1)' \in \Re^m$ be the unity vector, whence, $1_m' t$ is the sum of the components of t. Therefore, the experimental conditions are points in the probability simplex, which constitute the independent and controlled variables with the experimental domain being the simplex,

$$\mathrm{T} = \{t \in [0,1]^m ; 1_m' t = 1\} \qquad (1.2)$$

Under experimental conditions $t \in \mathrm{T}$, the experimental response Y_t is taken to be a scalar random variable. Replications under identical experimental conditions or response from distinct experimental conditions are assumed to be of equal (unknown) variance, σ^2 and uncorrelated.

An experimental design τ is a probability measure on the experimental domain T_m with finite support points. If τ assigns weights w_1, w_2,… to its points of support in T_m, then the experimenter is directed to draw proportions w_1, w_2,… of all observations under the respective experimental conditions. Furthermore, the observed response Y_t is expressed as $Y_t = \eta(t,\Theta) + \varepsilon(t)$, where $\eta(t,\Theta)$ is the expected response and $\varepsilon(t)$ is the error term. The expected response $\eta(t,\Theta)$ can be expressed as a function of t. For the second-degree model, Draper and Pukelsheim (1998) proposed a representation involving the Kronecker square t⊗t. Its regression functions

$f : \mathrm{T}_m \rightarrow \Re^{m^2}, t = (t_1,\ldots,t_m)' \rightarrow t \otimes t = t_i t_j, i, j = 1,..m$ with the lexicographical order of the subscripts. This representation yields the model equation;

$$E[Y_t] = f(t)'\theta = \sum_{i,j=1}^{m} \theta_{ii} t_i^2 + \sum_{i,j=1} (\theta_{ij} + \theta_{ji}) t_i t_j \qquad (1.3)$$

Where Y_t, the observed response under the experimental conditions $t \in \mathrm{T}$, is taken to be a scalar random variable and $\Theta = (\theta_{11}, \theta_{22}, \ldots., \theta_{mm})' \in \Re^{m^2}$ is unknown parameter.

The Kronecker representation has several advantages which include more compact notations, more convenient invariance properties and the homogeneity of the regression terms. Draper and Pukelsheim (1998) and Prescott, *et al*., (2002). The moment matrix $M(\tau) = \int_{\mathrm{T}} f(t) f(t)' d\tau$ for the second-degree Kronecker-model has all moments homogeneous in degree four and reflects the statistical properties of a design τ. Graffke and Heilingers (1996) and Pukelsheim (2006) gave a review of the general design environment. Klein (2004) showed that the class of weighted centroid designs is essentially complete for m≥2 ingredients, for Kiefer ordering. As a consequence, the search for optimal designs may be restricted to weighted centroid designs for most criteria.

Kinyanjui (2007) and Ngigi (2009) showed that unique D-and A-optimal weighted centroid designs, second degree mixture experiments for maximal parameter subsystem with m≥2 ingredients exist for $K'\theta$ .Cherutich (2012), proved that D-and A-optimal weighted centroid design, second degree mixture experiments for non-maximal parameter subsystem with m≥2 ingredients also do exist for $K'\theta$. The study extends the work done by Kinyanjui (2007) and Ngigi (2009) by deriving E-optimal weighted centroid designs for second degree Kronecker model mixture experiments for maximal and non-maximal parameter subsystem respectively with m≥2 ingredients.

1.2 Statement of problem

The general problem here is to obtain a design with maximum information for the maximal and non-maximal parameter subsystem $K'\theta$. This is accomplished through the application of the E-optimality criterion to a weighted centroid design which follows from the Kiefer-Wolfowitz equivalence theorem.

1.3 Objectives

The specific objectives of the study are:

1. To derive E-optimal weighted centroid designs for a maximal and non-maximal parameter subsystem corresponding to two, three and four and generalize to m ingredients.

2. To obtain the smallest eigenvalues for two, three and four and generalize to m ingredient for non-maximal and maximal parameter subsystem.
3. To obtain numerical V_p-optimal values for weighted centroid design for $K'\theta$

1.4 Significance of the study

Many practical problems in mixture experiments are associated with the investigation of mixture of ingredients which are assumed to influence the response only through the proportions in which they are blended together. As a consequence, competing designs will arise, hence, this study will be desirable since it will help in identifying the optimal design.

CHAPTER TWO

LITERATURE REVIEW

2.1Introduction

Experiments based on mixtures were first discussed by Quenouille (1953). Later on, Scheffe’ (1958, 1963) made a systematic study and laid a strong foundation. Draper and Pukelsheim (1998) proposed a set of mixture models referred to as k-models. They are alternative representation of mixture models based on the Kronecker algebra of vectors and matrices. They offer alternative symmetries, compact notations and homogeneity in ingredients.

The first-degree model is given by the equation;

$$E[Y_t] = \sum_{i=1}^{m} t_i \theta_i = t'\theta \tag{2.1}$$

For the second-degree model, Draper and Pukelsheim (1998) proposed a representation involving the Kronecker square $t \otimes t$, the m^2x1 vector consisting of the squares and cross products of the components of t in the lexicographic order of the subscripts. This is referred to as Kronecker-model with a Kronecker-polynomial and expressed by the regression function

$$E[Y_t] = \sum_{i=1}^{m} \sum_{j=1}^{m} t_j t_i \theta_{ij} = (t \otimes t)'\theta \tag{2.2}$$

2.2Kronecker products

The Kronecker product approach is based on second-degree polynomial regression in m variables $t = (t_1,..., t_m)'$ on the matrix of all cross products:

$$tt' = \begin{matrix} & t_1 & t_2 & \cdots & t_m \\ t_1 & t_1^2 & t_1t_2 & \cdots & t_1t_m \\ t_2 & t_2t_1 & t_2^2 & \cdots & t_2t_m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_m & t_mt_1 & t_mt_2 & \cdots & t_m^2 \end{matrix}, \tag{2.3}$$

rather than reducing them to the Box-Hunter minimal set of polynomials $(t_1^2,\cdots,t_m^2,t_1t_2,\cdots,t_{m-1}t_m)$.The benefits enjoyed are; the distinct terms are repeated appropriately according to the number of times they can arise, the transformational rules with a conformable matrix R become simple, $(Rt)(Rt)' = R(tt')R'$ and that the approach extends to third degree polynomial regression.

For a $k \times m$ matrix A and a $l \times n$ matrix B, their Kronecker product $A \otimes B$ is defined to be the $kl \times mn$ block matrix

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1m}B \\ \vdots & \ddots & \vdots \\ a_{k1}B & \cdots & a_{km}B \end{pmatrix}. \tag{2.4}$$

The Kronecker product of a vector $s \in \Re^m$ and another vector $t \in \Re^n$ then is simply a special case,

$$\mathrm{s} \otimes \mathrm{t} = \begin{pmatrix} \mathrm{s_1 t} \\ \vdots \\ \mathrm{s_m t} \end{pmatrix} = (\mathrm{s_i t_j})_{\substack{i=1,\ldots,m,\, j=1,\ldots,n \in \Re^{mn} \\ in\ lexicographic\ order}} . \tag{2.5}$$

A key property is their product rule $(A \otimes B)(s \otimes t) = (As) \otimes (Bt)$.

This has nice implications for transposition, $(A \otimes B)' = (A') \otimes (B')$, for Moore-Penrose inversion, $(A \otimes B)^+ = (A^+) \otimes (B^+)$ and if possible for regular inversion $(A \otimes B)^{-1} = (A^{-1}) \otimes (B^{-1})$

It is of specific importance that the Kronecker product preserves orthogonality. That is, if A, and B are individual orthogonal matrices, then their Kronecker product $(A \otimes B)$ is also an orthogonal matrix. Thus, while the matrix tt' assembles the cross products $t_i t_j$ in an $m \times m$ array, the Kronecker square $t \otimes t$ arranges the same numbers as a long $m^2 \times 1$ vector. The transformation with a conformable matrix R simply amounts to $(Rt) \otimes (Rt) = (R \otimes R)(t \otimes t)$. This greatly facilitates our calculations when we now apply Kronecker product to response surface models.

2.3 Kiefer design ordering

Kiefer design ordering has two steps. The first step is the majorization ordering. The second step is an improvement relative to the usual Loewner matrix ordering within the class of exchangeable moment matrices. For the second-degree Kronecker-moment matrix homogeneous in degree four, the moment matrix for four factors exhausts all the moments. Given two moment matrices $M(\eta)$ and $M(\tau)$ in two factors, $M(\eta) \geq M(\tau)$ if and only if $M_2(\eta) \geq M_2(\tau)$ and $M_4(\eta) \geq M_4(\tau)$, (Draper and Pukelsheim,1998).

The vertex design points η_1 and the overall centroid design η_2 play a special role; they are used to generate weighted centroid designs in the following sense; for weights $\alpha_1, \alpha_2 \geq 0$ with $\alpha_1 + \alpha_2 = 1$, the design $\eta = \alpha_1 \eta_1 + \alpha_2 \eta_2$ will be called a weighted centroid design. In the second-degree mixture model for m$\geq$4 ingredients, the set of weighted centroid designs $\eta = \{\alpha_1 \eta_1 + ... + \alpha_m \eta_m ; (\alpha_1, ..., \alpha_m)' \in \mathrm{T}\}$ is convex and constitutes a minimal complete class for the Kiefer ordering.

2.4 Kiefer Optimality

The set of weighted centroid designs constitute a minimal complete class of designs for the Kiefer ordering. Completeness of C (set of weighted centroid designs) means that for every design τ not in C, there is a member ξ in C that is Kiefer better than τ. That is it must be shown that ξ is more informative than τ, M (ξ)>M (τ), and that the two are not Kiefer equivalent. The weighted centroid design must be shown to satisfy

$M(\xi) \geq M(\bar{\tau}) \prec M(\tau)$, that is, $M(\xi) > M(\tau)$ hence satisfying the Kiefer optimality of $M(\xi)$.

Let H be a subgroup of nonsingular $s \times s$ matrices. No assumption will be placed on the set $M \subseteq NN(k)$ of competing moment matrices. A moment matrix $\mathrm{M} \in M$ is called Kiefer optimal for $k'\theta$ in M relative to the group H⊆GL(s) when the information matrix C_k(M) is H-invariant and satisfies

$$C_k(M) >> C_k(A) \text{ for all } A \in M, \tag{2.6}$$

where>> is the Kiefer ordering on sym(s) relative to H.

Draper and Pukelsheim (1998) proved that the assumption $M(\xi) \geq M(\tau)$ cannot hold true, rendering the class C minimal complete. Thus any design that is not a weighted centroid can be improved upon in terms of symmetry and Loewner ordering. Within the class of weighted centroid designs, however, other criteria will be needed to attain further improvement for example, the determinant criteria.

2.5 The Quadratic subspace $\mathrm{sym}(\mathbf{s}, \mathbf{H})$

In the theory of statistical experiments, quadratic subspaces of symmetric matrices arise when certain invariance properties of information matrices involved in the design are considered. We analyze a specific example of such a quadratic subspace and demonstrate how to apply the results of this analysis to designs in a second-degree polynomial regression model for mixture experiments, for $m \geq 2$, we denote the canonical unit vectors in $\Re^m$ by $e_1, e_2, \cdots, e_m$. The canonical unit vectors in $\Re^{\binom{m}{2}}$ are denoted by E_{ij} with lexicographically ordered index pairs (i,j), $1 \leq i < j \leq m$. Let ϑ_m denote the symmetric group of degree m, and let $perm(m)$ be the group of $m \times m$ permutation matrices.

We define

$$H = \left\{ H_\pi = \begin{pmatrix} R_\pi & 0 \\ 0 & S_\pi \end{pmatrix} : \pi \in \vartheta_m \right\} \tag{2.7}$$

with

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

and

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

Where $(\pi(i), \pi(j)) \uparrow$ denotes the pair of indices $\pi(i),\quad \pi(j)$ in ascending order. The set H is a subgroup of $perm\left(\binom{m+1}{2}\right)$ and is isomorphic to ϑ_m. It acts on the space $sym\left(\binom{m+1}{2}\right)$ through the congruence transformation $(H, C) \mapsto HCH'$ and induces subspace

$$sym\left(\binom{m+1}{2}, H\right) = \left\{C \in sym\left(\binom{m+1}{2}\right) : HCH \qquad for \quad all \quad H \in H\right\} \tag{2.8}$$

of H-invariant symmetric matrices. Since H is a subgroup of the permutation matrix group, H-invariance of a matrix $C \in sym(s)$ means that certain entries of C coincide. The following lemma from Draper and Pukelsheim (1998) describing the linear structure of $sym(s, H)$, shows that an H-invariant symmetric matrix has at most seven distinct elements.

Lemma 2.5

We define the identity matrices $U_1 = I_m$ and $W_1 = I_{\binom{m}{2}}$, and write $1_m = (1,1,\cdots,1)' \in \Re^m$.

Furthermore, we define

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

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

$$V_2 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k=1 \\ k \notin \{i,j\}}}^{m} E_{ij} e_k' \in \Re^{\binom{m}{2}\times m},$$

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

$$W_3 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k,l=1 \\ k<l \\ \{i,j\}\cap\{k,l\}=\phi}}^{m} E_{ij} E_{kl}' \in sym\left(\binom{m}{2}\right).$$

Then any matrix $C \in sym(s,H)$ can be uniquely represented in the form

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \tag{2.9}$$

With coefficients $a,\cdots,g \in \Re$. The terms containing V_2, W_2 and W_3only occur for $m \geq 3$ and $m \geq 4$ respectively.

In particular,

$$\dim sym(s,H) = \begin{cases} 4 & for \quad m = 2 \\ 6 & for \quad m = 3 \\ 7 & for \quad m \geq 4 \end{cases}.$$

Proof

Given a symmetric matrix $C \in sym(s,H)$, we partition this matrix according to the block structure of matrices in H, that is

$$C = \begin{pmatrix} C_{11} & C_{21}' \\ C_{21} & C_{22} \end{pmatrix} \tag{2.10}$$

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

Then, H-invariance of C can be expressed by the block wise conditions;

$$R_\pi C_{11} R_\pi' = C_{11},\ S_\pi C_{21} R_\pi' = C_{21}.\ S_\pi C_{22} S_\pi' = C_{22} \text{ for all } \pi \in \vartheta_m \tag{2.11}$$

Straightforward multiplication shows that the blocks given in (2.9) satisfy these conditions. For the reverse direction, we compare the entries of the matrices on both sides of the equations in (2.11) and obtain

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

Uniqueness of this representation in (2.9) follows from the linear independence of the sets $\{U_1, U_2\}, \quad \{V_1, V_2\} \quad and \quad \{W_1, W_2, W_3\}$ ▪

We now turn to the quadratic structure of $sym(s, H)$, that is, the additional property that $sym(s, H)$ is closed under formation of matrix powers. The block representation given in (2.9) implies that, powers of H-invariant symmetric matrices involve products of U_i, V_j and W_k. The following lemma presents a multiplication table for these matrices.

Lemma 2.6

The results of multiplication of the matrices U_i, V_j and W_k are as follows:

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

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

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

$$V_1U_2 = V_1 + 2V_2, \quad V_2U_2 = (m-2)V_1 + (m-3)V_2,$$
$$W_2V_1 = (m-2)V_1 + 2V_2, \quad W_2V_2 = (m-2)V_1 + 2(m-3)V_2,$$
$$W_3V_1 = (m-3)V_2, \quad W_3V_2 = \binom{m-2}{2}V_1 + \binom{m-3}{2}V_2.$$

(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

The equations are verified by elementary calculations and by occasionally using the 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 (2.6), products of matrices in $sym(s,H)$ can be calculated by mere symbolic manipulation and by multiplication of scalars. It is this result that allows us to perform the calculations involved in the design problem in an effective way. Furthermore, the multiplication table can be implemented in a computer-algebra system like maple.

As a side result of lemma (2.6) and the fact that $traceU_2 = traceW_2 = traceW_3 = 0$, the basis matrices;

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

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

implicitly given in (lemma 2.5) form an orthogonal basis of $sym(s,H)$ with respect to Euclidean matrix scalar product $(A,B) \mapsto traceAB$.(Lemma 2.6), also implies the following results on Moore-Penrose inverses, denoted by a superscript $+$ sign and on schur compliments:

Corollary 2.5

For any $m \geq 2$, suppose the matrix $C \in sym(s,H)$ is partitioned as in (2.10) with diagonal blocks C_{11}, $C_{22}$and off diagonal block C_{21}. Then we have

$$C_{11}^{+} \in span\{U_1, U_2\}\ ,\ C_{11} - C_{21}' C_{22}^{+} C_{21} \in span\{U_1, U_2\}$$

$$C_{22}^{+} \in span\{W_1, W_2, W_3\},\ C_{22} - C_{21} C_{11}^{+} C_{21}' \in span\{W_1, W_2, W_3\}\ .$$

Proof

The assertions on C_{11}^{+} and C_{22}^{+} follow from $\begin{pmatrix} C_{11} & 0 \\ 0 & C_{22} \end{pmatrix} \in sym(s, H)$ and the fact that quadratic subspaces are closed under Moore-Penrose inversion, Rao and Rao (1998), corollary 13.2.2.3). Together with lemma (2.6), these results imply the claims on the schur complements of C_{11} and C_{22}.

CHAPTER THREE

PROBLEM DESIGN

3.1Parameter Subsystem

We adopt the regression model for mixture experiments in which the experimental conditions are nonnegative quantities summing to one. The experimental conditions are points in the probability simplex $T_m = \{t \in \Re^m : 1_m' t = 1\}$, with $1_m = (1,...,1)' \in \Re^m$. In a polynomial regression function, a real-valued quantity Y_t observed under the experimental conditions $t \in T_m$ is assumed to be random with expected value $E[Y_t]$ which is a polynomial in t. The polynomial coefficients are unknown and have to be estimated from the observations. One instance of such a model introduced by Draper and Pukelsheim (1998), is the second-degree Kronecker model,

$$E[Y_t] = f(t)'\theta = (t \otimes t)'\theta = \sum_{i=1}^{m} \theta_{ii} t_i^2 + \sum_{\substack{i,\ j=1 \\ i<j}}^{m} (\theta_{ij} + \theta_{ji}) t_i t_j \qquad (3.1)$$

with the regression function $f(t) = t \otimes t$ and unknown parameter vector $\Theta = (\theta_{11}, \theta_{12}, \ldots, \theta_{mm})' \in \Re^{m^2}$. All observations taken in an experiment are assumed to be uncorrelated and to have common unknown variance. Since the Kronecker model's with parameter vector $\theta \in \Re^{m^2}$ is estimable, we consider a maximal parameter subsystem where all the parameters can be estimated and a non-maximal parameter subsystem where not all the parameters can be estimated.

3.1.1Maximal parameter subsystem

Definition

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

(i) $M \cap A(K) \neq \phi$ (3.2)

(Where $A(K)$ represent feasibility cone)

(ii) $rank\, K = r_M$. (3.3)

In this case, we have $r_M = \binom{m+1}{2}$ and K is called a maximal coefficient matrix for M .

If the set, M contains regular moment matrices, that is, $K = r_M$, the full parameter vector θ or any regular transform of it, is a maximal parameter subsystem for M .

We henceforth assume the set M to be convex. Then there is a matrix $M_0 \in \mathrm{M}$ with maximal range, that is, $\Re(M) \in \Re(M_0)$ for all $M_0 \in \mathrm{M}$, Pukelsheim (2006). While there may be many matrices M_0 with this property, the maximal range $R_m = \Re(M_0)$ is unique, and we have $\dim R_m = r_M$. This construction is analogous to that of a minimal nullspace in LaMotte, (1977).

In this study we define the matrix $K = (K_1, K_2) \in \Re^{m \times \binom{m+1}{2}}$ under maximal parameter subsystem. The coefficient matrix ,

$$K \in \Re^{m^2 \times \binom{m+1}{2}} \tag{3.4}$$

is assumed to have full column rank.

Where

$K_1 = \sum_{i=1}^{m} e_{ii} e_i'$ and $K_2 = \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E_{ij}'$,Kinyanjui (2007)

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

As such, 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 $K'\theta$.

If M be a set of moment matrices. We say that 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 $K \in \Re^{k \times \binom{m+1}{2}}$ of parameter subsystems $K'\theta$ that are estimable within M satisfy $rank\, K \leq r_M$, necessarily. We now consider the extreme case $rank\, K = r_M$, capturing the idea of estimating as many parameters as possible, within given set M of moment matrices.

3.1.2 Non-Maximal Parameter Subsystem

Definition

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

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

and

(ii) $rank\, K < r_M$. (3.5)

In this case an experimenter may wish to study s out of k components rather than being interested with all of them or a single one. The possibility is allowed by studying linear parameters subsystems that have the form for some *k*x*s* matrix *K*;*K* is called the coefficient matrix of the parameter subsystem $K'\theta$. The coefficient matrices $K \in \Re^{kx(m+1)}$ of parameter subsystem $K'\theta$ that is estimable within M since it satisfies $rank\, K < r_M$. This study focuses on estimating a system of linear function, $K'\theta$, of the parameter vector $\theta \in \Re^k$, where the coefficient matrix $K \in \Re^{kx(m+1)}$ is assumed to have a full column rank.

In our case when fitting second degree Kronecker model to a set of observations, a parameter subsystem $K'\theta$ of interest is chosen, where $K \in \Re^{m^2 \times s}$.

We define the K matrix as

$$K = (K_1, K_2) \in \Re^{m^2 \times m+1} \tag{3.6}$$

where, $K_1 = \sum_{i=1}^{m} e_{ii} e_i'$

and $K_2 = \frac{1}{2\binom{m}{2}} \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji})$

An experimental design for a mixture experiment is a probability measure τ on T_m with finite support. Each support point $t \in supp\,\tau$ directs an experimenter to take a proportion

T({t}) of all observations under the experimental condition t. The statistical properties of a design τ are reflected by the moment matrix

$$M(\tau) = \int_{T_m} f(t) f(t)' d\tau \in NND(m^2)\,, \tag{3.7}$$

Where NND(m^2) denotes the cone nonnegative definite $m^2 \times m^2$ matrices. The amount of information which the design T contains on the parameter system $K'\theta$ is captured by the information matrix for $K'\theta$.

3.2 E-Optimal Weighted Centroid Design

We now derive optimal weighted centroid designs for the smallest eigenvalue criterion, $\phi_{-\infty}$, that is, E-optimality criteria. To forge our way forward, we need to adopt three theorems in Pukelsheim (2006), which specifically focuses on E-optimality.

Theorem 3.2.1

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

Theorem 3.2.2

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

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

(i) 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

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

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

(ii) 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 weighted design which is E-optimal for $K'\theta$ in T, then the information matrix $\tilde{C} = C_k(M(\eta(\beta)))$, satisfies

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

The following theorem dictates on the choice of the matrix E of theorem (3.2.2) above.

Theorem 3.2.3

Let $M \in M$ be a competing moment matrix that is feasible for $K'\theta$ and let $\pm z \in \Re^s$ be an eigenvector corresponding to the smallest eigenvalue of the information matrix, $C_k(M)$. 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 (3.2.2) 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

We show that the normality inequality of theorem (3.2.2) for $\phi_{-\infty} - optimality$ coincides with that of theorem (3.2.1) for scalar optimality.

With $E = \frac{zz'}{\|z\|^2}$, the normality inequality of theorem (3.2.1) 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 (3.2.1) is

$$k'G'AGk \le k'M^{-}k \text{ for all } A \in M$$

With $c = Kz$, the two left hand sides are the same. So are the right hand sides, because of

$$k'M^{-}k = z'K'M^{-}Kz = z'C^{-1}z = \frac{\|z\|^2}{\lambda_{\min}(C_k(M))}.$$

If the smallest eigenvalue of $C_k(M)$ has multiplicity 1, then the only choice for E is

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

Therefore in obtaining optimal designs for E-criterion, we need to obtain smallest eigenvalue and its corresponding eigenvector, of the information matrix for the weighted centroid design. We proceed as follows:

From the information matrices involved in our designs it can be uniquely partitioned as

$$C = \begin{pmatrix} C_{11} & C'_{21} \\ C_{21} & C_{22} \end{pmatrix}$$

For $\lambda \in \Re$, let

$$C - \lambda I_s = \begin{pmatrix} C_{11} - \lambda U_1 & C'_{21} \\ C_{21} & C_{22} - \lambda W_1 \end{pmatrix} \in sym(s, H).$$

Then the characteristic polynomial can be written as

$$\chi_c(\lambda) = \det(C - \lambda I_s) = \det(C_{11} - \lambda I_s)\det[(C_{22} - \lambda W_1) - C_{21}(C_{11} - \lambda U_1)^{-1} C'_{21}]$$

Where the matrix $(C_{22} - \lambda W_1) - C_{21}(C_{11} - \lambda U_1)^{-1} C'_{21}$ is the schur complement of $C_{11} - \lambda U_1$ and lies in the $span\{W_1 \quad W_2 \quad W_3\}$.

The roots of this polynomial are the eigenvalues of the information matrix C and are computed as follows:

Lemma 3.2.1

Let $a, \cdots, g \in \Re$ be the coefficients of the matrix $C \in sym(s, H)$, with d, f and g occurring only when $m \geq 3$ or $m \geq 4$ respectively.

Furthermore, define

$$D_1 = \left[a + (m-1)b - e - 2(m-2)f - \binom{m-2}{2} g \right]^2 + 2(m-1)\left[2c + (m-2)d\right]^2 \tag{3.8}$$

$$D_2 = \left[a - b - e - (m-4)f + (m-1)g\right]^2 + 4(m-2)(c-d)^2 \tag{3.9}$$

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

$\lambda_1 = e - 2f + g$,

$$\lambda_{2,3} = \frac{1}{2}\left[a + (m-1)b + e + 2(m-3)f + \binom{m-2}{2} g \pm \sqrt{D_1} \right] \tag{3.10}$$

and

$$\lambda_{4,5} = \frac{1}{2}\left[a - b + e + (m-4)f - (m-3)g \pm \sqrt{D_2}\right] \tag{3.11}$$

With multiplicities; $\frac{m(m-3)}{2}$, 1 and $(m-1)$ respectively.

In the case m=2, only the eigenvalues $\lambda_2, \lambda_3, \lambda_4$ occur, whereas for m=3 there are four eigenvalues $\lambda_2, \lambda_3, \lambda_4$ *and* λ_5.

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

CHAPTER FOUR

E-OPTIMAL DESIGNS FOR NON-MAXIMAL AND MAXIMAL PARAMETER SUBSYSTEMS

4.1 Introduction

In this chapter derivation of E-optimal weighted centroid designs for two, three, four and a generalization to m ingredients were obtained. Smallest eigenvalues for the corresponding ingredients and E-optimal values are obtained in the process. Information matrixes from Cherutich (2012) and Kinyanjui (2007) for non-maximal and maximal parameter subsystem respectively were used.

4.1.0 E-Optimal Designs For Non-Maximal Parameter Subsystem

Lemma 4.1.0

In the second-degree Kronecker model with m=2 ingredients, the Weighted Centroid Design

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.4545\,\eta_1 + 0.5455\,\eta_2 \tag{4.1}$$

is E-optimal for $K'\theta$ in T.

The maximum of the E-criterion for m=2 ingredients is $v(\phi_{-\infty}) = 0.09090909$.

Proof

Information matrix $C_k(M(\eta(\alpha)))$ is,

$$C = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{4} \end{pmatrix} \tag{4.2}$$

From equation (2.9) any matrix $C \in sym(s,H)$ can be uniquely represented in the form

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

For the case m=2, the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 \\ cV_1^{'} & eW_1 \end{pmatrix}$$

With coefficients; $a, b, c, e \in \Re$, since the terms containing V_2, $W_2$and W_3 only occur for m>2.

From lemma (2.4), we get

$$U_1 = I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ U_2 = 1_2 1_2' - I_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$V_1 = \sum_{\substack{i,j=1 \\ i<j}}^{2} E_{ij}(e_i + e_j)' \in \Re^{1\times 2} = E_{12}(e_1 + e_2)' = (1 \quad 1) \text{ and } W_1 = I_{\binom{2}{2}} = 1.$$

Thus the information matrix $C_k(M(\eta(\alpha)))$ in equation (4.2) can be written as

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 \\ cV'_1 & eW_1 \end{pmatrix} = \begin{bmatrix} a\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & c\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ c(1 \quad 1) & e(1) \end{bmatrix} = \begin{pmatrix} a & b & c \\ b & a & c \\ c & c & e \end{pmatrix} \tag{4.3}$$

Where; $a = \dfrac{8\alpha_1 + \alpha_2}{16}$, $b = \dfrac{\alpha_2}{16}$, $c = \dfrac{\alpha_2}{8}$ and $e = \dfrac{\alpha_2}{4}$

From lemma (3.2.1), we compute the eigenvalues of the above matrix as follows;

$$D_1 = [a + b - e]^2 + 2[2c]^2 = \frac{33\alpha_1^2 - 26\alpha_1 + 9}{64}$$

$$D_2 = [a - b - e]^2 = \left[\frac{3\alpha_1 - 1}{4}\right]^2$$

using equation (3.10) in lemma (3.2.1), we obtain

$$\lambda_{2,3} = \frac{1}{2}\left[a + b + e \pm \sqrt{D_1}\right] = \frac{1}{16}\left[\alpha_1 + 3 \pm \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right]$$

again, using equation (3.10) in lemma (3.2.1), we obtain

$$\lambda_4 = \frac{1}{2}\left[a - b + e + \sqrt{D_2}\right] = \frac{\alpha_1}{2}$$

Thus for the case m=2, the eigenvalues that occur are

$$\lambda_2 = \frac{1}{16}\left[\alpha_1 + 3 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right]$$

$$\lambda_3 = \frac{1}{16}\left[\alpha_1 + 3 - \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right]$$

$$\lambda_4 = \frac{\alpha_1}{2}$$

From theorem (3.2.3), if the smallest eigenvalue of $C_k(M)$ has multiplicity 1, then the only choice for the matrix E is $E = \frac{zz'}{\|z\|^2}$, where $z \in \Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$. In our case, the smallest eigenvalue is

$$\lambda_{\min} = \lambda_3 = \frac{1}{16}\left[\alpha_1 + 3 - \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right] \tag{4.4}$$

We therefore need to get an eigenvector, z corresponding to the smallest eigenvalue of the matrix, $C_k(M)$.

By definition, $\lambda \in \Re$, is an eigenvalue of matrix $C_k(M)$ if

$$(C - \lambda I)\vec{z} = \vec{0} \Leftrightarrow C\vec{z} = \lambda\vec{z} \text{ with } \vec{z} \neq \vec{0}$$

where $\vec{z} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, is an eigenvector of $C_k(M)$ corresponding to λ.

Thus, from equation (4.2) and equation (4.4), we have

$(C - \lambda_{\min} I)\vec{z} = \vec{0}$, implies that

$$\begin{pmatrix} \frac{6\alpha_1 - 2 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{6\alpha_1 - 2 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{1 - 5\alpha_1 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}}{16} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (4.5)$$

If we let

$p = 6\alpha_1 - 2 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}$, $q = \alpha_2 = 1 - \alpha_1$ and $r = 1 - 5\alpha_1 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}$, we obtain the equations

$$px + qy + 2qz = 0$$

$$qx + py + 2qz = 0$$

$$2qx + 2qy + rz = 0$$

Solving the above system of linear equations, we obtain the eigenvector corresponding to $\lambda_{\min}$ as;

$$\vec{z} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \frac{-4q}{r} \end{pmatrix} \quad (4.6)$$

Then the matrix

$$zz' = \begin{pmatrix} 1 & 1 & \frac{-4q}{r} \\ 1 & 1 & \frac{-4q}{r} \\ \frac{-4q}{r} & \frac{-4q}{r} & \frac{16q^2}{r^2} \end{pmatrix} \text{and} \|z\|^2 = \frac{2r^2 + 16q^2}{r^2} \quad (4.7)$$

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{2r^2+16q^2} & \frac{r^2}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} \\ \frac{r^2}{2r^2+16q^2} & \frac{r^2}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} \\ \frac{-4qr}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} & \frac{16q^2}{2r^2+16q^2} \end{pmatrix} \quad (4.8)$$

Multiplying

$$C_1 = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$, Cherutich (2012)

and matrix E, equation (4.8), we have

$$C_1E = \begin{pmatrix} \frac{r^2}{2(2r^2+16q^2)} & \frac{r^2}{2(2r^2+16q^2)} & \frac{-4qr}{2(2r^2+16q^2)} \\ \frac{r^2}{2(2r^2+16q^2)} & \frac{r^2}{2(2r^2+16q^2)} & \frac{-4qr}{2(2r^2+16q^2)} \\ 0 & 0 & 0 \end{pmatrix} \quad (4.9)$$

Thus $traceC_1E = \frac{r^2}{2r^2+16q^2}$ (4.10)

Now $traceC_1E = \lambda_{\min}(C)$, implies that

$$\frac{r^2}{2r^2+16q^2}=\frac{1}{16}\left[\alpha_1+3-\sqrt{33\alpha_1^2-26\alpha_1+9}\right] \quad (4.11)$$

This simplifies to

$$-33792\,\alpha_1^6+161792\,\alpha_1^5-314368\,\alpha_1^4+315392\,\alpha_1^3-171008\,\alpha_1^2+47104\,\alpha_1-5120=0 \quad (4.12)$$

upon substituting the values of q and r .

The roots of polynomial (4.12) are

$\alpha_1 = 1.0003, 0.9999, 0.4545, 0.3333$

Since, $\alpha_1 \in (0,1)$, then it implies that α_1 =0.9999 or $\alpha_1 = 0.4545$ or $\alpha_1 = 0.3333$

When, $\alpha_1 = 0.9999$, $\alpha_2 = 1-\alpha_1 = 0.0001$ and

$$\lambda_{\min}=\frac{1}{16}\left[\alpha_1+3-\sqrt{33\alpha_1^2-26\alpha_1+9}\right]=0.00000025$$

When, $\alpha_1 = 0.4545$, $\alpha_2 = 1-\alpha_1 = 0.5455$ and $\lambda_{\min}=\frac{1}{16}\left[\alpha_1+3-\sqrt{33\alpha_1^2-26\alpha_1+9}\right]=0.0909$

When, $\alpha_1 = 0.3333$, $\alpha_2 = 1-\alpha_1 = 0.6667$ and

$$\lambda_{\min}=\frac{1}{16}\left[\alpha_1+3-\sqrt{33\alpha_1^2-26\alpha_1+9}\right]=0.0833$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = 0.4545$ and $\alpha_2 = 0.5455$.

Thus for m=2, ingredients we have, $\alpha_1 = 0.4545$ and $\alpha_2 = 0.5455$.

From Pukelsheim (2006), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.4), the smallest eigenvalue is

$$\lambda_{\min}=\frac{1}{16}\left[\alpha_1+3-\sqrt{33\alpha_1^2-26\alpha_1+9}\right]=0.0909 \quad (4.13)$$

Hence the optimal value for the E-criterion for m=2 factors becomes

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.09090909 \;\blacksquare \quad (4.14)$$

Lemma 4.1.1

In the second-degree Kronecker model with m=3 ingredients, the weighted centroid design

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.5753\,\eta_1 + 0.4247\,\eta_2 \tag{4.15}$$

is E-optimal for $K'\theta$ in T.

The maximum of the E-criterion for m=3 ingredientsis $v(\phi_{-\infty}) = 0.073556541$.

Proof

In the second-degree Kronecker model with m=3 ingredients, the information matrix $C_k(M(\eta(\alpha)))$ can be written as

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

where; $a = \dfrac{8\alpha_1 + \alpha_2}{24}$, $b = \dfrac{\alpha_2}{48}$, $c = \dfrac{\alpha_2}{4}$, $d = \dfrac{\alpha_2}{12}$ and $f = 0$

with the matrices; U_1, U_2, V_1, V_2, W_1, $W_2$and W_3defined as in lemma (2.5).

The information matrix $C_k(M(\eta(\alpha)))$ for a mixture experiment design $\eta(\alpha)$ with m=3 ingredients, we have;

$$C = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{12} \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{12} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{12} \\ \frac{\alpha_2}{12} & \frac{\alpha_2}{12} & \frac{\alpha_2}{12} & \frac{\alpha_2}{4} \end{pmatrix} \tag{4.16}$$

From equation (2.9), any marix $C \in sym(s,H)$ can be represented in the form

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

with coefficients $a,\ldots,g \in \Re$. The terms containing V_2, $W_2$and W_3occurring for $m \geq 3$ or $m \geq 4$ respectively.

For the present case m=3 and so the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C = \begin{pmatrix} aI_3 + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_3 + fW_2 \end{pmatrix}$$

From lemma (2.5), we get

$$U_1 = I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ U_2 = 1_3 1_3' - I_3 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

$$V_1 = \sum_{\substack{i,j=1 \\ i<j}}^{3} E_{ij}(e_i + e_j)' \in \Re^{3\times 3}$$

$$V_1 = E_{12}(e_1 + e_2)' + E_{13}(e_1 + e_3)' + E_{23}(e_2 + e_3)'$$

Now,

$$(e_1 + e_2) = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},\ (e_1 + e_3) = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \text{ and } (e_2 + e_3) = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

The vectors, $E_{ij} \in \Re^3$, $i, j \in (1,2,3), i < j$, with index pairs (i,j), considered in their lexicographic order are E_{12}, E_{13} *and* E_{23}. These vectors form the standard basis for $\Re^3$ and are $E_{12} = (1 \quad 0 \quad 0)'$, $E_{13} = (0 \quad 1 \quad 0)'$ and $E_{23} = (0 \quad 0 \quad 1)'$.

We then obtain

$$V_1 = E_{12}(e_1+e_2)' + E_{13}(e_1+e_3)' + E_{23}(e_2+e_3)' = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}.$$

$$V_2 = \sum_{\substack{i,j=1 \\ i<j}}^{3} \sum_{\substack{k=1 \\ k\notin\{i,j\}}}^{3} E_{ij} e_k' \in \Re^{3\times 3}$$

$$V_2 = E_{12}e_3' + E_{13}e_2' + E_{23}e_1' = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$W_2 = \sum_{\substack{i,j=1 \\ I<L}}^{3} \sum_{\substack{k,l=1 \\ k<l}}^{3} E_{ij} E_{kl}' \in sym(3)$$
$$|\{i,j\} \cap \{k,l\}| = 1$$

$$W_2 = E_{12}E_{13}' + E_{12}E_{23}' + E_{13}E_{12}' + E_{13}E_{23}' + E_{23}E_{12}' + E_{23}E_{13}' = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

From the definition of W_3, we get that $W_3=0$, since the side condition $|\{i,j\} \cap \{k,l\}| = \phi$, cannot be satisfied for m=3.

Thus the information matrix for m=3 factors can be written as

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} & c\begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} + d\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \\ c\begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} + d\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} & e\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + f\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} a & b & b & d \\ b & a & b & d \\ b & b & a & d \\ d & d & d & c \end{pmatrix} \tag{4.17}$$

Where, $a=\dfrac{8\alpha_1+\alpha_2}{24}$, $b=\dfrac{\alpha_2}{48}$, $c=\dfrac{\alpha_2}{4}$, $d=\dfrac{\alpha_2}{12}$, $f=0$ and $e=\dfrac{\alpha_2}{4}$

From lemma (3.2.1), we compute the eigenvalues of the above matrix as follows

$$D_1=[a+2b-e]^2+4[2c+d]^2=\left[\frac{8\alpha_1+\alpha_2}{24}+\frac{2\alpha_2}{48}-\frac{\alpha_2}{4}\right]^2+4\left[\frac{2\alpha_2}{12}\right]^2=\frac{13\alpha_1^2-14\alpha_1+5}{36} \quad (4.18)$$

$$D_2=[a-b-c]^2+4(3-2)[d]^2=\left[\frac{8\alpha_1+\alpha_2}{24}-\frac{\alpha_2}{48}-\frac{\alpha_2}{4}\right]^2+4\left[\frac{\alpha_2}{12}\right]^2=\left(\frac{73\alpha_1^2-722\alpha_1+185}{48^2}\right)^2 \quad (4.19)$$

Using equation (3.10) in lemma (31), we obtain for m=3

$$\lambda_{2,3}=\frac{1}{2}\left[a+2b+c\pm\sqrt{D_1}\right]=\frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{24}-2\left[\frac{\alpha_2}{48}\right]+\left[\frac{\alpha_2}{4}\right]\pm\sqrt{\frac{13\alpha_1^2-14\alpha_1+5}{36}}\right]$$

$$=\frac{1}{12}\left[2\pm\sqrt{13\alpha_1^2-14\alpha_1+5}\right], \quad \text{with multiplicity 1} \quad (4.20)$$

Similarly, using equation (3.11) in lemma (3.2.1) we get

$$\lambda_{4,5}=\frac{1}{2}\left[a-b+c\pm\sqrt{D_2}\right]=\frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{24}-\frac{\alpha_2}{48}+\frac{\alpha_2}{4}\pm\sqrt{\frac{793\alpha_1^2-722\alpha_1+185}{48^2}}\right] \quad (4.21)$$

From lemma (3.2.1) the eigenvalues that λ_2, λ_3, λ_4 *and* λ_5 occur for the case m=3. These are

$$\lambda_2=\frac{1}{12}\left[2+\sqrt{13\alpha_1^2-14\alpha_1+5}\right], \text{ with multiplicity 1,}$$

$$\lambda_3=\frac{1}{12}\left[2-\sqrt{13\alpha_1^2-14\alpha_1+5}\right], \text{ with multiplicity 1,}$$

$$\lambda_4=\frac{1}{96}\left[3\alpha_1+13+\sqrt{793\alpha_1^2-722\alpha_1+185}\right], \text{ with multiplicity 2 and}$$

$$\lambda_5=\frac{1}{96}\left[3\alpha_1+13-\sqrt{793\alpha_1^2-722\alpha_1+185}\right], \text{ with multiplicity 2.}$$

From theorem (3.2.3), if the smallest eigenvector of $C_k(M)$ has multiplicity 1, then the only choice for the matrix Eis, $E = \frac{zz'}{\|z\|^2}$, where $z \in \Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$. In our case, the smallest eigenvalue is

$$\lambda_{\min} = \lambda_3 = \frac{1}{12}\left[2 - \sqrt{13\alpha_1^2 - 14\alpha_1 + 5}\right] \qquad (4.22)$$

We therefore need to get an eigenvector z, corresponding to the smallest eigenvalue of the matrix, $C_k(M)$.

By definition, $\lambda \in \Re$, is an eigenvalue of matrix C if

$$(C - \lambda I)\vec{z} = \vec{0} \Leftrightarrow C\vec{z} = \lambda\vec{z} \text{ with } \vec{z} \neq \vec{0}$$

Where, $\vec{z} = \begin{pmatrix} w & x & y & z \end{pmatrix}'$, is an eigenvector of C corresponding to λ.

Thus, from equation (4.17) and equation (4.22)

$(C - \lambda_{\min} I)\vec{z} = \vec{0}$, implies that

$$\begin{pmatrix} 2p & q & q & 4q \\ q & 2p & q & 4q \\ q & q & 2p & 4q \\ 4q & 4q & 4q & 4r \end{pmatrix}\begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{matrix} 0 \\ 0 \\ 0 \\ 0 \end{matrix} \qquad (4.23)$$

where, $p = 7\alpha_1 - 3 + \sqrt{13\alpha_1^2 - 14\alpha_1 + 5}$, $q = \alpha_2 = 1 - \alpha_1$ and

$r = -3\alpha_1 + 1 + \sqrt{13\alpha_1^2 - 14\alpha_1 + 5}$

$2pw + qx + qy + 4qz = 0$

$qw + 2px + qy + 4qz = 0$

$qw + qx + 2py + 4qz = 0$

$$4qw + 4qx + 4qy + 12rz = 0$$

Solving the above system of linear equations, we obtain the eigenvector corresponding to $\lambda_{\min}$ as;

$$\vec{z} = \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \frac{-3q}{r} \end{pmatrix} \tag{4.24}$$

Then the matrix

$$zz' = \begin{pmatrix} 1 & 1 & 1 & \frac{-3q}{r} \\ 1 & 1 & 1 & \frac{-3q}{r} \\ 1 & 1 & 1 & \frac{-3q}{r} \\ \frac{-3q}{r} & \frac{-3q}{r} & \frac{-3q}{r} & \frac{9q^2}{r} \end{pmatrix} \text{and} \|z\|^2 = \frac{3r^2 + 9q^2}{r^2}$$

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{3r^2+9q^2} & \frac{r^2}{3r^2+9q^2} & \frac{r^2}{3r^2+9q^2} & \frac{-3qr^2}{3r^2+9q^2} \\ \frac{r^2}{3r^2+9q^2} & \frac{r^2}{3r^2+9q^2} & \frac{r^2}{3r^2+9q^2} & \frac{-3qr^2}{3r^2+9q^2} \\ \frac{r^2}{3r^2+9q^2} & \frac{r^2}{3r^2+9q^2} & \frac{r^2}{3r^2+9q^2} & \frac{-3qr^2}{3r^2+9q^2} \\ \frac{-3qr^2}{3r^2+9q^2} & \frac{-3qr^2}{3r^2+9q^2} & \frac{-3qr^2}{3r^2+9q^2} & \frac{9q^2}{3r^2+9q^2} \end{pmatrix} \tag{4.25}$$

Multiplying

$C_1 = \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$, Cherutich (2012)and matrix E, equation (4.25), we have

$$C_1E = \begin{pmatrix} \frac{r^2}{3(3r^2+9q^2)} & \frac{r^2}{3(3r^2+9q^2)} & \frac{r^2}{3(3r^2+9q^2)} & \frac{-3qr^2}{3(3r^2+9q^2)} \\ \frac{r^2}{3(3r^2+9q^2)} & \frac{r^2}{3(3r^2+9q^2)} & \frac{r^2}{3(3r^2+9q^2)} & \frac{-3qr^2}{3(3r^2+9q^2)} \\ \frac{r^2}{3(3r^2+9q^2)} & \frac{r^2}{3(3r^2+9q^2)} & \frac{r^2}{3(3r^2+9q^2)} & \frac{-3qr^2}{3(3r^2+9q^2)} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.26)$$

Thus $traceC_1E = \frac{r^2}{3r^2+9q^2}$ (4.27)

Now

$traceC_1E = \lambda_{\min}(C)$, implies that

$$\frac{r^2}{3r^2+9q^2} = \frac{1}{12}\left[2-\sqrt{13\alpha_1^2 - 14\alpha_1 + 5}\right] \quad (4.28)$$

This simplifies to

$$-32656\,\alpha_1^6 + 165792\,\alpha_1^5 - 346032\,\alpha_1^4 + 379328\,\alpha_1^3 - 229872\,\alpha_1^2 + 72864\,\alpha_1 - 9424 = 0 \quad (4.29)$$

upon substituting the values of q and r .

The roots of polynomial (4.29) are

$$\alpha_1 = 0.5753, 0.5016$$

Since, $\alpha_1 \in (0,1)$, then it implies that α_1=0.5753 or $\alpha_1 = 0.5016$

When, $\alpha_1 = 0.5753$, $\alpha_2 = 1-\alpha_1 = 0.4247$ and

$$\lambda_{\min} = \frac{1}{12}\left[2-\sqrt{13\alpha_1^2 - 14\alpha_1 + 5}\right] = 0.073556541$$

When, $\alpha_1 = 0.5016$, $\alpha_2 = 1-\alpha_1 = 0.4984$ and

$$\lambda_{\min} = \frac{1}{12}\left[2-\sqrt{13\alpha_1^2 - 14\alpha_1 + 5}\right] = 0.073556528$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = 0.5753$ and $\alpha_2 = 0.4247$.

Thus for m=3, ingredients we have, $\alpha_1 = 0.5753$ and $\alpha_2 = 0.4247$.

From Pukelsheim (2006), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.22), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{12}\left[2 - \sqrt{13\alpha_1^2 - 14\alpha_1 + 5}\right] = 0.073556541 \qquad (4.30)$$

Hence the optimal value for the E-criterion for m=3 factors becomes

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.073556541 \ ▪ \qquad (4.31)$$

Lemma 4.1.2

In the second-degree Kronecker model with m=4 ingredients, the weighted centroid design

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.9998\,\eta_1 + 0.0002\,\eta_2 \qquad (4.32)$$

is E-optimal for $K'\theta$ in T.

The maximum of the E-criterion for m=4 ingredients is $v(\phi_{-\infty}) = 0.0018823$.

Proof

In the second-degree Kronecker model any matrix $C \in \text{sym}(s,H)$ can be uniquely represented in the form

$$C = \begin{pmatrix} aU_1 + bU_2 & dV_1 \\ dV_1' & c\dfrac{V'V}{m} \end{pmatrix}$$

And for the case m=4 ingredients the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C = \begin{pmatrix} aU_1 + bU_2 & dV_1 \\ dV'_1 & c\dfrac{V'V}{m} \end{pmatrix}$$

With coefficients $a, b, c, d \in \Re$,

where; $a = \dfrac{8\alpha_1 + \alpha_2}{32}$, $b = \dfrac{\alpha_2}{96}$, $c = \dfrac{\alpha_2}{4}$, and $d = \dfrac{\alpha_2}{16}$

with the matrices; U_1, U_2, V_1, V_2, W_1, $W_2$and W_3defined as in lemma (4.2).

The information matrix $C_k(M(\eta(\alpha)))$ for a mixture experiment design, $\eta(\alpha)$ with m=4 ingredients is,

$$C = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} \\ \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{4} \end{pmatrix} \quad (4.33)$$

From equation (2.9), any marix $C \in sym(s, H)$ can be represented in the form

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

with coefficients $a,\ldots,g \in \Re$. The terms containing V_2, $W_2$and W_3occurring for $m \geq 3$ or $m \geq 4$ respectively.

For the present case m=4 the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C = \begin{pmatrix} aI_3 + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_3 + fW_2 \end{pmatrix}$$

From lemma (2.4), we get

$$U_1 = I_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$U_2 = 1_4 1_4' - I_4 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix},$$

$$V = \sum_{\substack{i,j=1 \\ i<j}}^{4} (e_i) \in \Re^{4\times 1} = (e_1 + e_2 + e_3 + e_4) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

Thus the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} aU_1 + bU_2 & dV_1 \\ dV'_1 & c\dfrac{V'V}{m} \end{pmatrix} = \left[\begin{matrix} a\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} & d\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \\ d\begin{pmatrix} 1 & 1 & 1 & 1 \end{pmatrix} & c(1) \end{matrix}\right] \quad (4.34)$$

Where, where; $a = \dfrac{8\alpha_1 + \alpha_2}{32}$, $b = \dfrac{\alpha_2}{96}$, $c = \dfrac{\alpha_2}{4}$, and $d = \dfrac{\alpha_2}{16}$

From lemma (3.2.1), we compute the eigenvalues of the above matrix as follows

$$D_1 = [a + 3b - c]^2 + 6[2d]^2 = \left[\frac{8\alpha_1 + \alpha_2}{24} + \frac{3\alpha_2}{96} - \frac{\alpha_2}{24}\right]^2 + 6\left[\frac{2\alpha_2}{16}\right]^2 = \frac{73\alpha_1{}^2 - 90\alpha_1 + 33}{16^2} \quad (4.35)$$

$$D_2 = [a - b - c]^2 + 4(4-2)[d]^2 = \left[\frac{8\alpha_1 + \alpha_2}{32} - \frac{\alpha_2}{96} - \frac{\alpha_2}{4}\right]^2 + 4(2)\left[\frac{\alpha_2}{16}\right]^2 = \left(\frac{601\alpha_1^2 - 650\alpha_1 + 193}{48^2}\right)^2 \quad (4.36)$$

Using equation (3.10) in lemma (3.2.1), we obtain for m=4

$$\lambda_{2,3}=\frac{1}{2}\left[a+3b+c\pm\sqrt{D_1}\right]=\frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{32}+3\left[\frac{\alpha_2}{96}\right]+\left[\frac{\alpha_2}{4}\right]\pm\sqrt{\frac{73\alpha_1^2-90\alpha_1+33}{16^2}}\right]$$

$$=\frac{1}{32}\left[-\alpha_1+5\pm\sqrt{73\alpha_1^2-90\alpha_1+33}\right],\quad \text{with multiplicity 1} \qquad (4.37)$$

Similarly, using equation (3.11) in lemma (3.2.1) we get

$$\lambda_{4,5}=\frac{1}{2}\left[a-b+c\pm\sqrt{D_2}\right]=\frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{32}-\frac{\alpha_2}{96}+\frac{\alpha_2}{4}\pm\sqrt{\frac{601\alpha_1^2-650\alpha_1+193}{48^2}}\right]$$

$$=\frac{1}{96}\left[-2\alpha_1+26\pm\sqrt{601\alpha_1^2-650\alpha_1+193}\right],\ \text{with multiplicity 2} \qquad (4.38)$$

The smallest eigenvalue is $=\frac{1}{32}\left[-\alpha_1+5\pm\sqrt{73\alpha_1^2-90\alpha_1+33}\right]$ (4.39)

From lemma (3.2.1) the eigenvalues that $\lambda_2,\ \lambda_3,\ \lambda_4\ and\ \lambda_5$ occur for the case m=4. These are

$\lambda_2=\frac{1}{32}\left[-\alpha_1+5+\sqrt{73\alpha_1^2-90\alpha_1+33}\right]$, with multiplicity 1,

$\lambda_3=\frac{1}{32}\left[-\alpha_1+5-\sqrt{73\alpha_1^2-90\alpha_1+33}\right]$, with multiplicity 1,

$\lambda_4=\frac{1}{96}\left[-2\alpha_1+26+\sqrt{601\alpha_1^2-650\alpha_1+193}\right]$,withmultiplicity2 and

$\lambda_5=\frac{1}{96}\left[-2\alpha_1+26-\sqrt{601\alpha_1^2-650\alpha_1+193}\right]$, with multiplicity 2.

From theorem (3.2.3), if the smallest eigenvector of $C_k(M)$ has multiplicity 1, then the only choice for the matrix E is, $E=\frac{zz'}{\|z\|^2}$, where $z\in\Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$. In our case, the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{32}\left[-\alpha_1 + 5 - \sqrt{73\alpha_1^2 - 90\alpha_1 + 33}\right], \tag{4.40}$$

We therefore need to get an eigenvector z, corresponding to the smallest eigenvalue of the matrix, $C_k(M)$.

By definition, $\lambda \in \Re$, is an eigenvalue of matrix C if

$(C - \lambda I)\vec{z} = \vec{0} \Leftrightarrow C\vec{z} = \lambda\vec{z}$ with $\vec{z} \neq \vec{0}$

Where, $\vec{z} = (v \quad w \quad x \quad y \quad z)'$, is an eigenvector of C corresponding to λ.

Thus, from equation (4.33) and equation (4.40)

$(C - \lambda_{\min} I)\vec{z} = \vec{0}$, implies that

$$\begin{pmatrix} 3p & q & q & q & 6q \\ q & 3p & q & q & 6q \\ q & q & 3p & q & 6q \\ q & q & q & 3p & 6q \\ 6q & 6q & 6q & 6q & 3r \end{pmatrix}\begin{pmatrix} v \\ w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{4.41}$$

where, $p = 8\alpha_1 - 4 + \sqrt{73\alpha_1^2 - 90\alpha_1 + 33}$, $q = \alpha_2 = 1 - \alpha_1$ and

$r = -7\alpha_1 + 3 + \sqrt{73\alpha_1^2 - 90\alpha_1 + 33}$

$3pv + qw + qx + qy + 6qz = 0$

$qv + 3pw + qx + qy + 6qz = 0$

$qv + qw + 3px + qy + 6qz = 0$

$qv + qw + qx + 3py + 6qz = 0$

$6qv + 6qw + 6qx + 6qy + 3rz = 0$

Solving the above system of linear equations, we obtain the eigenvector corresponding to $\lambda_{\min}$ as;

$$\vec{z} = \begin{pmatrix} v \\ w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \frac{-8q}{r} \end{pmatrix} \tag{4.42}$$

Then the matrix

$$zz' = \begin{pmatrix} 1 & 1 & 1 & 1 & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} \end{pmatrix} \text{ and } \|z\|^2 = \frac{4r^2 + 64q^2}{r^2}$$

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{-8qr}{4r^2+64q^2} \\ \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{-8qr}{4r^2+64q^2} \\ \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{-8qr}{4r^2+64q^2} \\ \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{r^2}{4r^2+64q^2} & \frac{-8qr}{4r^2+64q^2} \\ \frac{-8qr}{4r^2+64q^2} & \frac{-8qr}{4r^2+64q^2} & \frac{-8qr}{4r^2+64q^2} & \frac{-8qr}{4r^2+64q^2} & \frac{64q^2r^2}{4r^2+64q^2} \end{pmatrix} \tag{4.43}$$

$$C_1 = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

, Cherutich (2012) and matrix E, equation (4.43), we have

$$C_1E = \begin{pmatrix} \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{-8qr}{4(4r^2+64q^2)} \\ \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{-8qr}{4(4r^2+64q^2)} \\ \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{-8qr}{4(4r^2+64q^2)} \\ \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{r^2}{4(4r^2+64q^2)} & \frac{-8qr}{4(4r^2+64q^2)} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.44}$$

Thus $traceC_1E = \frac{r^2}{4r^2+64q^2}$

Now

$traceC_1E = \lambda_{\min}(C)$, implies that

$$\frac{r^2}{4r^2+64q^2} = \frac{1}{32}\left[-\alpha_1 + 5 - \sqrt{73\alpha_1^2 - 90\alpha_1 + 33}\right] \tag{4.45}$$

This simplifies to

$$\begin{aligned} &-340992\alpha_1^6 + 1786880\alpha_1^5 - 3868672\alpha_1^4 + 4425728\alpha_1^3 \\ &-2819072\alpha_1^2 + 947200\alpha_1 - 131072 = 0 \end{aligned} \tag{4.46}$$

Upon substituting the values of q and r.

The roots of polynomial (4.46) are

$\alpha_1 = 1.0002, 0.9998$

Since, $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.9998$

When $\alpha_1 = 0.9998, \alpha_2 = 1 - \alpha_1 = 0.0002$ and

$$\lambda_{\min} = \frac{1}{32}\left[-\alpha_1 + 5 - \sqrt{73\alpha_1^2 - 90\alpha_1 + 33}\right] = 0.0018823$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = 0.9998, \alpha_2 = 1 - \alpha_1 = 0.0002$.

Thus for m=4 ingredients we have, $\alpha_1 = 0.99976469$ and $\alpha_2 = 0.00023531$

From Pukelsheim (2006), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.40), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{32}\left[-\alpha_1 + 5 - \sqrt{73\alpha_1^2 - 90\alpha_1 + 33}\right] = 0.0018823$$

Hence the optimal value for the E-criterion for m=4 factors becomes

$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.0018823$.

4.1.1 Generalization of E-optimal design for non-maximal parameter subsystem

Theorem 4.1.1

In the second degree Kronecker model with m-ingredients the weighted centroid design

$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2$ is E-optimal for $K'\theta$ in T. (4.47)

The maximum value of the E-criterion for $K'\theta$ with m ingredients is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{8m}\left[(-m+3)\alpha_1 + m + 1 \pm \sqrt{D}\right] \tag{4.48}$$

Where $D = (m^2 + 14m + 1)\alpha_1^2 - (2m^2 + 20m - 22)\alpha_1 + (m^2 + 6m - 7)$

Proof

From equation (2.9) any matrix $C \in sym(s, H)$ can be uniquely represented in the form

$$C = \begin{pmatrix} aU_1 + bU_2 & dV_1 \\ dV'_1 & c\dfrac{V'V}{m} \end{pmatrix}$$

For the case of m ingredients the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C = \begin{pmatrix} aU_1 + bU_2 & dV \\ dV' & c\dfrac{V'V}{m} \end{pmatrix}$$

With coefficients $a, b, c, d \in \Re$,

From lemma(2.5) we get

$$U_1 = I_m = \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} \tag{4.49}$$

$$U_2 = I_m I'_m - I_m = \begin{pmatrix} 1 & . & . & . & 1 \\ . & . & & & . \\ . & & . & & . \\ . & & & . & . \\ 1 & . & . & . & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & . & . & . & 1 \\ 0 & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 1 & & . & . & . & 0 \end{pmatrix}, \text{ and}$$

$$V = \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_i) \in \Re^{m\times 1} = (e_1 + e_2 + \ldots + e_m) = \begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \end{pmatrix}$$

Hence the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} aU_1 + bU_2 & dV \\ dV' & c\dfrac{V'V}{m} \end{pmatrix} = \left[\begin{matrix} a\begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 & . & . & . & 1 \\ 1 & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 1 & & . & . & . & 0 \end{pmatrix} & d\begin{pmatrix} 1 \\ \\ . \\ . \\ . \\ 1 \end{pmatrix} \\ d\begin{pmatrix} 1 & . & . & . & 1 \end{pmatrix} & c(1) \end{matrix} \right]$$

$$= \begin{pmatrix} \dfrac{8\alpha_1 + \alpha_2}{8m} U_1 + \dfrac{\alpha_2}{8m(m-1)} U_2 & \dfrac{\alpha_2}{4m} V \\ \dfrac{\alpha_2}{4m} V' & \dfrac{\alpha_2}{4} \dfrac{V'V}{m} \end{pmatrix} \tag{4.50}$$

Where $a = \dfrac{8\alpha_1 + \alpha_2}{8m}$, $b = \dfrac{\alpha_2}{8m(m-1)}$, $c = \dfrac{\alpha_2}{4}$ and $d = \dfrac{\alpha_2}{4m}$

From (lemma 3.2.1) for m ingredients we have

$$D_1 = [a + (m-1)b - c]^2 + 2(m-1)[2d]^2$$

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

$$= \frac{(4m^2 + 56m + 4)\alpha_1{}^2 - (8m^2 + 80m - 88)\alpha_1 + (4m^2 + 24m - 28)}{64m^2}$$

The eigenvalues are;

$$\lambda_{2,3} = \frac{1}{2}\left[a + (m-1)b + c \pm \sqrt{D_1}\right]$$

$$= \frac{1}{2}\left[\frac{8\alpha_1 + \alpha_2}{8m} + \frac{(m-1)\alpha_2}{8m(m-1)} + \frac{\alpha_2}{4} \pm \sqrt{D_1}\right] \tag{4.51}$$

$$= \frac{1}{8m}\left[(-m+3)\alpha_1 + (m+1) - \sqrt{D}\right] \tag{4.52}$$

Where $D = (m^2 + 14m + 1)\alpha_1{}^2 - (2m^2 + 20m - 22)\alpha_1 + (m^2 + 6m - 7)$ with multiplicity 1.

Hence the smallest eigenvalue is $\lambda_{\min} = \dfrac{1}{8m}\left[(-m+3)\alpha_1 + (m+1) - \sqrt{D}\right]$ where D is as defined above.

Now let $\lambda_{\min} = \frac{1}{8m}\left[(-m+3)\alpha_1 + (m+1) - \sqrt{D}\right]$ then $\lambda_{\min}$ is an eigenvalue for C if for corresponding eigenvector, say $\bar{z}$, we have $(C-\lambda I)\bar{z} = \bar{0}$ or $(C\bar{z} = \lambda\bar{z})$ with $\bar{z} \neq \bar{0}$

Now let

$$\bar{z} = \begin{pmatrix} z_1 \\ . \\ . \\ . \\ z_{m+1} \end{pmatrix}$$, be the eigenvector of C corresponding to λ.

We therefore have $(C-\lambda I)$, as

$$\begin{pmatrix} \frac{(m+4)\alpha_1 - m + \sqrt{D}}{8m}U_1 + \frac{\alpha_2}{8m(m-1)}U_2 & \frac{\alpha_2}{4m}V \\ \frac{\alpha_2}{4m}V' & \frac{(-m-3)\alpha_1 + (m-1) + \sqrt{D}}{8m}\frac{V'V}{m} \end{pmatrix} \quad (4.53)$$

Let $p_1 = \left[(m+4)\alpha_1 - m + \sqrt{D}\right]$, $q_1 = \alpha_2^{\ 2}$, $r_1 = \left[(-m-3)\alpha_1 + (m-1) + \sqrt{D}\right]$

Where $D = \left(m^2 + 14m + 1\right)\alpha_1^{\ 2} - \left(2m^2 + 20m - 22\right)\alpha_1 + \left(m^2 + 6m - 7\right)$

We get $(C-\lambda I)\bar{z} = \bar{0}$

$$\frac{1}{8m}\begin{pmatrix} (m-1)p_1U_1 + q_1U_2 & 2(m-1)q_1V \\ 2(m-1)q_1V' & (m-1)r_1\frac{V'V}{m} \end{pmatrix}$$

Solving these equations for z_i we get,

$$\bar{z} = \begin{pmatrix} z_1 \\ . \\ . \\ . \\ z_{m+1} \end{pmatrix} = \begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \\ \frac{-cmq}{r} \end{pmatrix}$$

Where c=2 for even number of ingredients and c=1 for odd number of ingredients as the eigenvector corresponding to $\lambda_{\min}$

Thus

$$\bar{z}\bar{z}' = \begin{pmatrix} U_1 + U_2 & -cmqV \\ \frac{cmq}{r}V' & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix}, \text{ and}$$

$$\|z\|^2 = \frac{mr^2 + c^2m^2q^2}{r^2} \tag{4.54}$$

Therefore

$$E = \frac{\bar{z}\bar{z}'}{\|z\|^2} = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} U_1 + U_2 & -cmqV \\ \frac{cmq}{r}V' & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix} \tag{4.55}$$

And from equation (4.50) and equation (4.55),

$$C_1E = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} \frac{1}{m}U_1 + \frac{1}{m}U_2 & -cqV \\ 0 & 0 \end{pmatrix} \tag{4.56}$$

From (Theorem 3.2.2) a weighted centroid design $\eta(\alpha)$ is E-optimal for $K'\theta$ in T if and only if $traceC_jE = \lambda_{\min}(C)$.

For j=1

$$traceC_jE = \frac{r^2}{m(mr^2 + c^2m^2q^2)} + \ldots + .\frac{r^2}{m(mr^2 + c^2m^2q^2)} = \frac{r^2}{(mr^2 + c^2m^2q^2)}$$

Hence $traceC_jE = \lambda_{\min}(C) \Leftrightarrow \frac{r^2}{(mr^2 + c^2m^2q^2)} = \frac{1}{8m}\left[(-m+3)\alpha_1 + (m+1) - \sqrt{D}\right]$ (4.57)

Putting $q = \alpha_2$, $r_1 = \left[(-m-3)\alpha_1 + (m-1) + \sqrt{D}\right]$ and

$D = \left(m^2 + 14m + 1\right)\alpha_1^{\,2} - \left(2m^2 + 20m - 22\right)\alpha_1 + \left(m^2 + 6m - 7\right)$ reduces equation (4.57) to

$$-i\alpha_1^{\,6} + j\alpha_1^{\,5} - k\alpha_1^{\,4} + l\alpha_1^{\,3} - m\alpha_1^{\,2} + n\alpha_1^{\,1} - o = 0 \qquad (4.58)$$

Where

$i = -320m^4 - 4672m^3 + 2880m^2 - 1664m^1 + 512$

$j = 1920\,m^4 + 25728\,m^3 - 25984\,m^2 + 17664\,m^1 - 6144$

$k = -4800m^4 - 58560m^3 + 83648m^2 - 63360m + 23040$

$l = 6400m^4 + 70400m^3 - 132352m^2 + 110080m - 40960$

$m = -4800m^4 - 47040m^3 + 111808m^2 - 101760m + 38400$

$n = 1920m^4 + 16512m^3 - 48512m^2 + 48384m - 18432$

$o = -320m^4 - 2368m^3 + 8512m^2 - 9344m + 3584$

Solving the above polynomial yields the values of α_1 from which we choose α_1,such that $\alpha_1 \in (0,1)$; we substitute this values to $\lambda_{\min}$ and take the values that minimizes the $\lambda_{\min}$, hence the optimal E-criterion is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{8m}\left[(-m+3)\alpha_1 + m + 1 - \sqrt{D}\right]$$

Where $D = \left(m^2 + 14m + 1\right)\alpha_1^{\,2} - \left(2m^2 + 20m - 22\right)\alpha_1 + \left(m^2 + 6m - 7\right)$

4.1.2 E-optimal design for maximal parameter subsystem

Lemma 4.2.0

In the second-degree Kronecker model with m=2 ingredients, the weighted centroid design

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.0662\,\eta_1 + 0.9338\,\eta_2 \tag{4.59}$$

is E-optimal for $K'\theta$ in T.

The maximum of the E-criterion for m=2 ingredients is $v(\phi_{-\infty}) = 0.026314645$.

Proof

We obtained the information matrix, $C_k(M(\eta(\alpha)))$, Kinyanjui (2007) as;

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \end{pmatrix} \tag{4.60}$$

From equation (2.9), any matrix $C \in sym(s,H)$ can be uniquely represented in the form

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

For the case m=2, the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 \\ cV_1' & eW_1 \end{pmatrix}$$

With coefficients; $a,b,c,e \in \Re$, since the terms containing V_2, $W_2$and W_3 only occur for m>2.

From lemma (2.4), we get

$$U_1 = I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ U_2 = 1_2 1_2' - I_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$V_1 = \sum_{\substack{i,j=1 \\ i<j}}^{2} E_{ij}(e_i + e_j)' \in \Re^{1\times 2} = E_{12}(e_1 + e_2)' = (1 \quad 1) \text{ and } W_1 = I_{\binom{2}{2}} = 1.$$

Thus the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 \\ cV_1' & eW_1 \end{pmatrix} = \begin{bmatrix} a\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & c\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ c(1 \quad 1) & e(1) \end{bmatrix} = \begin{pmatrix} a & b & c \\ b & a & c \\ c & c & e \end{pmatrix} \tag{4.61}$$

Where; $a = \frac{8\alpha_1 + \alpha_2}{16}$, $b = \frac{\alpha_2}{16}$, $c = \frac{\alpha_2}{16}$ and $e = \frac{\alpha_2}{16}$

From lemma (3.2.1), we compute the eigenvalues of the above matrix as follows;

$$D_1 = [a + b - e]^2 + 2[2c]^2 = \frac{57\alpha_1^2 - 2\alpha_1 + 9}{256}$$

$$D_2 = [a - b - e]^2 = \left[\frac{9\alpha_1 - 1}{16}\right]^2$$

using equation (3.10) in lemma (3.2.1), we obtain

$$\lambda_{2,3} = \frac{1}{2}\left[a + b + e \pm \sqrt{D_1}\right] = \frac{1}{32}\left[(5\alpha_1 + 3) \pm \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] \tag{4.62}$$

again, using equation (3.11) in lemma (3.2.1), we obtain

$$\lambda_4 = \frac{1}{2}\left[a - b + e + \sqrt{D_2}\right] = \frac{\alpha_1}{2} \tag{4.63}$$

Thus for the case m=2, the eigenvalues that occur are

$$\lambda_2 = \frac{1}{32}\left[(5\alpha_1 + 3) + \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] \tag{4.64}$$

$$\lambda_3 = \frac{1}{32}\left[(5\alpha_1 + 3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] \tag{4.65}$$

$$\lambda_4 = \frac{\alpha_1}{2}$$

From theorem (3.2.3), if the smallest eigenvalue of $C_k(M)$ has multiplicity 1, then the only choice for the matrix E is $E = \frac{zz'}{\|z\|^2}$, where $z \in \Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$. In our case, the smallest eigenvalue is

$$\lambda_{\min} = \lambda_3 = \frac{1}{32}\left[(5\alpha_1 + 3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] \qquad (4.66)$$

We therefore need to get an eigenvector, z corresponding to the smallest eigenvalue of the matrix, $C_k(M)$.

By definition, $\lambda \in \Re$, is an eigenvalue of matrix C if

$$(C - \lambda I)\vec{z} = \vec{0} \Leftrightarrow C\vec{z} = \lambda\vec{z} \text{ with } \vec{z} \neq \vec{0}$$

where $\vec{z} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, is an eigenvector of C corresponding to λ.

Thus, from equation (4.60) and equation (4.66), we have

$(C - \lambda_{\min} I)\vec{z} = \vec{0}$, implies that

$$\begin{pmatrix} \frac{(9\alpha_1 - 1) + \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}}{32} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{(9\alpha_1 - 1) + \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}}{32} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{(-7\alpha_1 - 1) + \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}}{32} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \qquad (4.67)$$

If we let

$p = (9\alpha_1 - 1) + \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}$, $q = \alpha_2 = 1 - \alpha_1$ and $r = (-7\alpha_1 - 1) + \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}$,

we obtain the equations

$$px + 2qy + 2qz = 0$$

$$2qx + py + 2qz = 0$$

$$2qx + 2qy + rz = 0$$

Solving the above system of linear equations, we obtain the eigenvector corresponding to $\lambda_{\min}$ as;

$$\vec{z} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \dfrac{-4q}{r} \end{pmatrix} \tag{4.68}$$

Then the matrix

$$zz' = \begin{pmatrix} 1 & 1 & \dfrac{-4q}{r} \\ 1 & 1 & \dfrac{-4q}{r} \\ \dfrac{-4q}{r} & \dfrac{-4q}{r} & \dfrac{16q^2}{r^2} \end{pmatrix} \text{and} \|z\|^2 = \frac{2r^2 + 16q^2}{r^2}$$

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \dfrac{r^2}{2r^2 + 16q^2} & \dfrac{r^2}{2r^2 + 16q^2} & \dfrac{-4qr}{2r^2 + 16q^2} \\ \dfrac{r^2}{2r^2 + 16q^2} & \dfrac{r^2}{2r^2 + 16q^2} & \dfrac{-4qr}{2r^2 + 16q^2} \\ \dfrac{-4qr}{2r^2 + 16q^2} & \dfrac{-4qr}{2r^2 + 16q^2} & \dfrac{16q^2}{2r^2 + 16q^2} \end{pmatrix} \tag{4.69}$$

Multiplying

$$C_1 = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$, Kinyanjui (2007)

and equation (4.69), we have

$$C_1E = \begin{pmatrix} \frac{r^2}{2(2r^2+16q^2)} & \frac{r^2}{2(2r^2+16q^2)} & \frac{-4qr}{2(2r^2+16q^2)} \\ \frac{r^2}{2(2r^2+16q^2)} & \frac{r^2}{2(2r^2+16q^2)} & \frac{-4qr}{2(2r^2+16q^2)} \\ 0 & 0 & 0 \end{pmatrix} \quad (4.70)$$

Thus $traceC_1E = \frac{r^2}{2r^2+16q^2}$

Now

$traceC_1E = \lambda_{\min}(C)$, implies that

$$\frac{r^2}{2r^2+16q^2} = \frac{1}{32}\left[(5\alpha_1+3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] \quad (4.71)$$

This simplifies to

$$-39914624\ \alpha_1^6 - 373568\ \alpha_1^5 - 283059600\ \alpha_1^4 + 121760\ \alpha_1^3 - 11152\ \alpha_1^2 - 26048\ \alpha_1 + 7168 = 0 \quad (4.72)$$

upon substituting the values of q and r.

The root of polynomial (4.72) is

$$\alpha_1 = 0.0662$$

Since, $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.0662$

When, $\alpha_1 = 0.0662$, $\alpha_2 = 1 - \alpha_1 = 0.9338$ and

$$\lambda_{\min} = \frac{1}{32}\left[(5\alpha_1 + 3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] = 0.02631464 \tag{4.73}$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = 0.0662$ and $\alpha_2 = 0.9338$.

Thus for m=2, ingredients we have, $\alpha_1 = 0.0662$ and $\alpha_2 = 0.9338$.

From Pukelsheim (2006), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.66), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{32}\left[(5\alpha_1 + 3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] = 0.026314645$$

Hence the optimal value for the E-criterion for m=2 factors becomes

$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.026314645$ ▪

Lemma 4.2.1

In the second-degree Kronecker model with m=3 ingredients, the weighted centroid design

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.1012\,\eta_1 + 0.8988\,\eta_2 \tag{4.74}$$

is E-optimal for $K'\theta$ in T.

The maximum of the E-criterion for m=3 ingredients is

$$v(\phi_{-\infty}) = 0.01455548 \; . \tag{4.75}$$

Proof

From the information matrix $C_k(M(\eta(\alpha)))$ Kinyanjui (2007), we compute the eigenvalues of the above matrix as follows;

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & 0 \\ \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 \\ 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{48} \end{pmatrix} \tag{4.76}$$

From equation (2.9) any matrix $C \in sym(s,H)$ can be uniquely represented in the form

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

For the case m=3, the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1 \\ cV'_1 & eW_1 \end{pmatrix}$$

With coefficients; $a,b,c,e \in \Re$, since the terms containing V_2, $W_2$and W_3 only occur for m>2.

From lemma (2.4), we get

$$U_1 = I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ U_2 = 1_2 1_2' - I_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$V_1 = \sum_{\substack{i,j=1 \\ i<j}}^{2} E_{ij}(e_i + e_j)' \in \Re^{1\times 2} = E_{12}(e_1 + e_2)' = (1 \quad 1) \text{ and } W_1 = I_{\binom{2}{2}} = 1.$$

Thus the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C_k(M(\eta(\alpha)))\begin{pmatrix} aI_m+bU_2 & cV_1 \\ cV_1^{'} & eW_1 \end{pmatrix} = \begin{pmatrix} a\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}+b\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix} & & c\begin{pmatrix}1&1&0\\1&0&1\\0&1&1\end{pmatrix}+d\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix} \\ c\begin{pmatrix}1&1&0\\1&0&1\\0&1&1\end{pmatrix}+d\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix} & & e\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}+f\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}+g\begin{pmatrix}0&0&0\\0&0&0\\0&0&0\end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ c & c & d & e & f & f \\ c & d & c & f & e & f \\ d & c & c & f & f & e \end{pmatrix} \quad (4.77)$$

where; $a=\frac{8\alpha_1+\alpha_2}{24}$, $b=\frac{\alpha_2}{48}$, $c=\frac{\alpha_2}{48}$, $d=\frac{\alpha_2}{48}$, $e=\frac{\alpha_2}{48}$ and $f=0$

with the matrices; U_1, U_2, V_1, V_2, W_1, $W_2$and W_3defined as in lemma (2.4).

$$D_1=[a+2b-c]^2+4[2d]^2=\left[\frac{8\alpha_1+\alpha_2}{24}+\frac{2\alpha_2}{48}-\frac{\alpha_2}{48}\right]^2+4\left[\frac{2\alpha_2}{48}\right]^2=\frac{185\alpha_1^2+46\alpha_1+25}{2304} \quad (4.78)$$

$$D_2=[a-b-c]^2+4(3-2)[d]^2=\left[\frac{8\alpha_1+\alpha_2}{24}-\frac{\alpha_2}{48}-\frac{\alpha_2}{48}\right]^2+4\left[\frac{\alpha_2}{48}\right]^2=\left(\frac{260\alpha_1^2-8\alpha_1+4}{2304}\right) \quad (4.79)$$

Using equation (3.10) in lemma (3.2.1), we obtain for m=3

$$\lambda_{2,3}=\frac{1}{2}\left[a+2b+c\pm\sqrt{D_1}\right]=\frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{24}-2\left[\frac{\alpha_2}{48}\right]+\left[\frac{\alpha_2}{4}\right]\pm\sqrt{\frac{13\alpha_1^2-14\alpha_1+5}{36}}\right]$$

$$=\frac{1}{96}\left[(11\alpha_1+5)\pm\sqrt{185\alpha_1^2+46\alpha_1+25}\right], \quad \text{with multiplicity 1}$$

Similarly, using equation (3.11) in lemma (3.2.1) we get

$$\lambda_{4,5}=\frac{1}{2}\left[a-b+c\pm\sqrt{D_2}\right]=\frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{24}-\frac{\alpha_2}{48}+\frac{\alpha_2}{48}\pm\sqrt{\frac{260\alpha_1^2-8\alpha_1+4}{48^2}}\right]$$

$$= \frac{1}{48}\left[(7\alpha_1 + 1) \pm \sqrt{65\alpha_1{}^2 - 2\alpha_1 + 1}\right]$$

From lemma (3.2.1) the eigenvalues that $\lambda_2, \lambda_3, \lambda_4\ and\ \lambda_5$ occur for the case m=3. These are

$\lambda_2 = \frac{1}{96}\left[(11\alpha_1 + 5) + \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right]$, with multiplicity 1,

$\lambda_3 = \frac{1}{96}\left[(11\alpha_1 + 5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right]$, with multiplicity 1,

$\lambda_4 = \frac{1}{96}\left[(7\alpha_1 + 1) + \sqrt{65\alpha_1^2 - 2\alpha_1 + 1}\right]$, with multiplicity 2 and

$\lambda_5 = \frac{1}{48}\left[(7\alpha_1 + 1) - \sqrt{65\alpha_1^2 - 2\alpha_1 + 1}\right]$, with multiplicity 2.

From theorem (3.2.3), if the smallest eigenvector of $C_k(M)$ has multiplicity 1, then the only choice for the matrix E is, $E = \frac{zz'}{\|z\|^2}$, where $z \in \Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$. In our case, the smallest eigenvalue is

$$\lambda_3 = \frac{1}{96}\left[(11\alpha_1 + 5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right] \qquad (4.80)$$

We therefore need to get an eigenvector z, corresponding to the smallest eigenvalue of the matrix, $C_k(M)$.

By definition, $\lambda \in \Re$, is an eigenvalue of matrix C if

$$(C - \lambda I)\vec{z} = \vec{0} \Leftrightarrow C\vec{z} = \lambda\vec{z} \text{ with } \vec{z} \neq \vec{0}$$

Where, $\left(\vec{z} = u \quad v \quad w \quad x \quad y \quad z\right)$, is an eigenvector of C corresponding to λ.

Thus, from equation (4.76) and equation (4.80)

$(C-\lambda_{\min}I)\vec{z}=\vec{0}$, implies that

$$\begin{pmatrix} p & 2q & 2q & 2q & 2q & 0 \\ 2q & p & 2q & 2q & 0 & 2q \\ 2q & 2q & p & 0 & 2q & 2q \\ 2q & 2q & 0 & r & 0 & 0 \\ 2q & 0 & 2q & 0 & r & 0 \\ 0 & 2q & 2q & 0 & 0 & r \end{pmatrix}\begin{pmatrix} u \\ v \\ w \\ x \\ y \\ z \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{4.81}$$

where, $p=7\alpha_1-3+\sqrt{13\alpha_1^2-14\alpha_1+5}$, $q=\alpha_2=1-\alpha_1$ and

$r=-13\alpha_1+3+\sqrt{13\alpha_1^2-14\alpha_1+5}$

$pu+2qv+2qw+2qx+2qy+2qz=0$

$2qu+pv+2qw+2qx+2qz=0$

$2qu+2qv+pw+2qy+2qz=0$

$2qu+2qw+ry=0$

$2qv+2qw+rz=0$

Solving the above system of linear equations, we obtain the eigenvector corresponding to $\lambda_{\min}$ as;

$$\vec{z}=\begin{pmatrix} u \\ v \\ w \\ x \\ y \\ z \end{pmatrix}=\begin{pmatrix} 1 \\ 1 \\ 1 \\ \frac{-4q}{r} \\ \frac{-4q}{r} \\ \frac{-4q}{r} \end{pmatrix} \tag{4.82}$$

Then the matrix

$$zz' = \begin{pmatrix} 1 & 1 & 1 & \frac{-4q}{r} & \frac{-4q}{r} & \frac{-4q}{r} \\ 1 & 1 & 1 & \frac{-4q}{r} & \frac{-4q}{r} & \frac{-4q}{r} \\ 1 & 1 & 1 & \frac{-4q}{r} & \frac{-4q}{r} & \frac{-4q}{r} \\ \frac{-4q}{r} & \frac{-4q}{r} & \frac{-4q}{r} & \frac{16q^2}{r^2} & \frac{16q^2}{r^2} & \frac{16q^2}{r^2} \\ \frac{-4q}{r} & \frac{-4q}{r} & \frac{-4q}{r} & \frac{16q^2}{r^2} & \frac{16q^2}{r^2} & \frac{16q^2}{r^2} \\ \frac{-4q}{r} & \frac{-4q}{r} & \frac{-4q}{r} & \frac{16q^2}{r^2} & \frac{16q^2}{r^2} & \frac{16q^2}{r^2} \end{pmatrix} \text{ and } \|z\|^2 = \frac{3r^2 + 48q^2}{r^2}$$

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} \\ \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} \\ \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} \end{pmatrix} \quad (4.83)$$

Multiplying

$$C_1 = \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

, Kinyanjui (2007) and equation (4.83), we have

$$C_1E = \begin{pmatrix} \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} \\ \frac{r^2}{3(3r^2+12q^2)} & \frac{r^2}{3(3r^2+12q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} \\ \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} & \frac{-4qr}{3(3r^2+48q^2)} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

(4.84)

Thus $traceC_1E = \frac{r^2}{3r^2+48q^2}$

Now

$traceC_1E = \lambda_{\min}(C)$, implies that

$$\frac{r^2}{3r^2+48q^2} = \frac{1}{96}\left[(11\alpha_1+5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right] \quad (4.85)$$

This simplifies to

$$-1360035616\alpha_1^6 - 5193036\alpha_1^5 - 957013797\alpha_1^4 + 347618\alpha_1^3 + 1496439\alpha_1^2 - 792600\alpha_1 + 164864 = 0 \quad (4.86)$$

upon substituting the values of q and r .

The root of polynomial (4.80) is

$\alpha_1 = 0.1012$

Since, $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.1012$

When, $\alpha_1 = 0.1012$, $\alpha_2 = 1 - \alpha_1 = 0.8988$ and

$$\lambda_{\min} = \frac{1}{96}\left[(11\alpha_1+5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right] = 0.01455548 \quad (4.87)$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = 0.1012$

Thus for m=3, ingredients we have, $\alpha_1 = 0.1012$ and $\alpha_2 = 0.8988$.

From Pukelsheim (2006), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (103), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{96}\left[(11\alpha_1 + 5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right] = 0.01455548$$

Hence the optimal value for the E-criterion for m=3 factors becomes
$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.01455548$ **.**

Lemma 4.2.2

In the second-degree Kronecker model with m=4 ingredients, the weighted centroid design

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.1231\,\eta_1 + 0.8769\,\eta_2 \qquad (4.88)$$

is E-optimal for $K'\theta$ in T.

The maximum of the E-criterion for m=4 ingredients is

$$v(\phi_{-\infty}) = 0.015525588 \quad . \qquad (4.89)$$

Proof

In the second-degree Kronecker model any matrix $C \in \mathrm{sym}(s,H)$ can be uniquely represented in the form

$$C = \begin{pmatrix} aU_1 + bU_2 & dV_1' \\ dV_1 & c\dfrac{V'V}{m} \end{pmatrix}$$

and for the case m=4 ingredients the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C=\begin{pmatrix} aU_1+bU_2 & dV_1 \\ dV_1' & c\dfrac{V'V}{m} \end{pmatrix}$$

With coefficients $\mathrm{a,b,c,d}\in\Re$,

where; $a=\dfrac{8\alpha_1+\alpha_2}{32}$, $b=\dfrac{\alpha_2}{96}$, $c=\dfrac{\alpha_2}{48}$, and $d=0$ $e=\dfrac{\alpha_2}{96}$ $f=0$ $g=0$

with the matrices; U_1, U_2, V_1, V_2, W_1, $W_2$and W_3defined as in lemma (2.4).

Information matrix $C_k(M(\eta(\alpha)))$, Kinyanjui (2007), for a mixture experiment design $\eta(\alpha)$ for m=4 ingredients is given as;

$$C_k=C_k(M(\eta(\alpha)))=\begin{pmatrix}
\frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & 0 \\
\frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 \\
\frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} \\
\frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} \\
\frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 & 0 & 0 & 0 \\
\frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 & 0 & 0 \\
\frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 & 0 \\
0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 \\
0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{96} & 0 \\
0 & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha_2}{96}
\end{pmatrix}$$

(4.90)

From equation (2.9), any marix $C\in sym(s,H)$ can be represented in the form

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

with coefficients $a,\ldots,g\in\Re$. The terms containing V_2, $W_2$and W_3occurring for $m\geq 3$ or $m\geq 4$ respectively.

For case when m=4, the information matrix $C_k(M(\eta(\alpha)))$ can be written as;

$$C=\begin{pmatrix} aI_3+bU_2 & cV_1'+dV_2' \\ cV_1+dV_2 & eI_3+fW_2 \end{pmatrix}$$

From lemma (2.4), we get

$$U_1=I_4=\begin{pmatrix} 1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix},$$

$$U_2=1_41_4'-I_4=\begin{pmatrix} 1&1&1&1\\1&1&1&1\\1&1&1&1\\1&1&1&1 \end{pmatrix}-\begin{pmatrix} 1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}=\begin{pmatrix} 0&1&1&1\\1&0&1&1\\1&1&0&1\\1&1&1&0 \end{pmatrix},$$

$$V=\sum_{\substack{i,j=1\\i<j}}^{4}(e_i)\in\Re^{4\times 1}=(e_1+e_2+e_3+e_4)=\begin{pmatrix}1\\1\\1\\1\end{pmatrix}$$

Thus the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C_k(M(\eta(\alpha)))=\begin{pmatrix} aU_1+bU_2 & dV_1 \\ dV_1' & c\dfrac{V'V}{m} \end{pmatrix}=\left[\begin{matrix} a\begin{pmatrix} 1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}+b\begin{pmatrix} 0&1&1&1\\1&0&1&1\\1&1&0&1\\1&1&1&0 \end{pmatrix} & d\begin{pmatrix}1\\1\\1\\1\end{pmatrix} \\ d\begin{pmatrix}1&1&1&1\end{pmatrix} & c(1) \end{matrix}\right]$$

Where; $a = \dfrac{8\alpha_1 + \alpha_2}{32}$, $b = \dfrac{\alpha_2}{96}$, $c = \dfrac{\alpha_2}{48}$, and $d = 0$ $e = \dfrac{\alpha_2}{96}$ $f = 0$ $g = 0$

From lemma (3.2.1), we compute the eigenvalues of the above matrix as follows

$$D_1 = [a + 3b - e]^2 + 6[2c]^2 = \left[\frac{8\alpha_1 + \alpha_2}{32} + \frac{3\alpha_2}{96} - \frac{\alpha_2}{96}\right]^2 + 6\left[\frac{2\alpha_2}{48}\right]^2 = \frac{385\alpha_1^2 + 142\alpha_1 + 49}{9216} \quad (4.91)$$

$$D_2 = [a - b - e]^2 + 4(4-2)[c]^2 = \left[\frac{8\alpha_1 + \alpha_2}{32} - \frac{\alpha_2}{96} - \frac{\alpha_2}{96}\right]^2 + 4(2)\left[\frac{\alpha_2}{48}\right]^2 = \left(\frac{561\alpha_1^2 - 156\alpha_1 + 36}{9216}\right) \quad (4.92)$$

Using equation (3.10) in lemma (3.2.1), we obtain for m=4

$$\lambda_{2,3} = \frac{1}{2}\left[a + 3b + e \pm \sqrt{D_1}\right] = \frac{1}{2}\left[\frac{8\alpha_1 + \alpha_2}{32} + 3\left[\frac{\alpha_2}{96}\right] + \left[\frac{\alpha_2}{96}\right] \pm \sqrt{\frac{385\alpha_1^2 + 142\alpha_1 + 49}{96^2}}\right] \quad (4.93)$$

$$= \frac{1}{192}\left[(17\alpha_1 + 7) \pm \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}\right], \quad \text{with multiplicity 1}$$

Similarly, using equation (3.11) in lemma (3.2.1) we get

$$\lambda_{4,5} = \frac{1}{2}\left[a - b + e \pm \sqrt{D_2}\right] = \frac{1}{2}\left[\frac{8\alpha_1 + \alpha_2}{32} - \frac{\alpha_2}{96} + \frac{\alpha_2}{96} \pm \sqrt{\frac{561\alpha_1^2 - 156\alpha_1 + 36}{96^2}}\right]$$

$$= \frac{1}{96}\left[21\alpha_1 + 3 \pm \sqrt{561\alpha_1^2 - 156\alpha_1 + 36}\right], \text{ with multiplicity 2} \quad (4.94)$$

The smallest eigenvalue is $= \dfrac{1}{192}\left[17\alpha_1 + 7 \pm \sqrt{385\alpha_1^2 - 142\alpha_1 + 49}\right]$, (120)

From lemma (3.2.1) the eigenvalues that λ_2, λ_3, λ_4 *and* λ_5 occur for the case m=4. These are

$$\lambda_2 = \frac{1}{192}\left[17\alpha_1 + 7 + \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}\right], \text{ with multiplicity 1,}$$

$$\lambda_3 = \frac{1}{192}\left[17\alpha_1 + 7 - \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}\right]$$, with multiplicity 1,

$$\lambda_4 = \frac{1}{96}\left[21\alpha_1 + 3 \pm \sqrt{561\alpha_1^2 - 156\alpha_1 + 36}\right]$$, ,withmultiplicity2 and

$$\lambda_5 = \frac{1}{96}\left[21\alpha_1 + 3 \pm \sqrt{561\alpha_1^2 - 156\alpha_1 + 36}\right]$$, with multiplicity 2.

From theorem (3.2.3), if the smallest eigenvector of $C_k(M)$ has multiplicity 1, then the only choice for the matrix E is, $E = \frac{zz'}{\|z\|^2}$, where $z \in \Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$. In our case, the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{192}\left[17\alpha_1 + 7 - \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}\right], \tag{4.95}$$

We therefore need to get an eigenvector z, corresponding to the smallest eigenvalue of the matrix, $C_k(M)$.

By definition, $\lambda \in \Re$, is an eigenvalue of matrix C if

$$(C - \lambda I)\vec{z} = \vec{0} \Leftrightarrow C\vec{z} = \lambda\vec{z} \text{ with } \vec{z} \neq \vec{0}$$

Where, $\vec{z} = \begin{pmatrix} g & h & s & t & u & v & w & x & y & z \end{pmatrix}'$, is an eigenvector of C corresponding to λ.

Thus, from equation (4.90) and equation (4.95)

$(C - \lambda_{\min} I)\vec{z} = \vec{0}$, implies that

$$\begin{pmatrix} p & 2q & 2q & 2q & 4q & 4q & 4q & 0 & 0 & 0 \\ 2q & p & 2q & 2q & 4q & 0 & 0 & 4q & 4q & 0 \\ 2q & 2q & p & 2q & 0 & 4q & 0 & 4q & 0 & 4q \\ 2q & 2q & 2q & p & 0 & 0 & 4q & 0 & 4q & 4q \\ 4q & 4q & 0 & 0 & r & 0 & 0 & 0 & 0 & 0 \\ 4q & 0 & 4q & 0 & 0 & r & 0 & 0 & 0 & 0 \\ 4q & 0 & 0 & 4q & 0 & 0 & r & 0 & 0 & 0 \\ 0 & 4q & 4q & 0 & 0 & 0 & 0 & r & 0 & 0 \\ 0 & 4q & 0 & 4q & 0 & 0 & 0 & 0 & r & 0 \\ 0 & 0 & 4q & 4q & 0 & 0 & 0 & 0 & 0 & r \end{pmatrix} \begin{pmatrix} g \\ h \\ s \\ t \\ u \\ v \\ w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

where, $p = 25\alpha_1 + 13 + \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}$, $q = \alpha_2 = 1 - \alpha_1$ and

$r = 19\alpha_1 - 5 + \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}$

$pg + 2qh + 2qs + 2qt + 4qu + 4qv + 4qw = 0$

$2qg + ph + 2qs + 2qt + 4qu + 4qx + 4qy = 0$

$2qg + 2qh + ps + 2qt + 4qv + 4qx + 4qz = 0$

$2qg + 2qh + 2qs + pt + 4qw + 4qy + 4qz = 0$

$4qg + 4qh + ru = 0$

$4qg + 4qs + rv = 0$

$4qg + 4qt + rw = 0$

$4qh + 4qs + rx = 0$

$4qh + 4qt + ry = 0$

$4qs + 4qt + rz = 0$

Solving the above system of linear equations, we obtain the eigenvector corresponding to

$\lambda_{\min}$ as;

$$\vec{z} = \begin{pmatrix} g \\ h \\ s \\ t \\ u \\ v \\ w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \end{pmatrix}$$

Then the matrix

$$zz' = \begin{pmatrix}
1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\
1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\
1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\
1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\
\frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\
\frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\
\frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\
\frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\
\frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\
\frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2}
\end{pmatrix}$$

and $\|z\|^2 = \frac{4r^2 + 384q^2}{r^2}$

Thus the matrix E is given as;

$$E=\begin{pmatrix}
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2}
\end{pmatrix} \tag{4.96}$$

Multiplying matrix

$$C_1=\begin{pmatrix}
\frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

, Kinyanjui (2007) and equation (4.96),we have

$$C_1E=\begin{pmatrix}
\frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} \\
\frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} \\
\frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} \\
\frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{r^2}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} & \frac{-8qr}{4(4r^2+384q^2)} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \tag{4.97}$$

Thus $traceC_1E = \frac{r^2}{4r^2 + 384q^2}$

Now

$traceC_1E = \lambda_{\min}(C)$, implies that

$$\frac{r^2}{4r^2 + 384\,q^2} = \frac{1}{192}\left[17\,\alpha_1 + 7 - \sqrt{385\,\alpha_1^2 - 142\,\alpha_1 + 49}\right]$$

(4.98)

This simplifies to

$$-5512679936\ \alpha_1^6 - 30324736\ \alpha_1^5 - 2271901952\ \alpha_1^4 + 2900480\ \alpha_1^3 + 10876672\ \alpha_1^2 - 4265984\ \alpha_1 + 897024\ = 0 \tag{4.99}$$

upon substituting the values of q and r.

The root of polynomial (4.99) is

$\alpha_1 = 0.1312$,

Since, $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.1312$

When $\alpha_1 = 0.1312$, $\alpha_2 = 1 - \alpha_1 = 0.8688$ and

$$\lambda_{\min} = \frac{1}{192}\left[17\alpha_1 + 7 - \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}\right] = 0.015525588$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = 0.1312$, $\alpha_2 = 1 - \alpha_1 = 0.8688$.

Thus for m=4 ingredients we have, $\alpha_1 = 0.1312$ and $\alpha_2 = 0.8688$

From Pukelsheim (2006), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.95), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{192}\left[17\alpha_1 + 7 - \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}\right] = 0.015525588$$

Hence the optimal value for the E-criterion for m=4 factors becomes

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.015525588 \ .$$

4.1.3 Generalization of E-optimal design for maximal parameter subsystem

Theorem 4.2.1

In the second degree Kronecker model with m-ingredients the weighted centroid design

$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2$ is E-optimal for $K'\theta$ in T. (4.100)

The maximum value of the E-criterion for $K'\theta$ with m ingredients is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{16m(m-1)}\left[(6m-7)\alpha_1 + 2m - 1 - \sqrt{D}\right] \qquad (4.101)$$

Where $D = (36m^2 - 52m + 17)\alpha_1^{\ 2} - (24m^2 - 72m + 46)\alpha_1 + (4m^2 - 4m + 1)$ (4.102)

Proof

From equation (2.9) any matrix $C \in sym(s,H)$ can be uniquely represented in the form

$$C = \begin{pmatrix} aU_1 + bU_2 & dV_1 \\ dV_1^{'} & c\dfrac{V'V}{m} \end{pmatrix}$$

For the case m ingredients the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C = \begin{pmatrix} aU_1 + bU_2 & dV_1 \\ dV_1^{'} & c\dfrac{V'V}{m} \end{pmatrix}$$

With coefficients $\mathrm{a,b,c,d} \in \Re$,

For lemma(2.5) we get

$$U_1 = I_m = \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0. & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix}$$

$$U_2 = I_m I'_m - I_m = \begin{pmatrix} 1 & . & . & . & 1 \\ . & . & & & . \\ . & & . & & . \\ . & & & . & . \\ 1 & . & . & . & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0. & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & . & . & . & 1 \\ 1. & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 1 & & . & . & . & 0 \end{pmatrix}, \text{ and}$$

$$V = \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_i) \in \Re^{m\times 1} = (e_1 + e_2 + \ldots + e_m) = \begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \end{pmatrix}$$

Hence the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} aU_1 + bU_2 & dV \\ dV' & c\dfrac{V'V}{m} \end{pmatrix} = \left[\begin{matrix} a\begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} + b \begin{pmatrix} 0 & 1 & . & . & . & 1 \\ 1 & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 1 & & . & . & . & 0 \end{pmatrix} & d\begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \end{pmatrix} \\ d\begin{pmatrix} 1 & . & . & . & 1 \end{pmatrix} & c(1) \end{matrix} \right]$$

$$= \begin{pmatrix} \dfrac{8\alpha_1 + \alpha_2}{8m} U_1 + \dfrac{\alpha_2}{8m(m-1)} U_2 & \dfrac{\alpha_2}{8m(m-1)} V \\ \dfrac{\alpha_2}{8m(m-1)} V' & \dfrac{\alpha_2}{8m(m-1)} \dfrac{V'V}{m} \end{pmatrix} \tag{4.103}$$

From lemma (3.2.1) for m ingredients we have

$$D_1 = [a+(m-1)b-c]^2 + 2(m-1)[2d]^2$$

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

$$= \frac{(36m^2-52m+17)\alpha_1{}^2 - (24m^2-72m+46)\alpha_1 + (4m^2-4m+1)}{64m^2}$$

The eigenvalues are;

$$\lambda_{2,3} = \frac{1}{2}\left[a+(m-1)b+c \pm \sqrt{D_1}\right]$$

$$= \frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{8m} + \frac{(m-1)\alpha_2}{8m(m-1)} + \frac{\alpha_2}{8m(m-1)} \pm \sqrt{D_1}\right]$$

$$= \frac{1}{16m(m-1)}\left[(6m-7)\alpha_1 + 2m - 1 - \sqrt{D}\right]$$

Where $D = (36m^2-52m+17)\alpha_1{}^2 - (24m^2-72m+46)\alpha_1 + (4m^2-4m+1)$ with multiplicity 1.

Hence the smallest eigenvalue is $\lambda_3 = \frac{1}{16m(m-1)}\left[(6m-7)\alpha_1 + 2m - 1 - \sqrt{D}\right]$ where D is as above.

Now let $\lambda_{\min} = \frac{1}{16m(m-1)}\left[(6m-7)\alpha_1 + 2m - 1 - \sqrt{D}\right]$ then $\lambda_{\min}$ is an eigenvalue for C if for corresponding eigenvector, say $\bar{z}$, we have $(C-\lambda I)\bar{z} = \bar{0}$ or $(C\bar{z} = \lambda\bar{z})$ with $\bar{z} \neq \bar{0}$

Now let

$$\bar{z} = \begin{pmatrix} z_1 \\ . \\ . \\ . \\ z_{m+1} \end{pmatrix}$$, be the eigenvector of C corresponding to λ.

We therefore have $(C-\lambda I)$, as

$$\begin{pmatrix} \frac{8m\alpha_1 - 5m + \sqrt{D}}{16m(m-1)} I_m + \frac{\alpha_2}{8m(m-1)} U_2 & \frac{\alpha_2}{8m(m-1)} V \\ \frac{\alpha_2}{8m(m-1)} V' & \frac{(5-6m)\alpha_1 - 2m + 3 + \sqrt{D}}{16m(m-1)} I_{\binom{m}{2}} \end{pmatrix}$$

$$= \frac{1}{16m(m-1)} \begin{pmatrix} 8m\alpha_1 - 5m + \sqrt{D} I_m + 2\alpha_2 U_2 & 2\alpha_2 V \\ 2\alpha_2 V' & (5-6m)\alpha_1 - 2m + 3 + \sqrt{D} I_{\binom{m}{2}} \end{pmatrix}$$

Let $p_1 = 8m\alpha_1 - 5m + \sqrt{D}$, $q_1 = \alpha_2^{\ 2}$, $r_1 = (5-6m)\alpha_1 - 2m + 3 + \sqrt{D}$

We get $(C-\lambda I)\bar{z} = \bar{0}$

$$= \frac{1}{16m(m-1)} \begin{pmatrix} (p_1 U_1 + 2q_1 U_2 & 2q_1 V \\ 2q_1 V' & r_1 \frac{V'V}{m} \end{pmatrix} \quad (4.104)$$

Solving these equations for z_i we get,

$$\bar{z} = \begin{pmatrix} z_1 \\ . \\ . \\ . \\ \\ z_{m+1} \end{pmatrix} = \begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \\ \frac{-cmq}{r} \end{pmatrix}$$

Where c=2 for even number of ingredients and varying fraction for odd number of ingredients as the eigenvector corresponding to $\lambda_{\min}$

Thus

$$\bar{z}\bar{z}' = \begin{pmatrix} U_1 + U_2 & -cmqV \\ \frac{cmq}{r}V' & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix}, \text{ and } \|z\|^2 = \frac{mr^2 + c^2m^2q^2}{r^2}$$

Therefore

$$E = \frac{\bar{z}\bar{z}'}{\|z\|^2} = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} U_1 + U_2 & -cmqV \\ \frac{cmq}{r}V' & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix} \tag{4.105}$$

And from equation (4.103) and equation (4.105)

$$C_1E = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} \frac{1}{m}U_1 + \frac{1}{m}U_2 & -cqV \\ 0 & 0 \end{pmatrix}$$

From theorem 3.2.2 a weighted centroid design $\eta(\alpha)$ is E-optimal for $K'\theta$ in T if and only if $traceC_jE = \lambda_{\min}(C)$.

For j=1

$$traceC_jE = \frac{r^2}{m(mr^2 + c^2m^2q^2)} + \ldots + .\frac{r^2}{m(mr^2 + c^2m^2q^2)} = \frac{r^2}{(mr^2 + c^2m^2q^2)}$$

Hence

$$traceC_j E = \lambda_{\min}(C) \Leftrightarrow \frac{r^2}{(mr^2 + c^2m^2q^2)} = \frac{1}{16m(m-1)}\left[(6m-7)\alpha_1 + (2m-1) - \sqrt{D}\right] \quad (4.106)$$

Putting $q = \alpha_2$, $r_1 = \left[(5-6m)\alpha_1 - 2m + 3 + \sqrt{D}\right]$ and

$D = (36m^2 - 52m + 17)\alpha_1^2 - (24m^2 - 72m + 46)\alpha_1 + (4m^2 - 4m + 1)$ reduces equation

(4.106) to

$$-i\alpha_1^6 - j\alpha_1^5 + k\alpha_1^4 + l\alpha_1^3 + m\alpha_1^2 - n\alpha_1^1 + o = 0$$

Where

$$i = -5225472m^5 - 18432m^4 + 44544m^3 - 9996832m^2 + 4608m + 2048$$

$$j = -10368m^6 + 33124m^5 - 149760m^4 + 328952m^3 - 313056m^2 + 135680m - 24576$$

$$k = 14260m^5 - 172049m^4 - 34987744m^3 - 178688m^2 - 119296m + 92160$$

$$l = 6888m^6 - 30840m^5 - 58926m^4 + 528976m^3 - 946368m^2 + 664064m - 163840$$

$$m = 3068m^6 - 14972m^5 + 157695m^4 - 618592m^3 + 952576m^2 - 633344m + 153600$$

$$n = 384m^6 - 1440m^5 - 65792m^4 + 289400m^3 - 447840m^2 + 299008m - 73728$$

$$o = 12288m^4 - 52224m^3 + 81408m^2 - 55808m + 14336$$

Solving the above polynomial yields the values of α_1 from which we choose α_1, such that $\alpha_1 \in (0,1)$; we substitute this values to $\lambda_{\min}C$ and take the values that maximizes the $\lambda_{\min}C$, hence the optimal E-criterion is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{16m(m-1)}\left[(6m-7)\alpha_1 + 2m - 1 - \sqrt{D}\right]$$

Where $D = (36m^2 - 52m + 17)\alpha_1^2 - (24m^2 - 72m + 46)\alpha_1 + (4m^2 - 4m + 1)$

CHAPTER FIVE

NUMERICAL RESULTS AND DISCUSSION

5.1 Numerical Results

In this chapter, numerically computed values for the two corresponding parameters of interest for $E-optimal$ weighted centroid designs for $K'\theta$ are presented. These include the two values α_1 and α_2. The optimality value, v_p for the corresponding number of ingredients are also presented. Smallest eigenvalues for two, three, four and generalized for m ingredient for non-maximal and maximal parameter subsystem is presented.

Table 5.1: E-optimal weights and values for $K'\theta$, $m = 2,3,\ldots,7$

m	**Parameter subsystem** $p=-\infty$	**Non-maximal**	**Maximal**
2	$\alpha_1^{(p)}$	0.4545	0.0662
	$\alpha_2^{(p)}$	0.5455	0.9338
	v_p	0.0909	0.0263
3	$\alpha_1^{(p)}$	0.5753	0.1012
	$\alpha_2^{(p)}$	0.4247	0.8988
	v_p	0.0735	0.0145
4	$\alpha_1^{(p)}$	0.9998	0.1312
	$\alpha_2^{(p)}$	0.0002	0.8688
	v_p	0.0018	0.0155
5	$\alpha_1^{(p)}$	0.0001	0.1424
	$\alpha_2^{(p)}$	0.0009	0.8760
	v_p	0.10002	0.0020
6	$\alpha_1^{(p)}$	0.9780	0.1619
	$\alpha_2^{(p)}$	0.0006	0.8381
	v_p	0.0001	0.0320
7	$\alpha_1^{(p)}$	0.9995	0.1827
	$\alpha_2^{(p)}$	0.0005	0.8173
	v_p	0.0001	0.0011

5.2 Discussion

Table 5.1 shows the computed weights and optimal values for two, three, four and a continuation of optimal values for five, six and seven obtained from the generalized formula derived. The values α_1 and α_2 are weights used to develop E-optimal weighted centroid design for m≥2 ingredients in the study. The value v_p represents optimal values for the weighted centroid design for every m-ingredient.

CHAPTER SIX

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

In this thesis, some E-optimal designs in the second-degree Kronecker model for mixture experiments were investigated for the non-maximal and maximal parameter subsystem. All considerations were restricted to weighted centroid designs due to the completeness result.

It was found that for second-degree Kronecker model with $m \geq 2$ ingredients the unique E-optimal weighted centroid designs for $K'\theta$, exist for Non-maximal and maximal parameter subsystem. In addition, a general formula for the computation of the smallest eigenvalues for m ingredient exists for the two parameters of interest hence this will help in obtaining the smallest eigenvalues for m number of ingredients.

6.2 Recommendations

Earlier work done for third-degree Kronecker model for non maximal parameter subsystem showed that there exists E-optimal weighted centroid design for $K'\theta$. It would therefore be very interesting to see whether there exists E-optimal weighted centroid design for maximal parameter subsystem for $K'\theta$.In line with the study it could be interesting to see practical results for the implementation of the designs suggested in this study is recommended.

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