OPTIMAL DESIGN FOR SECOND-DEGREE KRONECKER MODEL MIXTURE EXPERIMENTS FOR MAXIMAL PARAMETER SUBSYSTEM

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DECLARATION

Declaration by the student

This thesis is my original work and has not been presented for a degree in any other University. No part of this thesis may be reproduced without the prior written permission of the author and/or University of Eldoret.

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DEDICATION

To my beloved parent, friends and future family

ABSTRACT

Products in many disciplines frequently involve blending two or more ingredients together. The design factors in a mixture experiment are the proportions of the components of a blend, and the response variables vary as a function of these proportions making the total and not the actual quantity of each component. This study investigated optimal design for maximal parameter subsystem for second-degree Kronecker model mixture experiments put forward by Draper and Pukelsheim. Based on the completeness result, the investigations was restricted to weighted centroid designs. In mixture model on the simplex an improvement is obtained for a given design in terms of increasing symmetry as well as obtaining a larger moment matrix under the Loewner ordering. These two criteria constitute the Kiefer design ordering. The parameter subsystem of interest $K'\theta$ in the study was maximal parameter subsystem which is a subspace of the full parameter space θ. In this model the full parameter subsystem was not estimable. By a proper definition of parameter matrix, a maximal parameter subsystem in the model was selected. Canonical unit vectors and the concept of Kronecker products were employed to identify the parameter matrices as well as the information matrices. For the second degree mixture model with two, three, four and m ingredients, a set of weighted centroid designs were obtained for a characterization of the feasible weighted centroid designs for the maximal parameter subsystem. After obtaining the feasible weighted centroid designs the information matrix of the design was computed. Derivations of A-, D- and E-optimal weighted centroid designs were then obtained from the information matrix. The optimality criteria A, D and E were used to compute optimal centroid designs. The results based on maximal parameter subsystem, second degree mixture model with $m \geq 2$ ingredient for A-, D- and E-optimal weighted centroid design for $K'\theta$ exist for the choice of the coefficient matrix specifically in this study. Optimal weights and values for the weighted centroid designs were numerically computed using Matlab software.

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CHAPTER ONE

INTRODUCTION

1.1 Background Information

A mixture problem is one where two or more ingredients are mixed together to form a product. This product has desirable properties that are of interest to the manufacturers. Many practical problems are associated with investigation of a mixture of m factors, assumed to influence the response only through the proportions in which they are blended together. The response is a measurable quantity or property of interest on the product. It is assumed that, the experimenter can measure quantities of the ingredients in the mixture without error. It is further assumed that, the responses are functionally related to the product composition and that, by varying the composition through the changing of ingredients proportions, the responses will also vary. The experimenter's motives to studying the functional relationship between the response and the controllable variables are;

(i) To determine whether some combination of the factors can be considered best in some sense

(ii) To gain a better understanding of the overall system by studying the roles played by the different ingredients.

The aim of studying the functional relationship between the measured property (response) and the controllable variables is to determine the best combination of ingredients that yield the desired product.

Some examples are:

(i) Cake formulations using baking powder, shortening, flour, sugar and water.

(ii) Fruit punch consisting of juices from watermelon, pineapple and orange.

(iii) Building construction concrete formed by mixing sand, water and cement.

In each of the cases, one or more properties that are desirable are, fluffiness of the cake, such that fluffiness is related to the ingredient proportion, the fruitiness flavor of the punch, which depends on the percentages of water melon, pineapple and orange that are present in the punch, and the hardness or compression strength of the concrete, where the hardness is a function of the percentages of cement, sand and water in the mix (Cornell, 1990).

1.2 Mixture Experiment

A mixture experiment is an experiment which involves mixing of 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 of m factors, assumed to influence the response through the proportions in which they are blended together. The definitive text by Cornell (1990) lists numerous examples of applications of mixture experiments and provides a thorough discussion of both theory and practical. Early work was done by Scheffe' (1958, 1963) who suggested and analyzed canonical model forms when the regression function for the expected response is a polynomial of degree one, two or three.

For $i = 1,...,m$, let $t_i \in [0,1]$ be the proportion of ingredient i in the mixture. We assemble the individual components to form the vector of experimental conditions, $t = (t_1,...,t_m)'$, subject to the simplex restriction

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

Let $1_m = (1, ..., 1)' \in \Re^m$, be the unit vector. Thus, the experimental domain is then the standard probability simplex T_m, represented as;

$$T_m = \{t = (t_1,...,t_m)' \in [0,1]^m ; 1'_m t = 1\}$$

Under experimental conditions $t \in T_m$, the experimental response Y_t, is taken to be a scalar random variable. Replications under identical experimental conditions as well as responses from distinct experimental conditions are assumed to have equal (unknown) variance, σ^2 and to be uncorrelated.

An experimental design, τ on the experimental domain T_m, is a probability measure having a finite number of 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. Let the observed response Y_t be expressed as $Y_t = \eta(t,\Theta) + \varepsilon(t)$, where $\eta(t,\Theta)$ is the expected response and $\varepsilon(t)$, is the error term at t. we assume that for independent observations, the errors, $\varepsilon(t)$ are statistically independent and have mean zero and the same variance. Further we assume that, $\eta(t,\Theta)$ can be expressed as a polynomial function in t.

A particular polynomial regression model for mixture experiments suggested by Draper and Pukelsheim (1998) is the second-degree Kronecker model. Its regression function $f : T_m \to \Re^{m^2}; t = (t_1, ..., t_m)' \to t \otimes t = t_i t_j, \quad i, j = 1, ..., m$ with the index pairs (i,j), $1 \le i < j \le m$ ordered lexicographically yields the model equation;

$$E(Y_t) = f(t)'\theta = \sum_{i=1}^{m} \theta_{ii} t_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{m} (\theta_{ij} + \theta_{ji}) t_i t_j \; , \quad \text{...} \; (1.2)$$

where Y_t, the response under experimental condition $t \in T_m$, is taken to be a real valued random variable and $\theta = (\theta_{11}, \theta_{12}, ..., \theta_{mm})' \in \Re^{m^2}$ an unknown parameter. All observations taken in an experiment are assumed to be uncorrelated and to have common unknown variance $\sigma^2 \in (0, \infty)$.

1.3 Statement of the problem

The study investigates optimal designs in the second-degree Kronecker model for mixture experiments and obtained a design with maximum information on the parameter subsystem. Since the full parameter subsystem is not estimable, coefficient matrix $K'\theta$ of interest is chosen to make it estimable subject to the side condition. The full system θ is made estimable by dividing the interacting factors by the total number of interacting parameters in the model. This maximum is accomplished through the application of the ∅ -optimality criteria of a weighted centroid design following the Kiefer Wolfowitz equivalence theorem.

1.4 Study objectives

The objectives of the study are;

1.4.1 General objective

To obtain optimal weighted centroid designs for secord degree Kronecker model mixture experiments.

1.4.2 Specific objectives

1. To obtain optimal moment and information matrices for second degree Kronecker model for mixture experiments.
2. To derive D-, A- and E-criteria for optimal weighted centroid design for second-degree K-model.
3. To obtain a design with maximum information on the parameter subsystem $K'\theta$

1.5 Justification

Since the Kronecker model's full parameter subsystem $\theta \in \Re^{m^2}$ is not estimable, we consider a maximum parameter subsystem $K'\theta$ where the range $\Re(K)$ coincides with the span of the regression range $X = \{f(t) : t \in \tau_{\mathrm{m}}\}$. This formalizes the idea of estimating as many parameters as possible. This study is desirable since it helps in identifying the optimal design for second-degree Kronecker model mixture experiments.

CHAPTER TWO

LITERATURE REVIEW

2.1 Introduction

Mixture experiments were first discussed in Quenouille (1953). Later on, Scheffe' (1958, 1963) made a systematic study and laid a strong foundation. Pukelsheim (1993) and Gaffke and Heiligers (1996) gave a review of the general design environment on mixture experiments. Klein (2004) and Cheng (1995) showed that the class of weighted centroid designs is essentially complete for $m \geq 2$ for the Kiefer ordering. As a consequence, the search for optimal designs may be restricted to weighted centroid designs for most criteria particularly applied to mixture experiments, Kiefer (1959, 1975, 1978, 1985) and Galil and Kiefer (1977). Klein (2004) and Kinyanjui (2007) showed how invariance results can be applied to analytical derivations of optimal designs.

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 homogeneous in ingredients.

The first-degree model is;

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

where Y_t, the response under experimental condition $t \in T_m$, is taken to be a real valued random variable and $\theta = (\theta_{11}, \theta_{12}, ..., \theta_{mm})' \in \Re^{m^2}$ an unknown parameter. All observations taken in an experiment are assumed to be uncorrelated and to have common unknown variance $\sigma^2 \in (0, \infty)$.

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

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

2.2 Kronecker products

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

$$tt' = \begin{pmatrix} t_1^2 & t_1t_2 & \cdots & t_1t_m \\ t_2t_1 & t_2^2 & \cdots & t_2t_m \\ \vdots & \vdots & \ddots & \vdots \\ t_mt_1 & t_mt_2 & \cdots & t_m^2 \end{pmatrix}, \ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(2.3)}$$

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;

(i) That distinct term are repeated appropriately according to the number of times they can arise.

(ii) That transformational rules with a conformable matrix R become simple,

$(Rt)(Rt)' = R(tt')R'$

(iii)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

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

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

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

A key property is their product rule

$$(A \otimes B)(s \otimes t) = (As) \otimes (Bt) \quad . \qquad (2.6)$$

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 Draper and Pukelsheim (1998).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(η) and M(τ) in two factors, M(η)≥M(τ) if and only if $\mu_{(2)}(\eta) = \mu_{(2)}(\tau)$ and $\mu_4(\eta) \geq \mu_4(\tau)$. 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≥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. Draper and Pukelsheim (1998) suggested that within the class of weighted centroid designs, however, other criteria would be needed to attain further improvement, for example, the determinant criteria.

2.4 Model and notation

The linear model,

$$y = f(t)'\theta + \varepsilon \quad \text{...} \quad (2.7)$$

with a real valued response, y, experimental conditions, t chosen from the experimental domain, T_m , a regression function $f : T_m \mapsto \Re^k$, an unknown parameter vector, $\theta \in \Re^k$ and centered error term, ε. In an experiment with sample size n, errors are assumed to be uncorrelated with unknown variance σ^2.

The statistical properties of a design τ within model (2.7), are reflected by its moment matrix

$M(\tau)=\int_{\tau} f(t)f(t)'d\tau \in NND(k)$, where NND(k) denotes the cone of non-negative definite $k \times k$ matrices. We shall focus our attention to estimating a system of linear function, $K'\theta$ of the parameter subsystem $\theta \in \Re^k$, where the coefficient matrix $K \in \Re^{k \times \binom{m+1}{2}}$ is assumed to have full column rank.

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 that the range of K is included in the range of $M(\tau)$,

$$\Re(K) \subseteq \Re(M(\tau)) \qquad (2.8)$$

Thus, any moment matrix $A \in NND(k)$ with $\Re(K) \subseteq \Re(A)$ is called feasible for $K'\theta$. The set $A(k)=\{A \in NND(k) : \Re(K) \subseteq \Re(A)\}$ is called the feasibility cone for $K'\theta$.

Let M be a set of moment matrices in model (2.7). 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.

Definition

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

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

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

In this 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 (1993). 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 null space given by LaMotte (1977)

2.5 Information matrices

For a design τ with moment matrix M, the information matrix for $k'\theta$, with $k \times s$ coefficient matrix k of column rank s, is defined to be $C_k(M)$ where the mapping C_k from the cone NND(k) into the space sym(s)is given by;

$C_k(A) = \min_{L \in \Re^{s \times k} : Lk = I_s} LAL'$ for all A∈NND (k) with minimum taken relative to the Loewner ordering over all left inverses L of K Pukelsheim (1993)

2.6 Moment and Information matrices

The information matrix mapping

$$C_k(A) = \min\left\{LAL' : L \in \Re^{s\times k}, LK = I_s\right\} \in NND(s) \quad \text{.............................} \quad (2.9)$$

in Gaffke (1987 formula 2). This minimum is taken relative to the Loewner ordering on the space sym(s) of $s \times s$ symmetric matrices, defined by $A \le B$ if and only if $B - A \in NND(s)$, for $A, B \in sym(s)$. Pukelsheim (1993), showed that this minimum exists and that it is unique. The information matrix $C_k(M(\tau))$ of a design τ with moment matrix captures the amount of information that τ contains on $K'\theta$ (Pukelsheim, 1993).

Define

$$L_0 = (K'K)^{-1}K' \in \Re^{r_M \times k}, \quad \text{...} \quad (2.10)$$

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

If $K'\theta$ is an arbitrary parameter subsystem and $A \in NND(k)$ a given matrix, then there is always a left inverse $\tilde{L} = \tilde{L}(A)$ independent of A with $\Re(A) \subseteq R_m$ such that $C_k(A) = \tilde{L}A\tilde{L}'$, Pukelsheim (1993). The linearity of $C_k(M(\tau))$ as a function of $M(\tau)$ entails linearity of $C_k(M(\tau))$ as a function of τ. Furthermore, the linearity of C_k is a generalization of the obvious identity $C_{I_k}(A) = A$ for all $A \in NND(k)$, which states that moment matrices are information matrices for the full parameter vector. Whence, information matrices should be understood as modified moment matrices.

With the matrix $L_0 \in \Re^{r_M \times k}$ defined in equation (2.10), we now consider the model:

$$y = [L_0 f(t)]' \beta + \varepsilon, \qquad (2.11)$$

with the same experimental domain T_m as model (2.7), the regression function $L_0 f : T_m \mapsto \Re^{r_M}$, parameter vector $\beta \in \Re^{r_M}$ and moment matrix $\tilde{M}(\tau)$ of a design τ. Then, for every design τ on T_m with $\Re(M(\tau)) \subseteq R_m$, we have $\tilde{M}(\tau) = C_k(M(\tau))$ and the set $\tilde{M} = \{C_k(M); M \subseteq \mathrm{M}\} \subseteq NND(r_M)$ is a convex set of moment matrices in model (2.11). Thus the full parameter vector β is estimable within $\tilde{M}$, (Kinyanjui, 2007).

In order to study design problems for a parameter subsystem $K'\theta$ in model (2.7) we introduce an information function $\phi : NND(s) \mapsto [0, \infty]$. That is, ϕ is non-constant, positively homogeneous, superadditive with respect to the Loewner ordering and is upper semi continuous. It suffices to consider optimal moment matrices rather than optimal designs.

Let M be a subset of moment matrices in model (2.7). A moment matrix, $M_1 \in M$ is called $\phi - optimal$ for $K'\theta$ in M if and only if it solves the design problem

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

Subject to $M \in \mathrm{M} \cap A(k)$ ……………………………………………… (2.12)

Lemma 2.1

Let $M \neq \phi$ be a convex set of moment matrices in model (2.7) and let $K \in \Re^{k \times r_M}$ be maximal coefficient matrix for M. Define the set $\tilde{M} = \{C_k(M); M \subseteq \mathrm{M}\}$ of moment matrices in model (2.11). Finally, let $\phi : NND(r_M) \mapsto [0, \infty)$ be an information function. Then a moment matrix, $M_1 \in M$ in model (2.7) is $\phi - optimal$ for $K'\theta$ if and only if the moment matrix, $\tilde{M} = C_k(M_1)$ in model (2.11) is $\phi - optimal$ for the full parameter vector β in $\tilde{M}$, (Kinyanjui, 2007).

2.7 Nonnegative definite matrices

Let A be a symmetric $k \times k$ matrix with smallest eigenvalue $\lambda_{\min}(A)$. Then we have;

$$A \in NND(k) \Leftrightarrow \lambda_{\min}(A) \geq 0$$

$$\Leftrightarrow traceAB \geq 0 \text{ For all A,B} \in \text{NND(k)}$$

$$A \in PD(k) \Leftrightarrow \lambda_{\min}(A) > 0$$

$$\Leftrightarrow \text{trace AB>0 for all } 0 \neq B \in \text{NND(k)}$$

2.8 Feasibility cone

The most important case occurs if the full parameter vector θ is of interest, i.e. if k=I_k. Since the unique left inverse L of k is then the identity matrix I_k, the information matrix for θ reproduces the moment matrix M,

$$C_{I_k}(M) = M \quad .$$

In other words, for a design ξ, the matrix M(ξ) has two meanings; it is the moment matrix of ξ and it is the information matrix for θ.

But if the matrix M lies in the feasibility A(C), Gauss-Markov Theorem provides the representation

$$C_c(M) = (c'M^{-1}c)^{-1}$$

Here the information for $c'\theta$ is the scalar $(c'M^{-1}c)^{-1}$, in contrast to the moment matrix M.

The task of minimizing information sounds reasonable. For a parameter subsystem $k'\theta$, the feasibility cone $A(k)$ is defined by; $A(k) = \{A \in NND(k); rangek \subseteq rangeA\}$

A matrix Aϵsym(k) is called feasible for $k'\theta$ when $A \in A(k)$; a design ξ is called feasible for $k'\theta$ when $M(\xi) \in A(k)$. If k is of full rank s, the Gauss-Markov theorem provides the representation; $C_k(A) = (k'A^{-1}k)^{-1}$.

It is in this form that information matrices appear in statistical inference.

Gauss-Markov theorem state that, Let $q'y$ be a linear estimator of the scalar function $p'\beta$ of the regression parameters in the model $(y; X\beta, \sigma^2 I)$. Then $q'y$ is an unbiased estimator, such that $E(q'y) = q'E(y) = q'X\beta = p'\beta$ for all β, if and only if $q'X = p'$. Moreover, $q'y$ has the minimum variance in the class of all unbiased linear estimators if and only if

$$q'y = q'X(X'X)^{-1}X'y = p'(X'X)^{-1}X'y.$$

Therefore since p is arbitrary, it can be said that $\hat{\beta} = (X'X)^{-1}X'y$ is the minimum variance unbiased linear estimator of β.

2.9 Estimability

The subsystem $k'\theta$ is estimable if and only if there exist at least one $n \otimes s$ matrix U such that;

$E_{\theta,\sigma^2}[U'Y] = k'\theta$ for all $\theta \in \Theta$, $\sigma^2 > 0$

This entails $k = X'U$, or equivalently, $range k \subseteq range X' = range X'X$

2.10 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

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

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.

2.11 Polynomial regression

Response surface models apply to scalar responses Y_t, assuming that observations under identical or distinct experimental conditions t are of equal (unknown) variance, σ^2 and uncorrelated. Moreover, these models assume that the expected response $E(Y_t) = \eta(t, \Theta)$ permits a fit with a low-degree polynomial in t. Making use of the Kronecker product, the second-degree model then is $\eta(t, \Theta) = \theta_0 + t'\theta_{\{i\}} + (t \otimes t)'\theta_{\{ij\}}$, with the mean parameter vector,

$$\Theta = \begin{pmatrix} \theta_0 \\ \theta_{\{i\}} \\ \theta_{\{ij\}} \end{pmatrix}.$$

The individual components have the usual interpretation with θ_0 being the grand mean. The $m \times 1$ vector $\theta_{\{i\}} = (\theta_1, ..., \theta_m)'$ consists of the main effects θ_i. The $m^2 \times 1$ vector $\theta_{\{ij\}} = (\theta_{11}, \theta_{12}, ..., \theta_{mm})'$ consists of the pure quadratic effects θ_{ii} and the two-way interactions θ_{ij} with the evident second-degree restrictions $\theta_{ij} = \theta_{ji}$ for all i,j.

This model is of the form $\eta(t, \Theta) = f(t)'\theta$. The regression function $t \mapsto f(t)$ conforms to the parameter vector Θ and is, in turn

$$f(t) = \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix}$$

As t varies over the experimental domain T_m, the vector $f(t)$ spans a space of dimension $\frac{(m+1)(m+2)}{2}$. This number coincide with the components of the parameter vector Θ. Thus the Kronecker model of degree two is seen to be over parameterized.

An experimental design, τ, on the domain T_m is a probability measure that has finite support. Suppose the support points are; $t_1, t_2, \cdots, t_l$ and they have corresponding weights; $w_1, w_2, \cdots, w_l$, then the experimenter is directed to draw a proportion, w_j of all observations under experimental condition t_j. For a linear model with regression function $f(t)$, the statistical properties of a design, τ are captured by its moment matrix

$$M(\tau) = \sum_{j \le l} w_j f(t_j) f(t_j)' = \int_\tau f(t) f(t)' d\tau .$$

Because of overparametrization, any such moment matrix is rank deficient, and so is the dispersion matrix of the least squares estimator for Θ. Unfortunately then, regular matrix inverses do not exist. This compels the invoking of generalized inverses which performs equally well.

The dependence of the expected response on the experimental conditions, t is described by the model response surface, $t \mapsto \eta(t,\Theta)$. The parameter vector Θ is generally not known. When we replace the true parameter by its least squares estimate, $\hat{\Theta}$, we shift our interest to the estimated response surface, $t \mapsto \eta(t,\hat{\Theta}) = f(t)'\hat{\Theta}$. When $\hat{\Theta}$ is calculated from observations drawn according to the experimental design τ, the statistical properties of the estimated response surface are determined by the variance surface $t \mapsto v_\tau(t) = f(t)'M(\tau)^{-1} f(t)$, or equivalently by the information surface, $t \mapsto i_\tau(t) = \dfrac{1}{v_\tau(t)}$. These quantities do not depend on the choice of the generalized inverse, provided the vector, $f(t)$ lies in the range of the matrix $M(\tau)$; otherwise a continuity argument suggests setting $v_\tau(t) = \infty$ and $i_\tau(t) = 0$, which also makes good sense statistically. The information surface $i_\tau(t)$ ranges from zero to some finite maximum, whence it is easier graphically depicted than the variance surface (Draper and Pukelsheim, 1998).

CHAPTER THREE

METHODOLOGY

3.1 Introduction

This chapter presents the space of the moment and information matrices that were involved in our design problem under study.

3.2 Space of Design Matrices

3.2.1 Invariant symmetric block matrices for design of mixture experiments

A quadratic subspace of symmetric $n \times n$ matrices is a linear subspace ϑ of $sym(n)$ with additional feature that $C \in \vartheta$, implies $C^2 \in \vartheta$. Rao, et al. (1998), gave an introduction to the subset and some of its statistical applications. 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

$$H = \left\{ H_\pi = \begin{pmatrix} R_\pi & 0 \\ 0 & S_\pi \end{pmatrix} : \pi \in \vartheta_m \right\} \qquad (3.1)$$

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

$$sym\left(\binom{m+1}{2}, H\right) = \left\{ C \in sym\left(\binom{m+1}{2}\right) : HCH \quad for \quad all \quad H \in H \right\} \ldots\ldots\ldots\ldots\ldots\ldots(3.2)$$

of H-invariant symmetric matrices. Since H is a subgroup of the orthogonal group, the space $sym\left(\binom{m+1}{2}, H\right)$ is a quadratic subspace, Pukelsheim (1993). This quadratic subspace is the object of our study.

Draper *et al* (1991) characterize rotatable symmetric matrices in first and second-degree models, where rotatability means invariance under congruence transformation with matrices from a certain group isomorphic to the orthogonal group. Gafke and Heiligers (1996) considered moment matrices which are invariant under a finite subgroup of the orthogonal group including permutations and sign changes. Eigenvalues of invariant moment matrices are then used in numerical algorithm for finding optimal designs in certain cubic models.

In a similar fashion, Draper *et al.* (1996), compute numerically optimal designs in a rotatable cubic model. A particular example of H-invariance already occurs in Galil and Kiefer (1977) while Galils and Kiefers treatment of H-invariance is less formal and does not mention quadratic subspace, their numerical approach to optimal designs for mixture experiments is well aware of the structure and exploits eigenvalues of H-invariant symmetric matrices. Klein (2004) and Kinyanjui (2007), showed how invariance results can be applied to analytical derivations of optimal designs. The spectral analysis of invariant symmetric matrices yields both eigenvalues and eigenvectors.

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

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 describing the linear structure of $sym(s,H)$, ($s = \binom{m+1}{2}$), shows that an H-invariant symmetric matrix has at most seven distint elements.

Lemma 3.1

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

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

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

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

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

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

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

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \qquad (3.3)$$

With coefficients $a,\cdots,g \in \Re$. The terms containing V_2, W_2 and W_3 only 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

$$C = \begin{pmatrix} C_{11} & C'_{21} \\ C_{21} & C_{22} \end{pmatrix} \qquad (3.4)$$

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 blockwise conditions;

$$R_\pi C_{11} R'_\pi = C_{11}, S_\pi C_{21} R'_\pi = C_{21} . S_\pi C_{22} S'_\pi \text{ for all } \pi \in \vartheta_m \qquad (3.5)$$

Straightforward multiplication shows that the blocks given in equation (3.3) satisfy these conditions. For the reverse direction, we compare the entries of the matrices on both sides of the equations in (3.5) 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 equation (3.3) 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 equation (3.3) 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 3.2

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

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

$$V'_1 V_1 = (m-1)U_1 + U_2, \qquad V'_2 V_2 = \binom{m-1}{2} U_1 + \binom{m-2}{2} U_2,$$
$$V'_1 V_2 = V'_2 V_1 = (m-2)U_2, \qquad U_2^2 = (m-1)U_1 + (m-2)U_2.$$

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

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

(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 (3.2), 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 (2.12) in an effective way. Furthermore, the multiplication table can be implemented in a computer-algebra system like maple.

As a side result of lemma (3.2) and the fact that $traceU_2 = traceW_2 = traceW_3 = 0$, the basis matrices;

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

$$B_5 = \begin{pmatrix} 0 & 0 \\ 0 & W_1 \end{pmatrix},\ B_6 = \begin{pmatrix} 0 & 0 \\ 0 & W_2 \end{pmatrix} \text{ and } B_7 = \begin{pmatrix} 0 & 0 \\ 0 & W_3 \end{pmatrix}, \qquad (3.6)$$

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

Corollary 3.1

For any $m \geq 2$, suppose the matrix $C \in sym(s, H)$ is partitioned as in equation (3.4) 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, *et al*.1998, corollary 13.2.3). Together with lemma (3.2), these results imply the claims on the schur complements of C_{11} and C_{22}.

3.3 Optimality Criteria

The most prominent optimality criteria in the design of experiments are the Determinant criterion, (D-criterion), the Average-variance criterion, (A-criterion), the smallest eigenvalue criterion (E-criterion) and the trace criterion, (T-criterion). These are particular cases of the matrix means, ϕ_p, with parameter $p \in [-\infty, 1]$.

The optimality properties of designs are determined by their moment matrices, Pukelsheim (1993). The computation of optimal design for the second order Kronecker model involves searching for the optimum in a set of competing moment matrices. The matrix mean ϕ_p which is an information function, serves as a basic tool in this study.

The amount of information inherent to $C_k(M(\tau))$ is provided by Kiefers $\phi_p - criteria$ with $C_k(M(\tau)) \in PD\left(\binom{m+1}{2}\right)$, the set of $\binom{m+1}{2} \times \binom{m+1}{2}$ positive definite matrices. These are defined as follows

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

for all C in $PD\left(\binom{m+1}{2}\right)$, where $\lambda_{\min}(C)$ refers to the smallest eigenvalue of C.

By definition, $\phi_p(C)$ is a scalar measure which is a function of the eigenvalues of C for all $p \in [-\infty,1]$, (Pukelsheim,1993). The class of $\phi_p - criteria$ includes the prominently used T-, D-, A- and E-criteria corresponding to parameter values 1,0,-1 and $-\infty$ respectively. These are thus defined as:

The trace criterion, T-, $\phi_1(C) = \frac{1}{s} traceC$,

The determinant criterion, D-, $\phi_0(C) = (\det C)^{\frac{1}{s}}$, The average variance criterion, A-, $\phi_{-1}(C) = \left(\frac{1}{s} traceC^{-1}\right)^{-1}$ and,

The smallest eigenvalue criterion, E-, $\phi_{-\infty}(C) = \lambda_{\min}(C^{-1})$, where $s = \binom{m+1}{2}$.

The problem of finding a design with maximum information on the parameter subsystem $K'\theta$ can now be formulated as;

Maximize $\phi_p(C_k(M(\tau)))$ with $\tau \in T$

Subject to $C_k(M(\tau)) \in PD(s)$……………………………………………..(3.7)

where T denotes the set of all designs on T_m.

The side condition $C_k(M(\tau)) \in PD(s)$ is equivalent to the existence of an unbiased estimator for $K'\theta$ under τ, (Pukelsheim,1993). In this case, the design, τ is called feasible for $K'\theta$. Any design that solve problem (3.7) for fixed $p \in [-\infty,1]$, is called $\phi_p - optimal$ for $K'\theta$ in T. For all $p \in [-\infty,1)$, the existence of $\phi_p - optimal$ designs for $K'\theta$ is guaranteed in Pukelsheim (1993).

Definition

The j^{th} elementary centroid design $\eta_j, \quad j \in \{1,...,m\}, \quad m \geq 2$ is the uniform distribution on all points taking the form,

$$\frac{1}{j}\sum_{i=1}^{j} e_k \in T_m \text{ with } 1 \leq k_1 < k_2 < \cdots < k_j \leq m.$$

A convex combination, $\eta(\alpha) = \sum_{j=1}^{m} \alpha_j \eta_j$ with $\alpha = (\alpha_1,...,\alpha_m)' \in T_m$ is called a weighted centroid design with weight vector α restricted by $\sum_{i=1}^{m} \alpha_i = 1$.

These designs were introduced by Scheffe` (1963). Weighted centroid designs are exchangeable, that is, they are invariant under permutations.

Klein (2004) summarized the work by Draper and Pukelsheim (1999) and Draper, et al (2000) by putting forward an idea that affirms the importance of weighted centroid design for the Kronecker model. He showed that, in the second degree Kronecker model for mixture experiments with $m \geq 2$ ingredients, the set of weighted centroid designs is an essentially complete class. That is, for every $p \in [-\infty;1]$ and for every design $\tau \in \mathrm{T}$ there exists a weighted centroid design η with

$$(\phi_p \circ C_k \circ M)(\eta) \geq (\phi_p \circ C_k \circ M)(\tau).$$

Thus for every design, $\tau \in \mathrm{T}$ there is a weighted centroid design η whose moment matrix $M(\eta)$ improves upon $M(\tau)$ in the kiefer ordering. (Draper, et al. 1998) and (Pukelsheim, 1999).

Under the Kiefer ordering, we say a moment matrix M is more informative than a moment matrix N if M is greater than or equal to some intermediate matrix F under the Loewner ordering, and F is majorized by N under the group that leaves the problem invariant:

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

Two moment matrices M and N are said to be Kiefer equivalent when M>>N and N>>M. We call M Kiefer better than N when M>>N without M and N being equivalent. A design τ is kiefer better than a design ξ when M(τ) is Kiefer better than M(ξ).

As a consequence, we may restrict the set of competing designs in problem (3.7) to $\eta(T_m)$, thus obtaining a mere allocation problem for the weight vector $\alpha \in T_m$. Hence the problem of finding a design with maximum information simplifies to;

Maximize $(\phi_p \circ C_k \circ M \circ \eta)\alpha$ with $\alpha \in T_m$

subject to $M(\eta(\alpha)) \in A(K)$ ……………………………………………………..… (3.8)

Weighted centroid designs are exchangeable. This property points to H-invariance of information matrices,

$$HC_k(M(\eta))H' = C_k(M(\eta)) \text{ for all } H \in H,\ \eta \in \eta(T_m) \quad \text{………………………} \ (3.9)$$

where H is the matrix group defined in equation (3.1). Equivalently, we may say that the information matrix, $C_k(M(\eta))$, lies in the quadratic space $sym(s,H) = \{C \in sym(s) : HCH' = C \quad for \quad all \quad H \in H\}$ of H-invariant symmetric matrices, that is, a subspace of matrices closed under formation of matrix powers C^n, $n \in N$.

Definition

A weighted centroid design $\eta(\alpha)$, satisfying the side condition $M(\eta(\alpha)) \in A(K)$ in problem (3.8), is called a feasible weighted centroid design for $K'\theta$ in T.

An equivalent but more tractable condition is the regularity of $C_k(M(\eta(\alpha)))$, (Pukelsheim, 1993). From the linearity of the information mapping C_k in equation (3.14), we get, for every $\alpha \in T_m$,

$$C_k(M(\eta(\alpha))) = \sum_{j \in \partial(\alpha)} \alpha_j C_k(M(\eta_j)), \quad \text{…………………...………………..……} \ (3.10)$$

with $\partial(\alpha) = \{j = 1,2,...,m : \alpha_j > 0\}$.

Since the information matrices $C_j = C_k M(\eta_j)$ are non-negative definite, this implies;

$$\Re(C_k(M(\eta(\alpha)))) = \sum_{j \in \partial(\alpha)} \Re(C_j).$$

The above equation suggests studying the ranges of the information matrices;

C_1, C_2, …, C_m of the elementary centroid designs. These matrices can be calculated by invoking the linear transformation to moment matrices $M(\eta_j)$ given by (Draper et al, 2000).

For j=1,2, …, m, we obtain

$$C_j = \begin{pmatrix} C_{11,j} & C'_{21,j} \\ C_{21,j} & C_{22,j} \end{pmatrix} \qquad (3.11)$$

With blocks

$$C_{11,j} = \frac{1}{j^3 m} I_m + \frac{1}{j^3 m}\frac{j-1}{m-1} U_2,$$

$$C_{21,j} = \frac{2}{j^3 m}\frac{j-1}{m-1} V_1 + \frac{2}{j^3 m}\frac{j-1}{m-1}\frac{j-2}{m-2} V_2,$$

$$C_{22,j} = \frac{4}{j^3 m}\frac{j-1}{m-1} I_{\binom{m}{2}} + \frac{4}{j^3 m}\frac{j-2}{m-1}\frac{j-2}{m-2} W_2 + \frac{4}{j^3 m}\frac{j-1}{m-1}\frac{j-2}{m-2}\frac{j-3}{m-3} W_3,$$

where the matrices; U_2, V_1, V_2, W_2, W_3 are defined in lemma (3.1). The terms containing V_2, W_2 *and* W_3 only occur for $m \geq 3$ and $m \geq 4$ respectively.

3.4 Motivating design problem

Mixture experiments are experiments in which the experimental conditions are nonnegative quantities summing to one. Formerly, 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 $t \in T_m$ will be 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 (2) with the regression function $f(t) = t \otimes t$ and unknown parameter vector $\Theta = (\theta_{11}, \theta_{12}, ..., \theta_{mm})' \in \Re^{m^2}$. All observations taken in an experiment are assumed to be uncorrelated and to have common unknown variance.

When fitting this model to a set of observations, a parameter subsystem, say $K'\theta$, of interest will be chosen with $k \in \Re^{m^2 \times s}$.

We define the K matrix as

$$K = \left(K_1, K_2\right) \in \Re^{m^2 \times m+1} \qquad \text{……………………………………………………………… (3.12)}$$

where, $K_1 = \sum_{i=1}^{m} e_{ii} e_i'$ and $K_2 = \frac{1}{2\binom{m}{2}} \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E_{ij}'$

The parameter subsystem considered in this study can be written as

$$K'\theta = \left\{ \begin{matrix} (\theta_{ii})_{1 \le i \le m} \\ \frac{1}{2\binom{m}{2}} (\theta_{ij} + \theta_{ji}),_{1 \le i < j \le m} \end{matrix} \right\} \in \Re^{\binom{m+1}{2}} \qquad \text{…………………………………………… (3.13)}$$

The amount of information a design τ contains on $K'\theta$ is captured by the information matrix;

$$C_k(M(\tau)) = \min\left\{ LM(\tau)L' : L \in \Re^{\binom{m+1}{2}\times m^2} ; LK = I_{\binom{m+1}{2}} \right\}, \ldots\ldots\ldots\ldots\ldots\ldots \quad (3.14)$$

where $I_{\binom{m+1}{2}}$ denotes the $\binom{m+1}{2}\times\binom{m+1}{2}$ identity matrix and L is the left inverse of K.

The above minimum is understood relative to Loewner ordering on the space $sym\left(\binom{m+1}{2}\right)$ of symmetric $\binom{m+1}{2}\times\binom{m+1}{2}$ matrices, defined by $A \le B$ if and only if $B - A$ is non-negative definite.

An experimental design for a mixture experiment is a probability measure τ on T_m with finite support. Each support point t∈supτ 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

$$M(\tau) = \int_{T_m} f(t)f(t)'d\tau \in NND(m^2), \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \ (3.15)$$

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 subsystem $k'\theta$ is captured by the information matrix for $k'\theta$

$$C_k(M(\tau)) = (k'k)^{-1}k'M(\tau)k(k'k)^{-1} \in NND(s). \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (3.16)$$

The information matrix C_k (M (τ)) is the precision matrix of the best linear unbiased estimator for $k'\theta$ under the design τ Pukelsheim (1993). The equation (3.16) is a linear function of M (τ) and is due to the fact that $k'\theta$ is a maximal parameter system for Kronecker model (Klein 2001).

A family of scalar measurements for the amount of information inherent to C_k (M (τ)) is provided by Kiefer's $\phi_p - criteria$, with p∈[-∞,1] . These are defined by;

$$\phi_p(C) = \begin{cases} \lambda_{\min}(C) if p = -\infty \\ (\det C)^{\frac{1}{s}} if p = 0 \\ (\frac{1}{s} trce C^p)^{\frac{1}{p}} if p \in (-\infty, 1] \setminus \{0\} \end{cases}$$

for all C in PD(s), the set of positive definite $s \times s$ matrices. Here $\lambda_{\min}(C)$ stands for the smallest eigenvalue of C. By definition, $\phi_p - (C)$ is a function of the eigenvalues of C for all p∈[-∞,1] Pukelsheim(1993). The family of $\phi_p - criteria$ includes the often used A-, D-, T-, and E-criteria, corresponding to parameter values 1, 0, -1, and -∞ respectively.

The problem of finding a design with maximum information on the parameter subsystem $k'\theta$ can now be formulated as

Maximize $\phi_p(C_k(M(\tau)))$ with t∈T

Subject to $C_k(M(\tau)) \in PD(s)$

where T denotes the set of all designs T_m. The side condition $C_k(M(\tau)) \in PD(s)$ is equal to the existence of an unbiased linear estimator for $k'\theta$ under τ. In which case, the design τ will be called feasible for $k'\theta$. Any design having the above problem for a fixed p∈[-∞ ,1] is called $\phi_p - optimal$ for $k'\theta$ will be guaranteed by theorem 7.13 in (Pukelsheim, 1993).

The set of competitors in the design problem above can be substantially reduced. In a mixture experiment with m ingredients, the j^th elementary centroid design η_j with j∈

{1,…,m} in the uniform distribution on all points of the form $\frac{1}{j}\sum_{j=1}^{m} e_{ki} \in T_m$ with $0 \le k_1 \le ... \le k_j \le m$.

A convex combination $\eta(\alpha) = \sum_{j=1}^{m} \alpha_j \eta_j$ with weight vector $\alpha = (\alpha_1,...,\alpha_m)' \in T_m$ is called a weighted centroid design. The set $\eta(\tau_m)$ of weighted centroid designs constitute an essentially complete class of designs with respect to the target function of the design problem. That is, for every design $\tau \in$T there is a weighted centroid design $\eta \in \eta(T_m)$ with

$(\phi_p \circ C_k \circ M)(\eta) \ge (\phi_p \circ C_k \circ M)(\tau)$. Therefore, the design problem reduces to

Maximize $(\phi_p \circ C_k \circ M \circ \eta)$ with $\alpha \in T_m$

Subject to $C_k(M(\eta(\alpha))) \in PD(s)$.

A necessary and sufficient condition for $\phi_p - optimality$ of a weighted centroid design $\eta(\alpha)$ with weight vector $\alpha = (\alpha_1,...,\alpha_m)' \in T_m$ follows from the Kiefer-Wolfowitz equivalence theorem in (Pukelsheim, 1993) and given by (Klein, 2001). Suppose $\eta(\alpha)$ satisfies the side condition $C_k(M(\eta(\alpha))) \in PD(s)$ and C_j written as $C_j = C_k(M(\eta_j))$ for j=1,…,m. Then, $\eta(\alpha)$ solves above problem with p∈(-∞,1] if and only if

$$trace C_j C_k(M(\eta(\alpha)))^{p-1} \begin{cases} = trace C_k(M(\eta(\alpha)))^p & for \quad all \;\; j \in \delta(\alpha) \\ \le trace C_k(M(\eta(\alpha)))^p & otherwise \end{cases}$$

with $\delta(\alpha) = \{ j \setminus \alpha_j > 0 \}$. The case p=-∞, that is, E-optimality, has a similar optimality condition Klein (2001). Without further knowledge of the information matrices involved, the optimality condition above will be hard to solve. However, invariance arguments will help to considerably simplify the problem. (Pukelsheim, 1993) gave a general discussion of invariance methods in experimental design. Weighted centroid designs are exchangeable, that is, they are invariant under permutations of the ingredients. Formally, the group perm(m) of m×m permutation matrices acts on the set T of designs through $(R,\tau) \to T^R = T \circ R^{-1}$. Exchangeability of a design τ ∈T then means $\tau = \tau^R$ through congruence transformation. The group H defined acts on the space sym(s) through congruence transformation. This action is linked to that of perm(m) on T by equivalence property

$$C_k(M(T^{R_\Pi})) = C_k((R_\Pi \otimes R_\Pi)M(\tau)(R_\Pi \otimes R_\Pi)')$$

$$= H_\Pi C_k(M(\tau))H'_\Pi$$

for all $\prod \in \sigma$ and τ ∈T, with matrices R_Π and H_Π. As a consequence, information matrices of exchangeable designs and in particular, all information matrices involved in the design problem, lie in the quadratic subspace sym(s, H) defined in (Klein, 2004). Hence analysis of quadratic subspace may help in solving the design problem, and the optimality criteria serves as a guide for the analysis.

(Klein, 2004) and (Kinyanjui, 2007) showed how invariance results can be applied to analytical derivation of optimal designs. The spectral analysis of invariant symmetric matrices yielded both eigenvalues and eigenvectors. (Kinyanjui, 2007) investigated $\phi_p - optimal$ weighted centroid designs for $k'\theta$ by adopting the General equivalence theorem as given in Pukelsheim (1993) and derive the general forms for the unique A-optimal, D-optimal, T-optimal, and E-optimal designs for $k'\theta$. Later on, (Ngigi, 2009) gave the optimality criteria for $\phi_p - optimal$ weighted centroid designs for $k'\theta$ and found that for second-degree model with m≥2 ingredients, a unique A-optimal, D-optimal, and T-optimal weighted centroid designs for $k'\theta$ exist. E-optimal designs could only be derived for experiments with two ingredients. Cherutich M. (2012) also showed that second degree mixture experiments for non-maximal parameter subsystem unique D-and A-optimal weighted centroid designs for *K'θ* alsodo exist.

This study investigated mixture models on the simplex an improvement is obtained for a given design in terms of increasing symmetry as well as obtaining a larger moment matrix under the Loewner ordering. The study adopted the second-degree mixture model put forward by Draper and Pukelsheim (1998). The parameter subsystem of interest in the study was maximal parameter subsystem which is a subspace of the full parameter space. For this model the full parameter subsystem was not estimable. By a proper definition of parameter matrix, a maximal parameter subsystem in the model was selected. Canonical unit vectors and the concept of Kronecker products were employed to identify the parameter matrices as well as the information matrices. For the second degree mixture model with two, three, four and *m* ingredients, a set of weighted centroid designs was obtained for a characterization of the feasible weighted centroid designs for the maximal parameter subsystem. After computing the feasible weighted centroid designs the information matrix of the design was obtained. Derivations of A-, D- and E-optimal weighted centroid designs were then computed from the information matrix. The optimality criteria A, D and E were used to obtain optimal centroid designs. The results based on maximal parameter subsystem, second degree mixture model with $m \geq 2$ ingredient for A-, D- and E-optimal weighted centroid design for $K'\theta$ is obtained based on the choice of the coefficient matrix specifically in this study. Optimal weights and values for the weighted centroid designs are numerically computed using Matlab software.

CHAPTER FOUR

RESULTS

4.1 Introduction

This chapter contain information matrixes, A-, D- and E-optimal weighted centroid design of the designs under study for $m=2$, $m=3$, $m=4$ and $m \geq 2$ ingredients.

4.2 Information matrices

For a design τ with moment matrix M, the information matrix for $k'\theta$, with $k \times s$ coefficient matrix k of column rank s, is defined to be $C_k(M)$ where the mapping C_k from the cone NND(k) into the space sym(s)is given by;

$C_k(A) = \min_{L \in \Re^{s \times k} : Lk = I_s} LAL'$ For all A∈NND (k) with minimum taken relative to the Loewner ordering over all left inverses L of K Pukelsheim (1993)

4.2.1 Information matrix for $m=2$ ingredients

Table 4.1. Weighted centroid design for m=2 ingredients

Design points	t_1	t_2
1	1	0
2	0	1
3	½	½

The elementary centroid designs are;

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

Lemma 4.1

The K matrix for m=2 ingredients is given by;

$$K = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{bmatrix}$$

Proof

From equation (3.12), we have $K = (K_1, K_2) \in \Re^{m^2 \times s}$ where;

$$K_1 = \sum_{i=1}^{m} e_{ii} e_i' \qquad K_2 = \frac{1}{2\binom{m}{2}} \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E_{ij}'$$

For m=2 ingredients, then;

$$K_1 = \sum_{i=1}^{2} e_{ii} e_i' = e_{11} e_1' + e_{22} e_2' \quad \text{and} \quad K_2 = \frac{1}{2} \sum_{\substack{i,j=1 \\ i<j}}^{2} (e_{ij} + e_{ji}) E_{ij}' = (e_{12} + e_{21}) E_{12}' \text{ with}$$

$$E_{12} \in \Re^{\binom{2}{2}} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.1)$$

Define, $e_{ij} = e_i \otimes e_j$, i,j=1,2 , $e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

Thus

$$e_{11} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \; e_{22} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \; e_{12} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \text{ and}$$

$$e_{21} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Substituting these in equation (4.1), we obtain

$$K_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}, K_2 = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} \text{ giving } K = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{bmatrix}$$

Theorem 4.1

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

$$C_k = C_K(M(\eta(\alpha))) = \begin{bmatrix} \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{4} \end{bmatrix}$$

Proof

The moment matrix for the weighted centroid design with two ingredients is given as

$$M(\eta(\alpha)) = \begin{bmatrix} \mu_4 & \mu_{31} & \mu_{31} & \mu_{22} \\ \mu_{31} & \mu_{22} & \mu_{22} & \mu_{31} \\ \mu_{31} & \mu_{22} & \mu_{22} & \mu_{31} \\ \mu_{22} & \mu_{31} & \mu_{31} & \mu_4 \end{bmatrix},$$

where the fourth moments are defined as

$$\mu_4(\eta) = \int t_1{}^4 d\eta, \; \mu_{31}(\eta) = \int t_1^3 t_2 d\eta, \; \mu_{22}(\eta) = t_1^2 t_2^2 d\eta$$

For m-ingredients there are m elementary centroid designs placing equal weights $\frac{1}{\binom{m}{j}}$ on the points having j out of their m components equal to $\frac{1}{j}$ and zeros elsewhere. A convex combination $\eta(\alpha)=\sum_{j=1}^{m}\alpha_j\eta_j$ with $\alpha=(\alpha_1,\alpha_2,...,\alpha_m)\in T_m$ is called a weighed centroid design with weight vector α such that $\sum_{j=1}^{m}\alpha_j=1$.

For the case, m=2, $\eta(\alpha)=\sum_{j=1}^{2}\alpha_j\eta_j=\alpha_1\eta_1+\alpha_2\eta_2$ with $\alpha=(\alpha_1,\alpha_2,0,0)\in T_2$ and $\alpha_1+\alpha_2=1$.

The fourth order moments are for j=(1,2, …, m)

$\mu_4(\eta_j)=\frac{1}{j^3 m}$ and $\mu_{31}(\eta_j)=\mu_{22}(\eta_j)=\frac{j-1}{j^3 m(m-1)}$. When m=2 these moments are;

$\mu_4(\eta_1)=\frac{1}{2}$, $\mu_{31}(\eta_1)=\mu_{22}(\eta_1)=0$, $\mu_4(\eta_2)=\frac{1}{16}$ and $\mu_{31}(\eta_2)=\mu_{22}(\eta_2)=\frac{1}{16}$.

Thus the moment matrices for designs η_1 and η_2 are:

$$M(\eta_1)=\begin{bmatrix}\frac{1}{2}&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&\frac{1}{2}\end{bmatrix},\ M(\eta_2)=\begin{bmatrix}\frac{1}{16}&\frac{1}{16}&\frac{1}{16}&\frac{1}{16}\\\frac{1}{16}&\frac{1}{16}&\frac{1}{16}&\frac{1}{16}\\\frac{1}{16}&\frac{1}{16}&\frac{1}{16}&\frac{1}{16}\\\frac{1}{16}&\frac{1}{16}&\frac{1}{16}&\frac{1}{16}\end{bmatrix}.$$

From equation (3.16), we obtain the information matrix as follows;

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

For the design η_1, the information matrix is given as;

$$C_1 = C_k(M(\eta_1)) = \tilde{L}M(\eta_1)\tilde{L}' = \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots .... (4.2)$$

And for the design η_2, the information matrix is given as

$$C_2 = C_k(M(\eta_2)) = \tilde{L}M(\eta_2)\tilde{L}' = \begin{pmatrix} 1/16 & 1/16 & 1/8 \\ 1/16 & 1/16 & 1/8 \\ 1/8 & 1/8 & 1/4 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots .. (4.3)$$

From equations (4.2) and (4.3) we can obtain the information matrix for the design $\eta(\alpha)$ as;

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

This on simplification yields;

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{4} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.4)$$

4.2.2 Information matrix for $m = 3$ ingredients

Table 4.2. Weighted centroid design for m=3 ingredients

Design points	t_1	t_2	t_3
1	1	0	0
2	0	1	0
3	0	0	1
4	½	½	0
5	½	0	½
6	0	½	½
7	⅓	⅓	⅓

From definition above (under theorem 4.1), there are m-elementary centroid designs, η_j, placing equal weights $\frac{1}{\binom{m}{j}}$ on the points having j out of their m components equal to $\frac{1}{j}$ and zeros elsewhere. These are for, m=3

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

A convex combination $\eta(\alpha) = \sum_{j=1}^{m} \alpha_j \eta_j$ with $\alpha = (\alpha_1, \alpha_2, ..., \alpha_m) \in T_m$ is called a weighed centroid design with weight vector α such that $\sum_{j=1}^{m} \alpha_j = 1$.

For the case, m=3, $\eta(\alpha) = \sum_{j=1}^{3} \alpha_j \eta_j = \alpha_1\eta_1 + \alpha_2\eta_2 + \alpha_3\eta_3$ with $\alpha = (\alpha_1, \alpha_2, 0, 0)' \in T_2$ and

$\alpha_1 + \alpha_2 = 1$

Theorem 4.2

The K-matrix for m=3 ingredients is given by

$$K = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{6} & 0 \\ 0 & 0 & 0 & \frac{1}{6} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{6} \\ 0 & 0 & 0 & 0 & \frac{1}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{6} \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Proof

From equation (3.12), we have $K = (K_1, K_2) \in \Re^{m^2 \times s}$ where;

$$K_1 = \sum_{i=1}^{m} e_{ii} e_i' \qquad K_2 = \frac{1}{2\binom{m}{2}} \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E_{ij}'$$

For m=3 ingredients, then;

$$K_1 = \sum_{i=1}^{3} e_{ii} e_i' = e_{11} e_1' + e_{22} e_2' + e_{33} e_3' \quad \text{and}$$

$$K_2 = \frac{1}{6} \sum_{\substack{i,j=1 \\ i<j}}^{3} (e_{ij} + e_{ji}) E_{ij}'$$
$$= \frac{1}{6} [(e_{12} + e_{21}) E_{12}' + (e_{13} + e_{31}) E_{13}' + (e_{23} + e_{32}) E_{23}'] \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. \text{(4.5)}$$

with $E_{ij} \in \Re^{\binom{3}{2}}$

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

Thus

$e_{11} = e_1 \otimes e_1 = (1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)'$,

$e_{22} = e_2 \otimes e_2 = (0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0)'$,

$e_{33} = e_3 \otimes e_3 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1)'$,

$e_{12} = e_1 \otimes e_2 = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)'$,

$e_{21} = e_2 \otimes e_1 = (0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)'$,

$e_{13} = e_1 \otimes e_3 = (0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)'$,

$e_{31} = e_3 \otimes e_1 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0)'$,

$e_{23} = e_2 \otimes e_3 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0)'$,

$e_{32} = e_3 \otimes e_2 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)'$.

The vectors $E_{ij}'s$ are obtained by considering the index pairs {i,j}with $i, j \in \{1, 2, 3\}$ and i<j. They represent the standard basis of $\Re^3$ and the index pairs should be in a lexicographic order. They are;

$E_{12} = (1 \quad 0 \quad 0)'$

$E_{13} = (0 \quad 1 \quad 0)'$ and

$E_{23} = (0 \quad 0 \quad 1)'$

Therefore we obtain;

$$K_1 = e_{11}e_1' + e_{22}e_2' + e_{33}e_3' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and $K_2 = (e_{12} + e_{21})E'_{12} + (e_{13} + e_{31})E'_{13} + (e_{23} + e_{32})E'_{23} = \begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{6} & 0 \\ \frac{1}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{6} \\ 0 & \frac{1}{6} & 0 \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & 0 \end{pmatrix}$

Thus

$$K = \begin{pmatrix} K_1 & K_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{6} & 0 \\ 0 & 0 & 0 & \frac{1}{6} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{6} \\ 0 & 0 & 0 & 0 & \frac{1}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{6} \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} ▪$$

Theorem 4.3

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

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 \\ 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{4} \end{pmatrix}$$

Proof

For m=3, the moment matrix for the weighted centroid design $\eta(\alpha)$ is given by;

$$M(\eta(\alpha)) = \begin{pmatrix} \mu_4 & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} \\ \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\ \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\ \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\ \mu_{22} & \mu_{31} & \mu_{211} & \mu_{31} & \mu_4 & \mu_{31} & \mu_{211} & \mu_{31} & \mu_{22} \\ \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} \\ \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\ \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} \\ \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_4 \end{pmatrix}$$

The moments of order four are, for j=1, 2, …, m:

$$\mu_4(\eta_j) = \frac{1}{j^3 m} \ ,$$

$$\mu_{31}(\eta_j) = \mu_{22}(\eta_j) = \frac{j-1}{j^3 m(m-1)} \, ,$$

$$\mu_{211}(\eta_j) = \frac{(j-1)(j-2)}{j^3 m(m-1)(m-2)}.$$

When m=3, these moments are;

$$\mu_4(\eta_1) = \frac{1}{3},\ \mu_{31}(\eta_1) = \mu_{22}(\eta_1) = 0,\ \mu_{211}(\eta_1) = 0,\ \mu_4(\eta_2) = \frac{1}{24},\ \mu_{31}(\eta_2) = \mu_{22}(\eta_2) = \frac{1}{48}$$

and $\mu_{211}(\eta_2) = 0$.

Thus the moment matrices for the design η_1 and η_2 are:

$$M(\eta_1) = \begin{pmatrix} 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/3 \end{pmatrix}$$

and

$$M(\eta_2) = \begin{pmatrix} 1/24 & 1/48 & 1/48 & 1/48 & 1/48 & 0 & 1/48 & 0 & 1/48 \\ 1/48 & 1/48 & 0 & 1/48 & 1/48 & 0 & 0 & 0 & 0 \\ 1/48 & 0 & 1/48 & 0 & 0 & 0 & 1/48 & 0 & 1/48 \\ 1/48 & 1/48 & 0 & 1/48 & 1/48 & 0 & 0 & 0 & 0 \\ 1/48 & 1/48 & 0 & 1/48 & 1/24 & 1/48 & 0 & 1/48 & 1/48 \\ 0 & 0 & 0 & 0 & 1/48 & 1/48 & 0 & 1/48 & 1/48 \\ 1/48 & 0 & 1/48 & 0 & 0 & 0 & 1/48 & 0 & 1/48 \\ 0 & 0 & 0 & 0 & 1/48 & 1/48 & 0 & 1/48 & 1/48 \\ 1/48 & 0 & 1/48 & 0 & 1/48 & 1/48 & 1/48 & 1/48 & 1/24 \end{pmatrix}.$$

The fourth moments of the weighted centroid design $\eta(\alpha)$ are obtained as

$$\mu_4(\eta(\alpha)) = \frac{8\alpha_1 + \alpha_2}{24}$$

$$\mu_{31}(\eta(\alpha)) = \mu_{22}(\eta(\alpha)) = \frac{\alpha_2}{48}$$

$$\mu_{211}(\eta(\alpha)) = 0$$

The matrix $\widetilde{L} = (K'K)^{-1}K'$ with K from equation (3.12) is

$$\widetilde{L} = (K'K)^{-1}K' = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 0 & 3 & 0 \end{pmatrix}$$

The information matrices for the designs η_1 and η_2 are obtained as follows:

$$C_1 = C_k(M(\eta_1)) = \widetilde{L}(M(\eta_1))\widetilde{L}' = \begin{pmatrix} 1/3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots \quad (4.6)$$

and

$$C_2 = C_k(M(\eta_2)) = \widetilde{L}(M(\eta_2))\widetilde{L}' = \begin{pmatrix} 1/24 & 1/48 & 1/48 & 1/8 & 1/8 & 0 \\ 1/48 & 1/24 & 1/48 & 1/8 & 0 & 1/8 \\ 1/48 & 1/48 & 1/24 & 0 & 1/8 & 1/8 \\ 1/8 & 1/8 & 0 & 3/4 & 0 & 0 \\ 1/8 & 0 & 1/8 & 0 & 3/4 & 0 \\ 0 & 1/8 & 1/8 & 0 & 0 & 3/4 \end{pmatrix} \ldots\ldots \quad (4.7)$$

From equation (4.6) and equation (4.7) we obtain the information matrix for the design $\eta(\alpha)$ as follows

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

This on simplification becomes

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 \\ 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{4} \end{pmatrix} \text{.......... (4.8)}$$

4.2.3 Information matrix for $m = 4$ ingredients

Table 4.3. Weighted centroid design for m=4 ingredients

Design points	t_1	t_2	t_3	t_4
1	1	0	0	0
2	0	1	0	0
3	0	0	1	0
4	0	0	0	1
5	½	½	0	0
6	½	0	½	0
7	½	0	0	½
8	0	½	½	0
9	0	½	0	½
10	0	0	½	½
11	⅓	⅓	⅓	0
12	⅓	⅓	0	⅓
13	⅓	0	⅓	⅓
14	0	⅓	⅓	⅓
15	¼	¼	¼	¼

From definition (under theorem 4.1), we showed that there are m-elementary centroid design η_j, placing equal weights $\frac{1}{\binom{m}{j}}$ on the points having j out of their m components equal to $\frac{1}{j}$ and zeros elsewhere. These are for, $m = 4$

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

$$\eta_3 = \left\{ \begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \\ 0 \end{pmatrix}, \begin{pmatrix} 1/3 \\ 1/3 \\ 0 \\ 1/3 \end{pmatrix}, \begin{pmatrix} 1/3 \\ 0 \\ 1/3 \\ 1/3 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/3 \\ 1/3 \\ 1/3 \end{pmatrix} \right\} \text{ and } \eta_4 = \left\{ \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{pmatrix} \right\}.$$

For the case, m=4, $\eta(\alpha) = \sum_{j=1}^{4} \alpha_j \eta_j = \alpha_1\eta_1 + \alpha_2\eta_2 + \alpha_3\eta_3 + \alpha_4\eta_4$ with

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

Theorem 4.4

The K-matrix for m=4 ingredients is given by

$$K = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Proof

From equation (3.12), we have $K = (K_1, K_2) \in \Re^{m^2 \times s}$ where;

$$K_1 = \sum_{i=1}^{m} e_{ii} e_i' \qquad \text{and} \qquad K_2 = \frac{1}{2\binom{m}{2}} \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E_{ij}'$$

For m=4 ingredients, then;

$$K_1 = \sum_{i=1}^{4} e_{ii} e_i' = e_{11}e_1' + e_{22}e_2' + e_{33}e_3' + e_{44}e_4' \quad \text{and}$$

$$K_2 = \frac{1}{12} \sum_{\substack{i,j=1 \\ i<j}}^{4} (e_{ij} + e_{ji}) E_{ij}'$$

$$= \frac{1}{12}[(e_{12}+e_{21})E_{12}' + (e_{13}+e_{31})E_{13}' + (e_{14}+e_{41})E_{14}' + (e_{23}+e_{32})E_{23}' + (e_{24}+e_{42})E_{24}' + (e_{34}+e_{43})E_{34}']$$

with $E_{ij} \in \Re^{\binom{3}{2}}$ ………………………………………………………………….… (4.9)

Define, $e_{ij} = e_i \otimes e_j$, i, j=1,2,3 $e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, $e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, $e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ and $e_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Thus

$$e_{11} = e_1 \otimes e_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{22} = e_2 \otimes e_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{33} = e_3 \otimes e_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{44} = e_4 \otimes e_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}',$$

$$e_{12} = e_1 \otimes e_2 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{21} = e_2 \otimes e_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{13} = e_1 \otimes e_3 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{31} = e_3 \otimes e_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{14} = e_1 \otimes e_4 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{41} = e_4 \otimes e_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{23} = e_2 \otimes e_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{32} = e_3 \otimes e_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{24} = e_2 \otimes e_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$

$$e_{42} = e_4 \otimes e_2 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0)',$$

$$e_{34} = e_3 \otimes e_4 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0)' \text{ and}$$

$$e_{43} = e_4 \otimes e_3 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)'.$$

The vectors E_{ij}'s are obtained by considering the index pairs {i,j}with $i, j \in \{1,2,3,4\}$ and i<j. They represent the standard basis of $\Re^6$ and the index pairs should be in a lexicographic order. They are;

$$E_{12} = (1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$E_{13} = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0)',$$

$$E_{14} = (0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0)',$$

$$E_{23} = (0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0)',$$

$$E_{24} = (0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)' \text{ and}$$

$$E_{34} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1)'$$

Therefore we obtain;

$$K_1 = e_{11}e_1' + e_{22}e_2' + e_{33}e_3' + e_{44}e_4' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$K_2 = \frac{1}{12}\sum_{\substack{i,j=1 \\ i<j}}^{4}(e_{ij} + e_{ji})E_{ij}'$$

$$= \frac{1}{12}[(e_{12}+e_{21})E_{12}' + (e_{13}+e_{31})E_{13}' + (e_{14}+e_{41})E_{14}' + (e_{23}+e_{32})E_{23}' + (e_{24}+e_{42})E_{24}' + (e_{34}+e_{43})E_{34}']$$

$$K_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1/12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/12 & 0 & 0 & 0 \\ 1/12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/12 & 0 \\ 0 & 1/12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/12 \\ 0 & 0 & 1/12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/12 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Thus

$$K = (K_1, K_2) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/12 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \blacksquare$$

Theorem 4.5

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

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 \\ \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 \\ 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 \\ 0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} \end{pmatrix}$$

Proof

For m=4, the moment matrix for the weighted centroid design $\eta(\alpha)$ is given by;

$$M(\eta(\alpha)) =$$

$$\begin{pmatrix}
\mu_{4} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{31} \\
\mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} \\
\mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} \\
\mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{4} & \mu_{31} & \mu_{31} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} \\
\mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\
\mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} \\
\mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{31} & \mu_{31} & \mu_{4} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} \\
\mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{21} & \mu_{22} & \mu_{31} \\
\mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} \\
\mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\
\mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} \\
\mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{4}
\end{pmatrix}$$

The fourth order moments are:

$$\mu_4(\eta_j) = \frac{1}{j^3 m} \ ,$$

$$\mu_{31}(\eta_j) = \mu_{22}(\eta_j) = \frac{j-1}{j^3 m(m-1)} \, ,$$

$$\mu_{211}(\eta_j) = \frac{(j-1)(j-2)}{j^3 m(m-1)(m-2)} \, .$$

$$\mu_{1111}(\eta_j) = \frac{(j-1)(j-2)(j-3)}{j^3 m(m-1)(m-2)(m-3)}$$

for j=1, 2, …, m.

When m=4 these moments are;

$\mu_4(\eta_1) = \frac{1}{4}$, $\mu_{31}(\eta_1) = \mu_{22}(\eta_1) = 0$, and $\mu_{211}(\eta_1) = \mu_{1111}(\eta_1) = 0$, $\mu_4(\eta_2) = \frac{1}{32}$,

$\mu_{31}(\eta_2) = \mu_{22}(\eta_2) = \frac{1}{96}$, and $\mu_{211}(\eta_2) = \mu_{1111}(\eta_2) = 0$

and $\mu_{211}(\eta_2) = 0$.

Thus the moment matrices for the design η_1 and η_2 are:

$$M(\eta_1) = \begin{pmatrix}
1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4
\end{pmatrix}$$

and $M(\eta_2) =$

$$\begin{pmatrix}
\frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & \frac{1}{96} \\
\frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{96} & 0 & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & 0 & \frac{1}{96} \\
\frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} \\
0 & 0 & 0 & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} \\
\frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} \\
\frac{1}{96} & 0 & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & 0 & \frac{1}{96} \\
0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{96} & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} \\
\frac{1}{96} & 0 & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & \frac{1}{96} & 0 & 0 & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{32}
\end{pmatrix}$$

The fourth moments of the weighted centroid design $\eta(\alpha)$ are obtained as

$$\mu_4(\eta(\alpha)) = \frac{8\alpha_1 + \alpha_2}{32}$$

$$\mu_{31}(\eta(\alpha)) = \mu_{22}(\eta(\alpha)) = \frac{\alpha_2}{96}$$

$$\mu_{211}(\eta(\alpha)) = 0$$

$$\mu_{1111}(\eta(\alpha)) = 0$$

The matrix $\tilde{L} = (K'K)^{-1}K'$ with K from equation (3.12) is

$$\tilde{L} = (K'K)^{-1}K' = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 6 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 6 & 0 \end{pmatrix}$$

The information matrices for the designs η_1 and η_2 are obtained as follows:

$$C_1 = C_k(M(\eta_1)) = \tilde{L}(M(\eta_1))\tilde{L}' = \begin{pmatrix} 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \ldots (4.10)$$

and

$C_2 = C_k(M(\eta_2))$

$$= \tilde{L}(M(\eta_2))\tilde{L}' = \begin{pmatrix} \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & 0 & 0 & 0 \\ \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{8} & 0 & 0 & \frac{1}{8} & \frac{1}{8} & 0 \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & 0 & \frac{1}{8} & 0 & \frac{1}{8} & 0 & \frac{1}{8} \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & 0 & 0 & \frac{1}{8} & 0 & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{8} & 0 & \frac{1}{8} & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 \\ \frac{1}{8} & 0 & 0 & \frac{1}{8} & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{8} & \frac{1}{8} & 0 & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 \\ 0 & \frac{1}{8} & 0 & \frac{1}{8} & 0 & 0 & 0 & 0 & \frac{3}{2} & 0 \\ 0 & 0 & \frac{1}{8} & \frac{1}{8} & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} \end{pmatrix} \qquad \text{……………………} (4.11)$$

From equation (4.10) and equation (4.11) we obtain the information matrix for the design $\eta(\alpha)$ as follows

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

This on simplification becomes

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 \\ \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 \\ 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 \\ 0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} \end{pmatrix}$$

………………………………. (4.12)

4.2.4 Information matrix for $m \geq 2$ ingredients

For a given value of $m \geq 2$ ingredients, the matrices C_1 and C_2 can be expressed in terms of m. Also, the matrix C_k, which is a linear combination of the matrices C_1 and C_2, can be expressed in m, α_1 *and* α_2. Thus we find it a noble task to establish a general expression for the weight vectors and corresponding optimal values for a given number of ingredients, m.

From equation (3.3), any matrix $C \in sym(s, H)$ can be uniquely represented in the form

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \quad \text{……………………………………} (4.13)$$

With coefficients $a,...,g \in \Re$. The terms containing V_2 , W_2 and W_3 only occur for $m \geq 3$ or $m \geq 4$, respectively.

In the proof of equation (3.4), any given symmetric matrix $C \in sym(s)$, can be partitioned according to the block structure of matrices in H, that is

$$C = \begin{pmatrix} C_{11} & C'_{21} \\ C_{21} & C_{22} \end{pmatrix} \quad (4.14)$$

With $C_{11} \in sym(m)$, $C_{21} \in \Re^{\binom{m}{2}\times m}$ and $C_{22} \in sym\left(\binom{m}{2}\right)$. From equation (3.11), we obtain

for j=1;

$C_{11,1} = \frac{1}{m} I_m$, $C_{21,1}=0$ and $C_{22,1}=0$.

and, for j=2;

$C_{11,2} = \frac{1}{8m} I_m + \frac{1}{8m(m-1)} U_2$, $C_{21,2} = \frac{1}{8} V_1$ and $C_{22,2} = \frac{m(m-1)}{8} I_{\binom{m}{2}}$,

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

Thus we have

$$C_1 = \begin{pmatrix} \frac{1}{m} I_m & 0 \\ 0 & 0 \end{pmatrix} \quad (4.15)$$

and $$C_2 = \begin{pmatrix} \frac{1}{8m} I_m + \frac{1}{8m(m-1)} U_2 & \frac{1}{8} V'_1 \\ \frac{1}{8} V_1 & \frac{m(m-1)}{8} I\binom{m}{2} \end{pmatrix} \quad (4.16)$$

From which we obtain

$C(\alpha) = \alpha_1 C_1 + \alpha_2 C_2$

$$= \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{8m} I_m + \frac{\alpha_2}{8m(m-1)} U_2 & \frac{\alpha_2}{8} V_1' \\ \frac{\alpha_2}{8} V_1 & \frac{m(m-1)\alpha_2}{8} I_{\binom{m}{2}} \end{pmatrix} \cdots\cdots (4.17)$$

4.3 A-Optimal Weighted Centroid Design

We now derive optimal weighted centroid designs for the average variance criterion, ϕ_{-1}. We begin by adapting the general equivalence theorem as is given in Pukelsheim (1993). This theorem provides a necessary and sufficient condition applicable to our specific problem.

Theorem 4.6

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

$$trace\, C_j C^{p-1} \begin{cases} = traceC^p & for\ all\ \ j \in \partial(\alpha) \\ < traceC^p & otherwise \end{cases}$$

Proof

The two major arguments of the proof are the linearity of the information matrix mapping depicted by equation (2.8) and the fact that $\eta(T_m)$ is the convex hull of the elementary centroid designs $\eta_1, \eta_2, \cdots, \eta_m$. From Pukelsheim (1993), $\eta(\alpha)$ is $\phi_p - optimal$ for $K'\theta$ in T if and only if there exists a generalized inverse G of $M = M(\eta(\alpha))$ satisfying

$$traceM(\eta(\beta))GKC^{p+1}K'G' \le traceC^p \text{ for all } \beta \in T_m \cdots\cdots (4.18)$$

With $C = (K'K)^{-1} K'MK(K'K)^{-1}$, $M = K(K'K)^{-1}K'M$ and

$M(\eta(\beta)) = KC_k(M(\eta(\alpha)))K'$, the left-hand side may be written as

$$traceM(\eta(\beta))GKC^{p+1}K'G'$$

$$= trace(K'GMK(K'K)^{-1})'C_k(M(\eta(\beta)))(K'GMK(K'K)^{-1})C^{p-1} \quad \text{..... (4.19)}$$

Due to the feasibility of $\eta(\alpha)$, we have $\Re(K) = \Re(M)$. Hence $K = MZ$ for some Z and so $K'GMK(K'K)^{-1} = Z'MGMK(K'K)^{-1} = Z'MK(K'K)^{-1} = I_{\binom{m}{2}}$.

Now the right-hand side of equation (4.19) simplifies to $traceC_k(M(\eta(\beta)))C^{p-1}$ and equation (4.18) turns into $traceC_k(M(\eta(\beta)))C^{p-1} \le traceC^p$ for all $\beta \in T_m$.

According to equation (3.10), we can write the left-hand side as

$\sum_{j=1}^{m} \beta_j traceC_j C^{p-1}$. Giving $trace\,C_j C^{p-1} \le traceC^p$ for all $1 \le j \le m$.

Finally, equality must hold for any $j \in \partial(\alpha)$ ▪

In addition, the following theorem guarantees that, the weighted centroid designs with first and second weight positive are unique.

Theorem 4.7

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

i. If $\partial(\alpha) = \{1,2\}$, then there is no further design $\tau \in T$ that is $\phi_p - optimal$ for $K'\theta$ in T, that is, $\eta(\alpha)$ is the unique solution of problem (3.7).

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

If there is a non-exchangeable design which is $\phi_p - optimal$ for $K'\theta$, then all its support points are centroids of depths 1, 2 or 3. (Klein 2004)▪

We begin investigating A-optimal designs for a mixture experiment with two ingredients.

4.3.1 A-Optimal design for m=2 ingredients

Theorem 4.8

In the second-degree Kronecker model for mixture experiments with two ingredients, the unique A-optimal design for $K'\theta$ is

$$\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2 = (5-2\sqrt{5})\eta_1 + (-4+2\sqrt{5})\eta_2 .$$

The maximum of the A-criterion for m=2 ingredients is

$$v(\phi_{-1}) = \left(\frac{3(-20+9\sqrt{5})}{\sqrt{5}}\right) = 0.16718427 .$$

Proof

From theorem (4.6), putting p=-1, it implies that $\eta(\alpha)$ is $\phi_{-1} - optimal$ for $K'\theta$ in T if and only if $tracC_j C(\alpha)^{-2} = traceC(\alpha)^{-1}$ for all $j \in \{1,2\}$ .... (4.20)

The inverse of the information matrix provided in theorem (4.1) is as follows;

$$[C(M(\eta(\alpha)))]^{-1} = \begin{pmatrix} \frac{2}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & \frac{2}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{4\alpha_1+\alpha_2}{\alpha_1\alpha_2} \end{pmatrix} \quad \text{...} \quad (4.21)$$

Now

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

$$[C(\alpha)]^{-2} = \begin{pmatrix} \frac{5}{\alpha_1^2} & \frac{1}{\alpha_1^2} & \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} \\ \frac{1}{\alpha_1^2} & \frac{5}{\alpha_1^2} & \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} \\ \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} & \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} & \frac{16\alpha_1^2+8\alpha_1\alpha_2+3\alpha_2^2}{\alpha_1^2\alpha_2^2} \end{pmatrix} \qquad (4.22)$$

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

From equations (4.2) and (4.22), we have

$$C_1[C(\alpha)]^{-2} = \begin{pmatrix} \frac{5}{2\alpha_1^2} & \frac{1}{2\alpha_1^2} & \frac{-(4\alpha_1+3\alpha_2)}{2\alpha_1^2\alpha_2} \\ \frac{1}{2\alpha_1^2} & \frac{5}{2\alpha_1^2} & \frac{-(4\alpha_1+3\alpha_2)}{2\alpha_1^2\alpha_2} \\ 0 & 0 & 0 \end{pmatrix}$$

hence, $traceC_1[C(\alpha)]^{-2} = \frac{5}{2\alpha_1^2} + \frac{5}{2\alpha_1^2} + 0 = \frac{5}{\alpha_1^2}$

From equation (4.21),

$$trace[C(\alpha)]^{-1} = \frac{2}{\alpha_1} + \frac{2}{\alpha_1} + \frac{4\alpha_1+\alpha_2}{\alpha_1\alpha_2} = \frac{4\alpha_1+5\alpha_2}{\alpha_1\alpha_2} \qquad (4.23)$$

Thus, $traceC_1C(M(\eta(\alpha)))^{-2} = traceC(M(\eta(\alpha)))^{-1}$, implies that

$\frac{5}{\alpha_1^2} = \frac{4\alpha_1+5\alpha_2}{\alpha_1\alpha_2}$, from which we obtain

$\alpha_1^2 - 10\alpha_1 + 5 = 0$, after utilizing the fact that $\alpha_1 + \alpha_2 = 1$. Which upon solving gives

$\alpha_1 = 5 + 2\sqrt{5}$ or $\alpha_1 = 5 - 2\sqrt{5}$.

But since $\alpha_1 \in (0,1)$, then it implies that, $\alpha_1 = 5 - 2\sqrt{5}$.

Similarly, for j=2, equation (4.3) and (4.22) gives,

$$C_2[C(\alpha)]^{-2} = \begin{pmatrix} \frac{-1}{2\alpha_1\alpha_2} & \frac{-1}{2\alpha_1\alpha_2} & \frac{4\alpha_1+\alpha_2}{2\alpha\alpha_2^2} \\ \frac{1}{2\alpha_1\alpha_2} & \frac{-1}{2\alpha_1\alpha_2} & \frac{4\alpha_1+\alpha_2}{2\alpha\alpha_2^2} \\ \frac{-1}{\alpha_1\alpha_2} & \frac{-1}{\alpha_1\alpha_2} & \frac{4\alpha_1+\alpha_2}{\alpha_1\alpha_2^2} \end{pmatrix}.$$

$$traceC_2[C(\alpha)]^{-2} = \frac{-1}{2\alpha_1\alpha_2} + \frac{-1}{2\alpha_1\alpha_2} + \frac{4\alpha_1+\alpha_2}{\alpha_1\alpha_2^2} = \frac{4}{\alpha_2^2}$$

Thus, $traceC_2C(M(\eta(\alpha)))^{-2} = traceC(M(\eta(\alpha)))^{-1}$, implies that

$\frac{4}{\alpha_2^2} = \frac{4\alpha_1+5\alpha_2}{\alpha_1\alpha_2}$, from which we obtain,

$5\alpha_2^2 + 4\alpha_1\alpha_2 - 4\alpha_1 = 0$. Substituting $\alpha_1 = 1-\alpha_2$, yields

$\alpha_2^2 + 8\alpha_2 - 4 = 0$, which upon solving gives

$\alpha_2 = -4 + 2\sqrt{5}$ or $\alpha_2 = -4 - 2\sqrt{5}$.

But since $\alpha_2 \in (0,1)$, then it implies that $\alpha_2 = -4 + 2\sqrt{5}$.

Thus for m=2 ingredients, we have $\alpha_1 = 5 - 2\sqrt{5}$ and $\alpha_2 = -4 + 2\sqrt{5}$.

From Pukelsheim (1993), the average-variance criterion, is given by;

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

For m=2, we have $v(\phi_{-1}) = \left(\frac{1}{3} traceC(\alpha)^{-1}\right)^{-1}$,

From equation (4.23), we have, $trace[C(\alpha)]^{-1} = \frac{4\alpha_1+5\alpha_2}{\alpha_1\alpha_2} = \frac{\sqrt{5}}{-20+9\sqrt{5}}$,

Thus the optimal value becomes,

$$v(\phi_{-1}) = \left(\frac{1}{3} traceC(\alpha)^{-1}\right)^{-1} = \left(\frac{4\alpha_1 + 5\alpha_2}{3\alpha_1\alpha_2}\right)^{-1} = \frac{3(-20+9\sqrt{5})}{\sqrt{5}} = 0.16718427 \blacksquare$$

4.3.2 A-Optimal design for m=3 ingredients

Theorem 4.9

In the second-degree Kronecker model for mixture experiments with three ingredients, the unique A-optimal design for $K'\theta$ is

$$\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2 = \left(\frac{38-4\sqrt{38}}{22}\right)\eta_1 + \left(\frac{-16+4\sqrt{38}}{22}\right)\eta_2 .$$

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

$$v(\phi_{-1}) = \left(\frac{25.82882991}{6}\right)^{-1} = 0.23229856 .$$

Proof

From theorem (4.6), putting p=-1, it implies that $\eta(\alpha)$ is $\phi_{-1} - optimal$ for $K'\theta$ in T if and only if

$trace\, C_j C(\alpha)^{-2} = traceC(\alpha)^{-1}$ for all $j \in \{1,2\}$ ……………………………………(4.24)

The inverse of the information matrix provided in theorem (4.3) is as follows

$$[C(M(\eta(\alpha)))]^{-1} = \begin{pmatrix} \frac{3}{\alpha_1} & 0 & 0 & \frac{-1}{2\alpha_1} & \frac{-1}{2\alpha_1} & 0 \\ 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{2\alpha_1} & 0 & \frac{-1}{2\alpha_1} \\ 0 & 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{2\alpha_1} & \frac{-1}{2\alpha_1} \\ \frac{-1}{2\alpha_1} & \frac{-1}{2\alpha_1} & 0 & \frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2} & \frac{1}{12\alpha_1} & \frac{1}{12\alpha_1} \\ \frac{-1}{2\alpha_1} & 0 & \frac{-1}{2\alpha_1} & \frac{1}{12\alpha_1} & \frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2} & \frac{1}{12\alpha_1} \\ 0 & \frac{-1}{2\alpha_1} & \frac{-1}{2\alpha_1} & \frac{1}{12\alpha_1} & \frac{1}{12\alpha_1} & \frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2} \end{pmatrix} \ldots\ldots\ldots\ldots (4.25)$$

Now

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

$$[C(\alpha)]^{-2} = \begin{pmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ c & c & d & e & f & f \\ c & d & c & f & e & f \\ d & c & c & f & f & e \end{pmatrix} \ldots\ldots\ldots\ldots (4.26)$$

Where;

$a = \frac{19}{2\alpha_1^2}$, $b = \frac{1}{4\alpha_1^2}$, $c = \frac{-39\alpha_2 - 16\alpha_1}{24\alpha_1^2\alpha_2}$, $d = \frac{-1}{12\alpha_1^2}$, $e = \frac{74\alpha_2^2 + 4(8\alpha_1+\alpha_2)^2}{144\alpha_1^2\alpha_2^2}$ and

$f = \frac{41\alpha_2 + 32\alpha_1}{144\alpha_1^2\alpha_2}$

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

From equation (4.6) and (4.26) we have

$$C_1[C(\alpha)]^{-2} = \begin{pmatrix} \frac{19}{6\alpha_1^2} & \frac{1}{12\alpha_1^2} & \frac{1}{12\alpha_1^2} & \frac{-39\alpha_1-16\alpha_2}{72\alpha_1^2\alpha_2} & \frac{-39\alpha_1-16\alpha_2}{72\alpha_1^2\alpha_2} & \frac{-1}{36\alpha_1^2} \\ \frac{1}{12\alpha_1^2} & \frac{19}{6\alpha_1^2} & \frac{1}{12\alpha_1^2} & \frac{-39\alpha_1-16\alpha_2}{72\alpha_1^2\alpha_2} & \frac{-1}{36\alpha_1^2} & \frac{-39\alpha_1-16\alpha_2}{72\alpha_1^2\alpha_2} \\ \frac{1}{12\alpha_1^2} & \frac{1}{12\alpha_1^2} & \frac{19}{6\alpha_1^2} & \frac{-1}{36\alpha_1^2} & \frac{-39\alpha_1-16\alpha_2}{72\alpha_1^2\alpha_2} & \frac{-39\alpha_1-16\alpha_2}{72\alpha_1^2\alpha_2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Hence $traceC_1[C(\alpha)]^{-2} = \frac{19}{6\alpha_1^2} + \frac{19}{6\alpha_1^2} + \frac{19}{6\alpha_1^2} + 0 + 0 + 0 = \frac{19}{2\alpha_1^2}$

From equation (4.25) ,

$$trace[C(\alpha)]^{-1} = 3\left(\frac{3}{\alpha_1}\right) + 3\left(\frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2}\right) = \frac{8\alpha_1+19\alpha_2}{2\alpha_1\alpha_2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.27)}$$

Thus, $traceC_1C(M(\eta(\alpha)))^{-2} = traceC(M(\eta(\alpha)))^{-1}$, implies that

$\frac{19}{2\alpha_1^2} = \frac{8\alpha_1+19\alpha_2}{2\alpha_1\alpha_2}$, from which we obtain

$11\alpha_1^2 - 38\alpha_1 + 19 = 0$, after utilizing the fact that $\alpha_2 = 1-\alpha_1$,

which upon solving gives

$\alpha_1 = \frac{38+4\sqrt{38}}{22}$ or $\alpha_1 = \frac{38-4\sqrt{38}}{22}$.

But since $\alpha_1 \in (0,1)$, we have, $\alpha_1 = \frac{38-4\sqrt{38}}{22}$.

Similarly, for j=2, we have, from equation (4.7) and equation (4.26),

$$C_2[C(\alpha)]^{-2}=\begin{pmatrix} \frac{-1}{6\alpha_1\alpha_2} & \frac{-1}{12\alpha_1\alpha_2} & \frac{-1}{12\alpha_1\alpha_2} & \frac{16\alpha_1+3\alpha_2}{72\alpha_1\alpha_2^2} & \frac{16\alpha_1+3\alpha_2}{72\alpha_1\alpha_2^2} & \frac{1}{36\alpha_1\alpha_2} \\ \frac{-1}{12\alpha_1\alpha_2} & \frac{-1}{6\alpha_1\alpha_2} & \frac{-1}{12\alpha_1\alpha_2} & \frac{16\alpha_1+3\alpha_2}{72\alpha_1\alpha_2^2} & \frac{1}{36\alpha_1\alpha_2} & \frac{16\alpha_1+3\alpha_2}{72\alpha_1\alpha_2^2} \\ \frac{-1}{12\alpha_1\alpha_2} & \frac{-1}{12\alpha_1\alpha_2} & \frac{-1}{6\alpha_1\alpha_2} & \frac{1}{36\alpha_1\alpha_2} & \frac{16\alpha_1+3\alpha_2}{72\alpha_1\alpha_2^2} & \frac{16\alpha_1+3\alpha_2}{72\alpha_1\alpha_2^2} \\ \frac{-1}{2\alpha_1\alpha_2} & \frac{-1}{2\alpha_1\alpha_2} & 0 & \frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2^2} & \frac{1}{12\alpha_1\alpha_2} & \frac{1}{12\alpha_1\alpha_2} \\ \frac{-1}{2\alpha_1\alpha_2} & 0 & \frac{-1}{2\alpha_1\alpha_2} & \frac{1}{12\alpha_1\alpha_2} & \frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2^2} & \frac{1}{12\alpha_1\alpha_2} \\ 0 & \frac{-1}{2\alpha_1\alpha_2} & \frac{-1}{2\alpha_1\alpha_2} & \frac{1}{12\alpha_1\alpha_2} & \frac{1}{12\alpha_1\alpha_2} & \frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2^2} \end{pmatrix}$$

$$traceC_2[C(\alpha)]^{-2}=3\left(\frac{-1}{6\alpha_1\alpha_2}\right)+3\left(\frac{8\alpha_1+\alpha_2}{6\alpha_1\alpha_2^2}\right)=\frac{4}{\alpha_2^2}$$

Thus, $traceC_2C(M(\eta(\alpha)))^{-2}=traceC(M(\eta(\alpha)))^{-1}$, implies that

$\frac{4}{\alpha_2^2}=\frac{8\alpha_1+19\alpha_2}{2\alpha_1\alpha_2}$, from which we obtain,

$11\alpha_2^2+16\alpha_2-8=0$ after substituting $\alpha_1=1-\alpha_2$.

Which upon solving gives

$\alpha_2=\frac{-16+4\sqrt{38}}{22}$ or $\alpha_2=\frac{-16-4\sqrt{38}}{22}$.

But since $\alpha_2\in(0,1)$, we have, $\alpha_2=\frac{-16+4\sqrt{38}}{22}$.

Thus for m=3 ingredients, we have $\alpha_1=\frac{38-4\sqrt{38}}{22}=0.6064701081$

and $\alpha_2=\frac{-16+4\sqrt{38}}{22}=0.393529818$

From Pukelsheim (1993), the average-variance criterion, is given by;

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

For m=3, we have $v(\phi_{-1}) = \left(\frac{1}{6} traceC(\alpha)^{-1}\right)^{-1}$,

Substituting the values of α_1 and α_2 obtained above in equation (4.27), we have,

$$trace[C(\alpha)]^{-1} = \frac{8\alpha_1 + 19\alpha_2}{2\alpha_1\alpha_2} = 25.82882991.$$

Thus the optimal value becomes,

$$v(\phi_{-1}) = \left(\frac{1}{6} traceC(\alpha)^{-1}\right)^{-1} = \left(\frac{25.82882991}{6}\right)^{-1} = 0.23229856 \blacksquare$$

4.3.3 A-Optimal design for m=4 ingredients

Theorem 4.10

In the second-degree Kronecker model for mixture experiments with four ingredients, the unique A-optimal design for $K'\theta$ is

$$\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.668953748\eta_1 + 0.331046251\eta_2.$$

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

$$v(\phi_{-1}) = \frac{10}{36.49914091} = 0.273979051.$$

Proof

From theorem (4.6), putting p=-1, then $\eta(\alpha)$ is $\phi_{-1} - optimal$ for $K'\theta$ in T if and only if

$$tracC_j C(\alpha)^{-2} = traceC(\alpha)^{-1} \text{ for all } j \in \{1,2\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.28)$$

The inverse of the information matrix provided in theorem (4.5) is as follows

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

$$\begin{pmatrix}
\frac{4}{\alpha_1} & 0 & 0 & 0 & \frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} & 0 & 0 & 0 \\
0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{3\alpha_1} & 0 & 0 & \frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} & 0 \\
0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{3\alpha_1} & 0 & \frac{-1}{3\alpha_1} & 0 & \frac{-1}{3\alpha_1} \\
0 & 0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{3\alpha_1} & 0 & \frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} \\
\frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} & 0 & 0 & \frac{12\alpha_1+\alpha_2}{18\alpha_1\alpha_2} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & 0 \\
\frac{-1}{3\alpha_1} & 0 & \frac{-1}{3\alpha_1} & 0 & \frac{1}{36\alpha_1} & \frac{12\alpha_1+\alpha_2}{18\alpha_1\alpha_2} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & 0 & \frac{1}{36\alpha_1} \\
\frac{-1}{3\alpha_1} & 0 & 0 & \frac{-1}{3\alpha_1} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & \frac{12\alpha_1+\alpha_2}{18\alpha_1\alpha_2} & 0 & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} \\
0 & \frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} & 0 & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & 0 & \frac{12\alpha_1+\alpha_2}{18\alpha_1\alpha_2} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} \\
0 & \frac{-1}{3\alpha_1} & 0 & \frac{-1}{3\alpha_1} & \frac{1}{36\alpha_1} & 0 & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & \frac{12\alpha_1+\alpha_2}{18\alpha_1\alpha_2} & \frac{1}{36\alpha_1} \\
0 & 0 & \frac{-1}{3\alpha_1} & \frac{-1}{3\alpha_1} & 0 & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & \frac{1}{36\alpha_1} & \frac{12\alpha_1+\alpha_2}{18\alpha_1\alpha_2}
\end{pmatrix}$$

…………………………………………………………………………………..……… (4.29)

Now

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

$$[C(\alpha)]^{-2} = \begin{pmatrix}
a & b & b & b & c & c & c & d & d & d \\
b & a & b & b & c & d & d & c & c & d \\
b & b & a & b & d & c & d & c & d & c \\
b & b & b & a & d & d & c & d & c & c \\
c & c & d & d & e & f & f & f & f & g \\
c & d & c & d & f & e & f & f & g & f \\
c & d & d & c & f & f & e & g & f & f \\
d & c & c & d & f & f & g & e & f & f \\
d & c & d & c & f & g & f & f & e & f \\
d & d & c & c & g & f & f & f & f & e
\end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4.30)$$

Where;

$a = \frac{49}{3\alpha_1^2}$, $b = \frac{1}{9\alpha_1^2}$, $c = \frac{-(74\alpha_2 + 12\alpha_1)}{54\alpha_1^2\alpha_2}$, $d = \frac{-1}{54\alpha_1^2}$, $e = \frac{37\alpha_2^2 + 72\alpha_1^2 + 12\alpha_1\alpha_2}{162\alpha_1^2\alpha_2^2}$,

$f = \frac{75\alpha_2 + 14\alpha_1}{648\alpha_1^2\alpha_2}$ and $g = \frac{1}{324\alpha_1^2}$

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

From equation (4.10) and (4.30) we have

$$C_1[C(\alpha)]^{-2} = \begin{pmatrix} \frac{a}{4} & \frac{b}{4} & \frac{b}{4} & \frac{b}{4} & \frac{c}{4} & \frac{c}{4} & \frac{c}{4} & \frac{d}{4} & \frac{d}{4} & \frac{d}{4} \\ \frac{b}{4} & \frac{a}{4} & \frac{b}{4} & \frac{b}{4} & \frac{c}{4} & \frac{d}{4} & \frac{d}{4} & \frac{c}{4} & \frac{c}{4} & \frac{d}{4} \\ \frac{b}{4} & \frac{b}{4} & \frac{a}{4} & \frac{b}{4} & \frac{d}{4} & \frac{c}{4} & \frac{d}{4} & \frac{c}{4} & \frac{d}{4} & \frac{c}{4} \\ \frac{b}{4} & \frac{b}{4} & \frac{b}{4} & \frac{a}{4} & \frac{d}{4} & \frac{d}{4} & \frac{c}{4} & \frac{d}{4} & \frac{c}{4} & \frac{c}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Hence, $traceC_1[C(\alpha)]^{-2} = \frac{a}{4} + \frac{a}{4} + \frac{a}{4} + \frac{a}{4} + 0 + 0 + 0 + 0 = a = \frac{49}{3\alpha_1^2}$

From equation (4.29),

$$trace[C(\alpha)]^{-1} = 4\left(\frac{4}{\alpha_1}\right) + 6\left(\frac{12\alpha_1 + \alpha_2)}{18\alpha_1\alpha_2}\right) = \frac{12\alpha_1 + 49\alpha_2}{3\alpha_1\alpha_2} \quad \text{.............................. (4.31)}$$

Thus, $traceC_1C(M(\eta(\alpha)))^{-2} = traceC(M(\eta(\alpha)))^{-1}$, implies that

$\frac{49}{3\alpha_1^2} = \frac{12\alpha_1 + 49\alpha_2}{3\alpha_1\alpha_2}$, from which we obtain

$37\alpha_1^2 + 98\alpha_1 - 49 = 0$, after utilizing the fact that $\alpha_1 + \alpha_2 = 1$.

Which upon solving gives

$\alpha_1 = 1.9796949$ or $\alpha_1 = 0.668953748$.

But since $\alpha_1 \in (0,1)$, we have, $\alpha_1 = 0.668953748$.

Similarly, for j=2, from equation (4.11) and (4.30) we have,

$$C_2[C(\alpha)]^{-2} = \begin{pmatrix} a & b & b & b & c & c & c & d & d & d \\ b & a & b & b & c & d & d & c & c & d \\ b & b & a & b & d & c & d & c & d & c \\ b & b & b & a & d & d & c & d & c & c \\ k & k & l & l & e & f & f & f & f & g \\ k & l & k & l & f & e & f & f & g & f \\ k & l & l & k & f & f & e & g & f & f \\ l & k & k & l & f & f & g & e & f & f \\ l & k & l & k & f & g & f & f & e & f \\ l & l & k & k & g & f & f & f & f & e \end{pmatrix},$$

Where; $a = \frac{-1}{12\alpha_1\alpha_2}$, $b = \frac{-1}{36\alpha_1\alpha_2}$, $c = \frac{6\alpha_1 + \alpha_2}{108\alpha_1\alpha_2^2}$, $d = \frac{1}{216\alpha_1\alpha_2}$, $e = \frac{12\alpha_1 + \alpha_2}{18\alpha_1\alpha_2^2}$,

$f = \frac{1}{36\alpha_1\alpha_2}$, $g = 0$, $k = \frac{-1}{3\alpha_1\alpha_2}$ and $l = 0$.

$traceC_2[C(\alpha)]^{-2} = 4\left(\frac{-1}{12\alpha_1\alpha_2}\right) + 6\left(\frac{12\alpha_1 + \alpha_2}{18\alpha_1\alpha_2^2}\right) = \frac{4}{\alpha_2^2}$, using $\alpha_1 = 1 - \alpha_2$.

Thus, $traceC_2C(M(\eta(\alpha)))^{-2} = traceC(M(\eta(\alpha)))^{-1}$, implies that

$\frac{4}{\alpha_2^2} = \frac{12\alpha_1 + 49\alpha_2}{3\alpha_1\alpha_2}$, from which we obtain,

$37\alpha_2^2 + 24\alpha_2 - 12 = 0$ after substituting $\alpha_1 = 1 - \alpha_2$.

Solving this equation we obtain

$\alpha_2 = -0.9796949$ or $\alpha_2 = 0.331046251$.

But since $\alpha_2 \in (0,1)$, we have, $\alpha_2 = 0.331046251$.

Thus for m=4 ingredients, we have $\alpha_1 = 0.668953748$ and $\alpha_2 = 0.331046251$

From Pukelsheim (1993), the average-variance criterion, is given by;

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

For m=4, we have $v(\phi_{-1}) = \left(\frac{1}{10} traceC(\alpha)^{-1}\right)^{-1}$,

From equation (4.27), we have $traceC[C(\alpha)]^{-1} = \dfrac{12\alpha_1 + 49\alpha_2}{3\alpha_1\alpha_2} = 36.49914091$,

Thus the optimal value becomes,

$$v(\phi_{-1}) = \left(\frac{1}{10} traceC(\alpha)^{-1}\right)^{-1} = \frac{10}{36.49914091} = 0.273979051 \blacksquare$$

4.3.4 A-Optimal design for $m \geq 2$ ingredients

Theorem 4.11

In the second-degree Kronecker model for mixture experiments with $m \geq 2$ ingredients, the unique A-optimal design for $K'\theta$ is

$$\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2$$
$$= \frac{(m^3 - m^2 + 1) - 2\sqrt{m^4 - 2m^3 + m^2 + m - 1}}{(m^3 - m^2 - 4m + 5)}\eta_1 + \frac{-4(m-1) + 2\sqrt{m^4 - 2m^3 + m^2 + m - 1}}{m^3 - m^2 - 4m + 5}\eta_2$$

.

The maximum of the A-criterion for m ingredients is

$$v(\phi_{-1}) = \left\{\frac{2(m^3 - m^2 - 4m + 5)^2}{m(m+1)\left[(m^4 - 2m^3 + 5m^2 - 7m + 3) - 4(m-1)\sqrt{m^4 - 2m^3 + m^2 + m - 1}\right]}\right\}^{-1} .$$

Proof

Let $\alpha = (\alpha_1, \alpha_2, 0, ..., 0)' \in T_m$ be a weight vector with $\partial(\alpha) = \{1,2\}$ and suppose $\eta(\alpha)$ is A-optimal for $K'\theta$ in T. Let $C(\alpha) = C_k(M(\eta(\alpha)))$.

Theorem (4.6) implies that

$$trace(C_j C^{-2}) \begin{cases} = trace(C(\alpha)^{-1}) & for \quad j \in \{1,2\}, \\ < trace(C(\alpha)^{-1}) & otherwise \end{cases} \quad \text{...} \quad (4.32)$$

We now compute for the optimality candidates, α_1 and α_2 in (0,1) as follows.

An inverse of a matrix in $sym(s, H)$ can be computed by solving a system of linear equations. By the same approach we obtain the blocks of $C(\alpha)^{-1}$ as obtained in equation (4.16) in the partitioning suggested by lemma (3.1), namely

$$C(\alpha)^{-1} = \begin{pmatrix} \frac{m}{\alpha_1} I_m & \frac{-1}{(m-1)\alpha_1} V_1' \\ \frac{-1}{(m-1)\alpha_1} V_1 & \frac{2[4(m-1)\alpha_1 + \alpha_2]}{m(m-1)^2 \alpha_1 \alpha_2} I_{\binom{m}{2}} + \frac{1}{m(m-1)^2 \alpha_1} W_2 \end{pmatrix} \quad \text{.................} \quad (4.33)$$

We can now obtain $C(\alpha)^{-2}$ as

$$C(\alpha)^{-2} = [C(\alpha)^{-1}]^2 =$$

$$\begin{pmatrix} \frac{m^2(m-1)+1}{(m-1)\alpha_1^2} I_m + \frac{1}{(m-1^2)\alpha_1^2} U_2 & -\left(\frac{8(m-1)\alpha_1 + [m^2(m+1)^2 - m]\alpha_2}{m(m-1)^3 \alpha_1^2 \alpha_2} \right) V_1' - \frac{2}{m(m-1)^3 \alpha_1^2} V_2' \\ -\left(\frac{8(m-1)\alpha_1 + [m^2(m+1)^2 - m]\alpha_2}{m(m-1)^3 \alpha_1^2 \alpha_2} \right) V_1 & \frac{2[32(m-1)^2 \alpha_1^2 + 16(m-1)\alpha_1\alpha_2 + (m^2(m+1)^2 + 2m)\alpha_2^2]}{m^2(m-1)^4 \alpha_1^2 \alpha_2^2} I_{\binom{m}{2}} \\ -\frac{2}{m(m-1)^3 \alpha_1^2} V_2 & + \frac{16(m-1)\alpha_1 + [m^2(m-1)^2 + m + 2]\alpha_2}{m^2(m-1)^4 \alpha_1^2 \alpha_2} W_2 + \frac{4}{m^2(m-1)^4 \alpha_1^2} W_3 \end{pmatrix}$$

$$\text{..} \quad (4.34)$$

We now compute for the optimality candidates, α_1 and α_2 in (0,1) as follows.

For $j = 1$, we have $traceC_1 C(\alpha)^{-2} = traceC(\alpha)^{-1}$

Now from equations (4.15) and (4.34) we have

$$C_1C(\alpha)^{-2} = \begin{pmatrix} \dfrac{m^2(m-1)+1}{m(m-1)\alpha_1^2} I_m + \dfrac{1}{m(m-1)^2\alpha_1^2} U_2 & \begin{matrix} -\left(\dfrac{8(m-1)\alpha_1 + [m^2(m+1)^2 - m]\alpha_2}{m^2(m-1)^3\alpha_1^2\alpha_2}\right) V_1' \\ -\dfrac{2}{m^2(m-1)^3\alpha_1^2} V_2' \end{matrix} \\ 0 & 0 \end{pmatrix}$$

Hence

$$traceC_1C(\alpha)^{-2} = trace\left(\frac{m^2(m-1)+1}{m(m-1)\alpha_1^2} I_m + \frac{1}{m(m-1)^2\alpha_1^2} U_2\right)$$

$$= \frac{m^2(m-1)+1}{m(m-1)\alpha_1^2} trace(I_m) + \frac{1}{m(m-1)^2\alpha_1^2} trace(U_2)$$

$= \dfrac{m^2(m-1)+1}{(m-1)\alpha_1^2}$, since $trace(I_m) = m$ and $trace(U_2) = 0$.

From equation (4.33) we have

$$trace(C(\alpha)^{-1}) = trace\left(\frac{m}{\alpha_1} I_m\right) + trace\left(\frac{2[4(m-1)\alpha_1 + \alpha_2]}{m(m-1)^2\alpha_1\alpha_2} I_{\binom{m}{2}} + \frac{1}{m(m-1)^2\alpha_1} W_2\right)$$

$= \dfrac{4(m-1)\alpha_1 + [m^2(m-1)+1]\alpha_2}{(m-1)\alpha_1\alpha_2}$, since $trace\left(I_{\binom{m}{2}}\right) = \dfrac{m(m-1)}{2}$ and

trace $(W_2)=0$

Thus,

$traceC_1C(\alpha)^{-2} = traceC(\alpha)^{-2}$, implies that

$\dfrac{m^2(m-1)+1}{(m-1)\alpha_1^2} = \dfrac{4(m-1)\alpha_1 + [m^2(m-1)+1]\alpha_2}{(m-1)\alpha_1\alpha_2}$, from which we obtain

$$4(m-1)\alpha_1^2 + [m^2(m-1)+1]\alpha_1\alpha_2 - [m^2(m-1)+1]\alpha_2^2 = 0$$

or $(m^3 - m^2 - 4m + 5)\alpha_1^2 - 2(m^3 + m^2 + 1)\alpha_1 + (m^3 - m^2 + 1) = 0$, since $\alpha_2 = 1 - \alpha_1$.

this upon solving gives

$$\alpha_1 = \frac{(m^3 - m^2 + 1) - 2\sqrt{m^4 - 2m^3 + m^2 + m - 1}}{(m^3 - m^2 - 4m + 5)} .$$

Similarly, from equations (4.16) and (4.34) we have

$$C_2 C(\alpha)^{-2} =$$

$$\begin{pmatrix} \frac{-1}{m(m-1)\alpha_1\alpha_2} I_m - \frac{1}{m(m-1)^2\alpha_1\alpha_2} U_2 & \frac{8(m-1)\alpha_1 + m\alpha_2}{m^2(m-1)^3\alpha_1\alpha_2^2} V_1' + \frac{2}{m^2(m-1)^3\alpha_1\alpha_2} V_2' - \frac{1}{(m-1)\alpha_1\alpha_2} V_1 \\ \frac{8(m-1)\alpha_1 + m\alpha_2}{m^2(m-1)^3\alpha_1\alpha_2^2} V_1' + \frac{2}{m^2(m-1)^3\alpha_1\alpha_2} V_2' - \frac{1}{(m-1)\alpha_1\alpha_2} V & \frac{2[4(m-1)\alpha_1 + \alpha_2]}{m(m-1)^2\alpha_1\alpha_2^2} I_{\binom{m}{2}} + \frac{1}{m(m-1)^2\alpha_1^2\alpha_2} w_2 \end{pmatrix}$$

Hence

$$trace C_2 C(\alpha)^{-2} = trace\left(\frac{-1}{m(m-1)\alpha_1\alpha_2} I_m - \frac{1}{m(m-1)^2\alpha_1\alpha_2} U_2 \right) + trace\begin{pmatrix} \frac{2[4(m-1)\alpha_1 + \alpha_2]}{m(m-1)^2\alpha_1\alpha_2^2} I_{\binom{m}{2}} \\ + \frac{1}{m(m-1)^2\alpha_1^2\alpha_2} W_2 \end{pmatrix}$$

but $trace(I_m) = m$, $trace(U_2) = 0$, $trace(I_{\binom{m}{2}}) = \frac{m(m-1)}{2}$ and $trace(W_2) = 0$. Giving

$$trace C_2 C(\alpha)^{-2} = \frac{4}{\alpha_2^2} .$$

Thus

$trace C_2 C(\alpha)^{-2} = trace C(\alpha)^{-2}$, implies that

$\frac{4}{\alpha_2^2} = \frac{4(m-1)\alpha_1 + [m^2(m-1)+1]\alpha_2}{(m-1)\alpha_1\alpha_2}$, from which we obtain

$$[m^2(m-1)+1]\alpha_2^2 + 4(m-1)\alpha_1\alpha_2 + 4(m-1)\alpha_1 = 0$$

or $(m^3 - m^2 - 4m + 5)\alpha_2^2 + 8(m-1)\alpha_2 - 4(m-1) = 0$, using $\alpha_1 = 1 - \alpha_2$.

This upon solving gives

$$\alpha_2 = \frac{-4(m-1) + 2\sqrt{m^4 - 2m^3 + m^2 + m - 1}}{m^3 - m^2 - 4m + 5}.$$

Thus for m ingredients, we have the unique solution in (0, 1) as the weight vector given in the theorem as

$$\alpha_1 = \frac{(m^3 - m^2 + 1) - 2\sqrt{m^4 - 2m^3 + m^2 + m - 1}}{(m^3 - m^2 - 4m + 5)} \qquad \text{and}$$

$$\alpha_2 = \frac{-4(m-1) + 2\sqrt{m^4 - 2m^3 + m^2 + m - 1}}{m^3 - m^2 - 4m + 5}.$$

By construction, the weight vector $\alpha^{(A)} = (\alpha_1{}^{(A)}, \alpha_2{}^{(A)}, 0, ..., 0)'$ satisfies the two equations in condition in theorem (4.7).

Therefore, $\eta(\alpha^{(A)})$ is indeed A-optimal for $K'\theta$ in T.

To obtain the optimal value for m factors, we adapt the definition of Average-variance criterion as provided in Pukelsheim (1993). That is

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

For m-factors, we have $v(\phi_{-1}) = \left(\frac{m(m+1)}{2} traceC(\alpha)^{-1}\right)^{-1}$.

From equation, (4.33), $trace(C(\alpha)^{-1}) = \frac{4(m-1)\alpha_1 + [m^2(m-1)+1]\alpha_2}{(m-1)\alpha_1\alpha_2}$.

Substituting for the values of $\alpha_1 = \frac{(m^3 - m^2 + 1) - 2\sqrt{m^4 - 2m^3 + m^2 + m - 1}}{(m^3 - m^2 - 4m + 5)}$ and

$\alpha_2 = \dfrac{-4(m-1)+2\sqrt{m^4-2m^3+m^2+m-1}}{m^3-m^2-4m+5}$, we obtain

$$trace(C(\alpha)^{-1}) = \frac{(m^3-m^2-4m+5)^2}{(m^4-2m^3+5m^2-7m+3)-4(m-1)\sqrt{m^4-2m^3+m^2+m-1}}.$$

Hence the optimal value becomes

$$v(\phi_{-1}) = \left(\frac{1}{\frac{m(m+1)}{2}} trace\, C(\alpha)^{-1} \right)^{-1}$$

$$= \left\{ \frac{2(m^3-m^2-4m+5)^2}{m(m+1)\left[(m^4-2m^3+5m^2-7m+3)-4(m-1)\sqrt{m^4-2m^3+m^2+m-1}\right]} \right\}^{-1}$$ ▪

4.4 D-Optimal Weighted Centroid Design

This section contains the derivation of optimal weighted centroid design for the determinant criterion, ϕ_0.

4.4.1 D-optimal design for $m = 2$ ingredients

Theorem 4.12

In the second-degree Kronecker model for mixture experiments with two ingredients, the unique D-optimal design for $K'\theta$ is

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{2}{3}\eta_1 + \frac{1}{3}\eta_2.$$

The maximum of the D-criterion for m=2 factors is $v(\phi_0) = \left(\frac{1}{108}\right)^{\frac{1}{3}} = 0.20998684$.

Proof

From theorem (4.6), we have then $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if

$$trace\, C_j C^{p-1} \begin{cases} = traceC^p & for\ all\ \ j \in \partial(\alpha) \\ < traceC^p & otherwise \end{cases}$$

Putting, $p = 0$, we have that $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if

$$traceC_j C(\alpha)^{-1} = traceC(\alpha)^0 = traceI \quad for\ all\ \ j \in \{1,2\}.$$

The inverse of the matrix $C(\alpha)$ is given in equation (4.21).

From equations (4.2) and (4.21), we have;

$$C_1 C(\alpha)^{-1} = \begin{pmatrix} \frac{1}{\alpha_1} & 0 & \frac{-1}{2\alpha_1} \\ 0 & \frac{1}{\alpha_1} & \frac{-1}{2\alpha_1} \\ 0 & 0 & 0 \end{pmatrix}$$

Hence

$$trace\, C_1 C(\alpha)^{-1} = \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + 0 = \frac{2}{\alpha_1} \text{ and } traceI = 3.$$

Thus

$trace\, C_1 C(\alpha)^{-1} = traceI$, implies that

$$\alpha_1 = \frac{2}{3}.$$

Also from equations (4.3) and (4.21), we have

$$C_2C(\alpha)^{-1} = \begin{pmatrix} 0 & 0 & \frac{1}{2\alpha_2} \\ 0 & 0 & \frac{1}{2\alpha_2} \\ 0 & 0 & \frac{1}{\alpha_2} \end{pmatrix}.$$

Now

$$traceC_2C(\alpha)^{-1} = \frac{1}{\alpha_2}.$$

Thus

$traceC_2C(\alpha)^{-1} = traceI$, implies that

$$\alpha_2 = \frac{1}{3}.$$

Thus for m=2 ingredients we have $\alpha_1 = \frac{2}{3}$ and $\alpha_2 = \frac{1}{3}$ as provided in the theorem.

From Pukelsheim (1993), the determinant criterion is obtained as

$v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{s}}$, where, $s = \begin{pmatrix} m+1 \\ 2 \end{pmatrix}$.

For $m = 2$, we have $v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{3}}$.

From theorem (4.6), the information matrix for the design with two factors is

$$C(\alpha) = C_K(M(\eta(\alpha))) = \begin{bmatrix} \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{4} \end{bmatrix}.$$

Substituting for the values of $\alpha_1 = \frac{2}{3}$ and $\alpha_2 = \frac{1}{3}$ we get

$$C(\alpha) = \begin{pmatrix} \frac{17}{48} & \frac{1}{48} & \frac{1}{24} \\ \frac{1}{48} & \frac{17}{48} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{24} & \frac{1}{12} \end{pmatrix}$$

$$Det[C(\alpha)] = \frac{1}{108}.$$

Hence the optimal value becomes $v(\phi_0) = \left(\det[C(\alpha)]\right)^{\frac{1}{3}} = \left(\frac{1}{108}\right)^{\frac{1}{3}} = 0.20998684$.

4.4.2 D-optimal design for $m = 3$ ingredients

Theorem 4.13

In the second-degree Kronecker model for mixture experiments with three ingredients, the unique D-optimal design for $K'\theta$ is

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{1}{2}\eta_1 + \frac{1}{2}\eta_2.$$

The maximum of the D-criterion for m=3 factors is $v(\phi_0) = \left(\frac{1}{2^{12}}\right)^{\frac{1}{6}} = 0.25$.

Proof

From theorem (4.6), we have then $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if

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

Putting $p = 0$, we have that $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if

$$traceC_j C(\alpha)^{-1} = traceC(\alpha)^0 = traceI \qquad for \quad all \qquad j \in \{1,2\}.$$

The inverse of the matrix $C(\alpha)$ is given in equation (4.25).

From equations (4.6) and (4.25), we have;

$$C_1C(\alpha)^{-1}=\begin{pmatrix} \frac{1}{\alpha_1} & 0 & 0 & \frac{-1}{6\alpha_1} & \frac{-1}{6\alpha_1} & 0 \\ 0 & \frac{1}{\alpha_1} & 0 & \frac{-1}{6\alpha_1} & 0 & \frac{-1}{6\alpha_1} \\ 0 & 0 & \frac{1}{\alpha_1} & 0 & \frac{-1}{6\alpha_1} & \frac{-1}{6\alpha_1} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Hence

$$traceC_1C(\alpha)^{-1}=\frac{1}{\alpha_1}+\frac{1}{\alpha_1}+\frac{1}{\alpha_1}+0=\frac{3}{\alpha_1} \text{ and } trace(I)=6.$$

Thus

$traceC_1C(\alpha)^{-1}=trace(I)$, implies that

$$\alpha_1=\frac{1}{2}.$$

Also for equations (4.7) and (4.25), we have

$$C_2C(\alpha)^{-1}=\begin{pmatrix} 0 & 0 & 0 & \frac{1}{6\alpha_2} & \frac{1}{6\alpha_2} & 0 \\ 0 & 0 & 0 & \frac{1}{6\alpha_2} & 0 & \frac{1}{6\alpha_2} \\ 0 & 0 & 0 & 0 & \frac{1}{6\alpha_2} & \frac{1}{6\alpha_2} \\ 0 & 0 & 0 & \frac{1}{\alpha_2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} \end{pmatrix}.$$

Now

$$traceC_2C(\alpha)^{-1} = \frac{3}{\alpha_2}.$$

Thus $traceC_2C(\alpha)^{-1} = traceI$, implies that

$$\alpha_2 = \frac{1}{2}.$$

Thus for m=3 ingredients we have $\alpha_1 = \frac{1}{2}$ and $\alpha_2 = \frac{1}{2}$ as provided in the theorem.

From Pukelsheim (1993), the determinant criterion is obtained as

$v(\phi_0) = (\det C(\alpha))^{\frac{1}{s}}$, where, $s = \binom{m+1}{2}$.

For $m = 3$, we have $v(\phi_0) = (\det C(\alpha))^{\frac{1}{6}}$.

From theorem (4.3), the information matrix for the design with three factors is

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 \\ 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{4} \end{pmatrix}.$$

Substituting for the values of $\alpha_1 = \frac{1}{2}$ and $\alpha_2 = \frac{1}{2}$ we get

$$C(\alpha)=\begin{pmatrix} \frac{9}{48} & \frac{1}{96} & \frac{1}{96} & \frac{1}{16} & \frac{1}{16} & 0 \\ \frac{1}{96} & \frac{9}{48} & \frac{1}{96} & \frac{1}{16} & 0 & \frac{1}{16} \\ \frac{1}{96} & \frac{1}{96} & \frac{9}{48} & 0 & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & 0 & \frac{3}{8} & 0 & 0 \\ \frac{1}{16} & 0 & \frac{1}{16} & 0 & \frac{3}{8} & 0 \\ 0 & \frac{1}{16} & \frac{1}{16} & 0 & 0 & \frac{3}{8} \end{pmatrix}$$

$$Det[C(\alpha)]=\frac{1}{2^{12}}.$$

Hence the optimal value becomes, $v(\phi_0)=\left(\det[C(\alpha)]\right)^{\frac{1}{6}}=\left(\frac{1}{2^{12}}\right)^{\frac{1}{6}}=0.25$.

4.4.3 D-optimal design for $m=4$ ingredients

Theorem 4.14

In the second-degree Kronecker model for mixture experiments with four ingredients, the unique D-optimal design for $K'\theta$ is

$$\eta(\alpha^{(D)})=\alpha_1\eta_1+\alpha_2\eta_2=\frac{2}{5}\eta_1+\frac{3}{5}\eta_2.$$

The maximum of the D-criterion for m=4 factors is $v(\phi_0)=\left(\frac{9^6}{10^{10}}\right)^{\frac{1}{10}}=0.373719282$.

Proof

From theorem (4.6), we have then $\eta(\alpha)$ is $\phi_0-optimal$ for $K'\theta$ in T if and only if

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

Putting $p = 0$, we have that $\eta(\alpha)$ is $\phi_0 - optimal$ for $K'\theta$ in T if and only if

$$traceC_j C(\alpha)^{-1} = traceC(\alpha)^0 = traceI \quad for\ all\ \ j \in \{1,2\}$$

The inverse of the matrix $C(\alpha)$ is given in equation (4.29).

From equations (4.10) and (4.29), we have;

$$C_1 C(\alpha)^{-1} = \begin{pmatrix} \frac{1}{\alpha_1} & 0 & 0 & 0 & \frac{-1}{12\alpha_1} & \frac{-1}{12\alpha_1} & \frac{-1}{12\alpha_1} & 0 & 0 & 0 \\ 0 & \frac{1}{\alpha_1} & 0 & 0 & \frac{-1}{12\alpha_1} & 0 & 0 & \frac{-1}{12\alpha_1} & \frac{-1}{12\alpha_1} & 0 \\ 0 & 0 & \frac{1}{\alpha_1} & 0 & 0 & \frac{-1}{12\alpha_1} & 0 & \frac{-1}{12\alpha_1} & 0 & \frac{-1}{12\alpha_1} \\ 0 & 0 & 0 & \frac{1}{\alpha_1} & 0 & 0 & \frac{-1}{12\alpha_1} & 0 & \frac{-1}{12\alpha_1} & \frac{-1}{12\alpha_1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Hence

$traceC_1 C(\alpha)^{-1} = \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + \frac{1}{\alpha_1} + 0 = \frac{4}{\alpha_1}$ and $trace(I) = 10$.

Thus

$traceC_1 C(\alpha)^{-1} = trace(I)$, implies that

$\alpha_1 = \frac{2}{5}$.

Also for equations (4.11) and (4.29), we have

$$C_2C(\alpha)^{-1} = \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{12\alpha_2} & \frac{1}{12\alpha_2} & \frac{1}{12\alpha_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{12\alpha_2} & 0 & 0 & \frac{1}{12\alpha_2} & \frac{1}{12\alpha_2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{12\alpha_2} & 0 & \frac{1}{12\alpha_2} & 0 & \frac{1}{12\alpha_2} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{12\alpha_2} & 0 & \frac{1}{12\alpha_2} & \frac{1}{12\alpha_2} \\ 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\alpha_2} \end{pmatrix}.$$

Now

$$trace C_2C(\alpha)^{-1} = 0 + 6\left(\frac{1}{\alpha_2}\right) = \frac{6}{\alpha_2}.$$

Thus

$trace C_2C(\alpha)^{-1} = trace I$, implies that

$$\alpha_2 = \frac{3}{5}.$$

Thus for m=4 ingredients we have $\alpha_1 = \frac{2}{5}$ and $\alpha_2 = \frac{3}{5}$ as provided in the theorem.

From Pukelsheim (1993), the determinant criterion is obtained as

$v(\phi_0) = \left(\det C(\alpha)\right)^{\frac{1}{s}}$, where $s = \binom{m+1}{2}$.

For $m = 4$, we have $v(\phi_0) = \left(\det C(\alpha)\right)^{\frac{1}{10}}$.

From theorem (4.5), the information matrix for the design with four factors is

$$C(\alpha) = \begin{pmatrix}
\frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 \\
\frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\
\frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\
\frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\
\frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 & 0 \\
\frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 \\
\frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha}{2} & 0 & 0 & 0 \\
0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 \\
0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 \\
0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2}
\end{pmatrix}$$

.

Substituting for the values of $\alpha_1 = \frac{2}{5}$ and $\alpha_2 = \frac{3}{5}$ we get

$$C(\alpha) = \begin{pmatrix} \frac{19}{160} & \frac{1}{160} & \frac{1}{160} & \frac{1}{160} & \frac{3}{40} & \frac{3}{40} & \frac{3}{40} & 0 & 0 & 0 \\ \frac{1}{160} & \frac{19}{160} & \frac{1}{160} & \frac{1}{160} & \frac{3}{40} & 0 & 0 & \frac{3}{40} & \frac{3}{40} & 0 \\ \frac{1}{160} & \frac{1}{160} & \frac{19}{160} & \frac{1}{160} & 0 & \frac{3}{40} & 0 & \frac{3}{40} & 0 & \frac{3}{40} \\ \frac{1}{160} & \frac{1}{160} & \frac{1}{160} & \frac{19}{160} & 0 & 0 & \frac{3}{40} & 0 & \frac{3}{40} & \frac{3}{40} \\ \frac{3}{40} & \frac{3}{40} & 0 & 0 & \frac{9}{10} & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{40} & 0 & \frac{3}{40} & 0 & 0 & \frac{9}{10} & 0 & 0 & 0 & 0 \\ \frac{3}{40} & 0 & 0 & \frac{3}{40} & 0 & 0 & \frac{9}{10} & 0 & 0 & 0 \\ 0 & \frac{3}{40} & \frac{3}{40} & 0 & 0 & 0 & 0 & \frac{9}{10} & 0 & 0 \\ 0 & \frac{3}{40} & 0 & \frac{3}{40} & 0 & 0 & 0 & 0 & \frac{9}{10} & 0 \\ 0 & 0 & \frac{3}{40} & \frac{3}{40} & 0 & 0 & 0 & 0 & 0 & \frac{9}{10} \end{pmatrix}$$

$$Det[C(\alpha)] = \frac{9^6}{10^{10}}.$$

Hence the optimal value becomes, $v(\phi_0) = (\det C(\alpha))^{\frac{1}{10}} = \left(\frac{9^6}{10^{10}}\right)^{\frac{1}{10}} = 0.373719282$.

4.4.4 D-optimal design for $m \geq 2$ ingredients

We now derive the general expressions giving the optimality candidates in (0,1) and the optimal value for the D-criterion.

Theorem 4.15

In the second order Kronecker model for mixture experiments with $m \geq 2$ ingredients, the unique D-optimal design for $K'\theta$ is

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{2}{m+1}\eta_1 + \frac{m-1}{m+1}\eta_2 .$$

The maximum of the D-criterion for m factors is

$$v(\phi_0) = \left\{ \left[\frac{m(m-1)^2}{8(m+1)} \right]^{\binom{m}{2}} \left[\frac{2}{m(m+1)} \right]^m \right\}^{\frac{2}{m(m+1)}} .$$

Proof

From theorem (4.7), the proposed optimal design is unique. We start by first deriving the optimality candidate.

Let $\alpha = (\alpha_1, \alpha_2, 0, ..., 0)' \in T_m$ be a weight vector with $\partial(\alpha) = \{1,2\}$ and suppose $\eta(\alpha)$ is D-optimal for $K'\theta$ in T. Let $C(\alpha) = C_k(M(\eta(\alpha)))$.

Theorem (4.6) implies that

$$trace(C_j C^{-1}) \begin{cases} = trace(C(\alpha)^0) & for \;\; j \in \{1,2\} \\ < trace(C(\alpha)^0) & otherwise \end{cases}$$

after substituting for p=0.

From lemma (3.1), any matrix $C \in sym(s, H)$ can be uniquely represented in the form

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

With coefficients; $a, ..., g \in \Re$. The terms containing V_2 , W_2 and W_3 only occur for $m \geq 3$ or $m \geq 4$, respectively.

In the proof of lemma (3.1), any given symmetric matrix $C \in sym(s)$, can be partitioned according to the block structure of matrices in H , that is

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

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

For $j = 1$, we have

$$traceC_1C(\alpha)^{-1} = traceC(\alpha)^0 = trace(I)$$

Now from equations (4.15) and (4.33), we obtain

$$C_1C(\alpha)^{-1} = \begin{pmatrix} \frac{1}{\alpha_1} I_m & \frac{-1}{m(m-1)\alpha_1} V_1' \\ 0 & 0 \end{pmatrix}$$

Hence, $trace(C_1C(\alpha)^{-1}) = trace\left(\frac{1}{\alpha_1} I_m\right) = \frac{m}{\alpha_1}$, since $trace(I_m) = m$.

Also for m factors, $trace(I_s) = \frac{m(m+1)}{2}$, where $s = \binom{m+1}{2}$.

Thus $traceC_1C(\alpha)^{-1} = traceC(\alpha)^0 = trace(I)$, implies that

$$\frac{m}{\alpha_1} = \frac{m(m+1)}{2}.$$

From this we get $\alpha_1 = \frac{2}{m+1}$.

Similarly, from equations (4.16) and (4.33), we obtain

$$C_2C(\alpha)^{-1} = \begin{pmatrix} 0 & \frac{1}{m(m-1)\alpha_1} V_1' \\ 0 & \frac{1}{\alpha_2} I_{\binom{m}{2}} \end{pmatrix}.$$

Hence

$$trace(C_2C(\alpha)^{-1}) = trace\left(\frac{1}{\alpha_2} I_{\binom{m}{2}}\right) = \frac{m(m-1)}{2\alpha_2}.$$

Thus, $traceC_2C(\alpha)^{-1} = traceC(\alpha)^0 = trace(I)$, implies that

$\frac{m(m-1)}{2\alpha_2} = \frac{m(m+1)}{2}$. This gives, $\alpha_2 = \frac{m-1}{m+1}$.

Thus for m factors, we have the unique solution in (0, 1) as the weight vector given in the theorem when $\alpha_1 = \frac{2}{m+1}$ and $\alpha_2 = \frac{m-1}{m+1}$.

Secondly, we verify the D-optimality.

From equation (4.17), the information matrix for a design with m factors is given as

$$C(\alpha) = \begin{pmatrix} \frac{8\alpha_1 + \alpha_2}{8m} I_m + \frac{\alpha_2}{8m(m-1)} U_2 & \frac{\alpha_2}{8} V_1' \\ \frac{\alpha_2}{8} V_1 & \frac{m(m-1)\alpha_2}{8} I_{\binom{m}{2}} \end{pmatrix}.$$

Substituting the values of $\alpha_1 = \frac{2}{m+1}$ and $\alpha_2 = \frac{m-1}{m+1}$, we get

$$C(\alpha) = \begin{pmatrix} \frac{m+15}{8m(m+1)} I_m + \frac{1}{8m(m+1)} U_2 & \frac{m-1}{8(m+1)} V_1' \\ \frac{m-1}{8(m+1)} V_1 & \frac{m(m-1)^2}{8(m+1)} I_{\binom{m}{2}} \end{pmatrix}.$$

Now

$$\det(C(\alpha)) = \left[\frac{m(m-1)^2}{8(m+1)}\right]^{\binom{m}{2}} \left[\frac{2}{m(m+1)}\right]^m.$$

From Pukelsheim (1993), the determinant criterion is obtained as

$v(\phi_0) = (\det C(\alpha))^{\frac{1}{s}}$, where, $s = \binom{m+1}{2}$.

Hence the optimal value becomes

$$v(\phi_0) = \left(\det(C(\alpha))\right)^{\frac{2}{m(m+1)}} = \left\{ \left[\frac{m(m-1)^2}{8(m+1)} \right]^{\binom{m}{2}} \left[\frac{2}{m(m+1)} \right]^{m} \right\}^{\frac{2}{m(m+1)}} \blacksquare$$

4.5 E-Optimal Weighted Centroid Design

This section contains the derivation and calculation of optimal weighted centroid designs for the smallest eigenvalue criterion, $\phi_{-\infty}$, that is, E-optimality criteria. We need to adopt two theorems in Pukelsheim (1993), which specifically focuses on E-optimality.

Theorem 4.16

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

Theorem 4.17

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, ($\partial(\alpha) = \{ j = 1,\ldots,m : \alpha_j > 0\}$).

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

$\tilde{C}K = \lambda_{\min}(C)E$ ▪

The following theorem dictates on the choice of the matrix E of theorem (4.17) above.

Theorem 4.18

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 (4.17) 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 (4.17) for $\phi_{-\infty} - optimality$ coincides with that of theorem (4.16) for scalar optimality. With $E = \frac{zz'}{\|z\|^2}$, the normality inequality of theorem (4.17) 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 (4.16) is

$$c'G'AGc \le c'M^{-}c \quad \text{for all } A \in M$$

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

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

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-ctriterion, we need to obtain smallest eigenvalue and its corresponding eigenvector, of the information matrix for the weighted centroid design. We proceed as follows:

From equation (3.4), the information matrices involved in our designs can be uniquely partitioned as

$$C = \begin{pmatrix} C_{11} & C'_{21} \\ C_{21} & C_{22} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.35)$$

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

$$\chi_c(\lambda) = \det(C - \lambda I_s) = \det(C_{11} - \lambda I_s)\det[(C_{22} - \lambda W_1) - C_{21}(C_{11} - \lambda U_1)^{-1}C'_{21}] \ldots\ldots (4.36)$$

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 $span\{W_1 \quad W_2 \quad W_3\}$ (as shown in corollary (2.1)).

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

Lemma 4.2

Let $a,\cdots,g \in \Re$ be the coefficients of the matrix $C \in sym(s,H)$, as given in lemma(3.1) with d, f and g occurring only when $m \geq 3$ or $m \geq 4$ respectively.

Furthermore, define

$$D_1 = \left[a + (m-1)b - e - 2(m-2)f - \binom{m-2}{2} g \right]^2 + 2(m-1)\left[2c + (m-2)d\right]^2 \quad \text{……….} (4.37)$$

$$D_2 = \left[a - b - e - (m-4)f + (m-1)g\right]^2 + 4(m-2)(c-d)^2 \quad \text{…………………………} (4.38)$$

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

$$\lambda_1 = e - 2f + g, \quad \text{……………………………………………………………………} (4.39)$$

$$\lambda_{2,3} = \frac{1}{2}\left[a + (m-1)b + e + 2(m-3)f + \binom{m-2}{2} g \pm \sqrt{D_1} \right] \text{ and } \quad \text{……………………} (4.40)$$

$$\lambda_{4,5} = \frac{1}{2}\left[a - b + e + (m-4)f - (m-3)g \pm \sqrt{D_2}\right] \quad \text{……………………………………} (4.41)$$

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 poof of this lemma is provided by Klein (2004).

4.5.1 E-optimal design for $m = 2$ ingredients

Theorem 4.19

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

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.45454545\eta_1 + 0.54545454\eta_2$$

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

We begin by observing that the proposed optimal design is unique in view of theorem (4.7). From theorem (4.6), we obtained the information matrix

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{4} \end{pmatrix} \qquad (4.42)$$

From equation (3.3) 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 (3.1), 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 (4.37) can be written as

$$C=\begin{pmatrix} aI_m+bU_2 & cV_1' \\ cV_1 & eW_1 \end{pmatrix}=\begin{bmatrix} a\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}+b\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & c\begin{pmatrix}1\\ 1\end{pmatrix} \\ c(1 \quad 1) & e(1) \end{bmatrix}=\begin{pmatrix} a & b & c \\ b & a & c \\ c & c & e \end{pmatrix} \quad \ldots\ldots\ldots\ldots (4.43)$$

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 (4.2), 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 (4.43) and equation (4.40) in lemma (4.2), 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 (4.43) and equation (4.41) in lemma (4.2), 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 (4.18), 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

$$\lambda_{\min} = \lambda_3 = \frac{1}{16}\left[\alpha_1 + 3 - \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right]. \qquad (4.44)$$

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

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

where $\vec{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$, is an eigenvector of C corresponding to λ.

Thus, from equation (4.43) and equation (4.44), we have

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

$$\begin{pmatrix} \frac{6\alpha_1 - 2 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{6\alpha_1 - 2 + \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{1 - 5\alpha_1 + \sqrt{33\alpha_1^2 - 26\alpha_1}}{16} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

If we let

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

$$\begin{pmatrix} p & q & 2q \\ q & p & 2q \\ 2q & 2q & r \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

we obtain the equations

$$py_1 + qy_2 + 2qy_3 = 0$$

$$qy_1 + py_2 + 2qy_3 = 0$$

$$2qy_1 + 2qy_2 + ry_3 = 0$$

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

$$\vec{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \frac{-4q}{r} \end{pmatrix}$$

Then the matrix

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

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{2r^2+16q^2} & \frac{r^2}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} \\ \frac{r^2}{2r^2+16q^2} & \frac{r^2}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} \\ \frac{-4qr}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} & \frac{16q^2}{2r^2+16q^2} \end{pmatrix} \quad \text{……………………...……(4.45)}$$

from equation (4.2) and equation (4.45), we have

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

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

Now

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

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

This simplifies to

$$33\alpha_1^4 - 92\alpha_1^3 + 90\alpha_1^2 - 36\alpha_1 + 5 = 0, \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.46)}$$

upon substituting the values of q and r.

The roots of polynomial (4.46) are

$$\alpha_1 = 1, 1, 0.45454545 \, and \, 0.33333333$$

Since, $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.45454545$ or $\alpha_1 = 0.33333333$.

When, $\alpha_1 = 0.45454545$, $\alpha_2 = 1 - \alpha_1 = 0.54545454$ and

$$\lambda_{\min} = \frac{1}{16}\left[\alpha_1 + 3 - \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right] = 0.09090909$$

When, $\alpha_1 = 0.33333333$, $\alpha_2 = 1 - \alpha_1 = 0.66666667$ and

$$\lambda_{\min} = \frac{1}{16}\left[\alpha_1 + 3 - \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right] = 0.08333333$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = \frac{5}{11}$ and $\alpha_2 = \frac{6}{11}$.

Thus for m=2, ingredients we have, $\alpha_1 = 0.45454545$ and $\alpha_2 = 0.54545454$.

From Pukelsheim (1993), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.44), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{16}\left[\alpha_1 + 3 - \sqrt{33\alpha_1^2 - 26\alpha_1 + 9}\right] = 0.09090909$$

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

$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.09090909$ ▪

4.5.2 E-optimal design for $m = 3$ ingredients

Lemma 4.3

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

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.66666679\eta_1 + 0.33333321\eta_2$$

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

The maximum of the E-criterion for m=3 ingredients is $v(\phi_{-\infty}) = 0.16666667$.

The information matrix for second-degree Kronecker model with m=3 ingredients, $C_k(M(\eta(\alpha)))$ 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; $a = \frac{8\alpha_1 + \alpha_2}{24}$, $b = \frac{\alpha_2}{48}$, $c = \frac{\alpha_2}{8}$, $d = 0$, $e = \frac{3\alpha_2}{4}$ and $f = 0$

with the matrices; U_1, U_2, V_1, V_2, W_1, W_2 and W_3 defined as in lemma (3.1).

Proof

In theorem (4.3), we have obtained the information matrix $C_k(M(\eta(\alpha)))$ for a mixture experiment design $\eta(\alpha)$ with m=3 ingredients as

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{3\alpha_2}{4} & 0 \\ 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{4} \end{pmatrix}$$

From equation (3.3), 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 $a,...,g \in \Re$. The terms containing V_2, W_2 and W_3 occurring 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 (3.1), 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 $E_{23} = (0 \quad 0 \quad 1)'$.

Thus

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

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

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

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

$$\left|\{i, j\} \cap \{k, l\}\right| = 1$$

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

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

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

$$= \begin{pmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ c & c & d & e & f & f \\ c & d & c & f & e & f \\ d & c & c & f & f & e \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.47)}$$

where; $a = \dfrac{8\alpha_1 + \alpha_2}{24}$, $b = \dfrac{\alpha_2}{48}$, $c = \dfrac{\alpha_2}{8}$, $d = 0$, $e = \dfrac{3\alpha_2}{4}$ and $f = 0$.

Theorem 4.20

In the second-degree Kronecker model with m=3 factors, there is a weighted centroid design, $\eta(\alpha)$ with $\partial(\alpha) \subseteq \{1,2\}$ which is E-optimal for $K'\theta$ in T.

Proof

From lemma (4.2), we compute the eigenvalues of the above matrix as follows

$$D_1 = [a + 2b - e]^2 + 4[2c - d]^2 = \frac{720\alpha_1^2 - 1056\alpha_1 + 400}{576} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.48)}$$

$$D_2 = [a-b-e]^2 + 4(c-d)^2 = \frac{2745\alpha_1^2 - 3558\alpha_1 + 1369}{2304} \qquad (4.49)$$

Using equation (4.47) and equation (4.37) in lemma (4.2), we obtain for m=3

$$\lambda_{2,3} = \frac{1}{2}\left[a+2b+e \pm \sqrt{D_1}\right] = \frac{1}{48}\left[-12\alpha_1 + 20 \pm \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right]$$

Similarly, using equation (4.47) and equation (4.49) in lemma (4.2) we get

$$\lambda_{4,5} = \frac{1}{2}\left[a-b+e \pm \sqrt{D_2}\right] = \frac{1}{96}\left[-21\alpha_1 + 37 \pm \sqrt{2745\alpha_1^2 - 3558\alpha_1 + 1369}\right]$$

From lemma (4.2) the eigenvalues that $\lambda_2, \lambda_3, \lambda_4$ *and* λ_5 occur for the case m=3. These are

$\lambda_2 = \frac{1}{48}\left[-12\alpha_1 + 20 + \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right]$, with multiplicity 1,

$\lambda_3 = \frac{1}{48}\left[-12\alpha_1 + 20 - \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right]$, with multiplicity 1,

$\lambda_4 = \frac{1}{96}\left[-21\alpha_1 + 37 + \sqrt{2745\alpha_1^2 - 3558\alpha_1 + 1369}\right]$, with multiplicity 2 and

$\lambda_5 = \frac{1}{96}\left[-21\alpha_1 + 37 - \sqrt{2745\alpha_1^2 - 3558\alpha_1 + 1369}\right]$, with multiplicity 2.

From theorem (4.17), 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

$$\lambda_{\min} = \lambda_3 = \frac{1}{48}\left[-12\alpha_1 + 20 - \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right] \qquad (4.50)$$

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, $\vec{z}=\begin{pmatrix} y_1 & y_2 & y_3 & y_4 & y_5 & y_6 \end{pmatrix}'$, is an eigenvector of C corresponding to λ.

Thus, from equation (4.47) and equation (4.50)

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

$$\begin{pmatrix} p & q & q & 6q & 6q & 0 \\ q & p & q & 6q & 0 & 6q \\ q & q & p & 0 & 6q & 6q \\ 6q & 6q & o & r & 0 & 0 \\ 6q & 0 & 6q & 0 & r & 0 \\ 0 & 6q & 6q & 0 & 0 & r \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

where, $p=26\alpha_1-18+\sqrt{720\alpha_1^2-1056\alpha_1+400}$, $q=\alpha_2=1-\alpha_1$ and

$r=-24\alpha_1+16+\sqrt{720\alpha_1^2-1056\alpha_1+400}$

$py_1+qy_2+qy_3+6qy_4+6qy_5=0$

$qy_1+py_2+qy_3+6qy_4+qy_6=0$

$qy_1+qy_2+py_3+6qy_5+6qy_6=0$

$6qy_1+6qy_2+ry_4=0$

$6qy_1+6qy_3+ry_5=0$

$6qy_2+6qy_3+ry_6=0$

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

$$\vec{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \frac{-12q}{r} \\ \frac{-12q}{r} \\ \frac{-12q}{r} \end{pmatrix} \quad \text{(4.51)}$$

Then the matrix

$$zz' = \begin{pmatrix} 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ 1 & 1 & 1 & \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \\ \frac{-12q}{r} & \frac{-12q}{r} & \frac{-12q}{r} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} & \frac{144q^2}{r^2} \end{pmatrix} \text{and} \|z\|^2 = \frac{3r^2 + 432q^2}{r^2}$$

Thus the matrix E is given as;

$$E=\frac{zz'}{\|z\|^2}=\begin{pmatrix} \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} \\ \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} \\ \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{r^2}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} \\ \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} \\ \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} \\ \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{-12qr}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} & \frac{144q^2}{3r^2+432q^2} \end{pmatrix}$$

.... (4.52)

From equation (4.6)

$$C_1=\begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$ and equation (4.52), we have

$$C_1E=\begin{pmatrix} a & a & a & b & b & b \\ a & a & a & b & b & b \\ a & a & a & b & b & b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$ .... (4.53)

Where $a=\frac{r^2}{3(3r^2+432q^2)}$ $b=\frac{-12qr}{3(3r^2+432q^2)}$

Thus $traceC_1E=3a=3\left[\frac{r^2}{3(3r^2+432q^2)}\right]$

Now

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

$$\frac{r^2}{3r^2 + 432q^2} = \frac{1}{48}\left[-12\alpha_1 + 20 - \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4.54)$$

This simplifies to

$$\begin{aligned} &-2149908480\alpha_1^6 + 117528833020\alpha_1^5 - 26658865150\alpha_1^4 + 32105299970\alpha_1^3 \\ &-21642412040\alpha_1^2 + 7739670532\alpha_1 - 1146617856 = 0 \end{aligned} \quad \ldots. (4.55)$$

Upon substituting the values of q and r.

The roots of polynomial (4.55) are $\alpha_1 = 0.79999697 and 0.66666679$

Since, $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.79999697$ or $\alpha_1 = 0.66666679$.

When, $\alpha_1 = 0.79999697$, $\alpha_2 = 1 - \alpha_1 = 0.20000303$ and

$$\lambda_{\min} = \frac{1}{48}\left[-12\alpha_1 + 20 - \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right] = 0.133334848$$

When, $\alpha_1 = 0.66666679$, $\alpha_2 = 1 - \alpha_1 = 0.33333321$ and

$$\lambda_{\min} = \frac{1}{48}\left[-12\alpha_1 + 20 - \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right] = 0.16666667$$

We observe that $\lambda_{\min}$ is maximum when $\alpha_1 = 0.66666679$ and $\alpha_2 = 0.33333321$.

Thus for m=3, ingredients we have, $\alpha_1 = 0.66666679$ and $\alpha_2 = 0.33333321$.

From Pukelsheim (1993), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.50), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{48}\left[-12\alpha_1 + 20 - \sqrt{720\alpha_1^2 - 1056\alpha_1 + 400}\right] = 0.16666667$$

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

$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.16666667$ ▪

4.5.3 E-optimal design for design $m = 4$ ingredients

Lemma 4.4

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

$$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = ,0.81818901\eta_1 + 0.18181099\eta_2$$

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

The maximum of the E-criterion for m=4 ingredients is $v(\phi_{-\infty}) = 0.18181818$.

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

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

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

where; $a = \dfrac{8\alpha_1 + \alpha_2}{32}$, $b = \dfrac{\alpha_2}{96}$, $c = \dfrac{\alpha_2}{8}$, and $d = 0$ $e = \dfrac{3\alpha_2}{2}$ $f = 0$ $g = 0$

with the matrices; U_1, U_2, V_1, V_2, W_1, $W_2$and W_3defined as in lemma (3.1).

Information matrix $C_k(M(\eta(\alpha)))$ equation (4.12) for a mixture experiment design $\eta(\alpha)$ with m=4 ingredients as

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 \\ \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{8} & 0 & 0 & \frac{\alpha_2}{8} & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 & 0 \\ 0 & \frac{\alpha_2}{8} & 0 & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} & 0 \\ 0 & 0 & \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & 0 & 0 & 0 & 0 & 0 & \frac{3\alpha_2}{2} \end{pmatrix}$$

…………………………………………………………………………………… (4.56)

From equation (3.3), 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 $a,\dots,g \in \Re$. 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 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 (3.1), 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

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

Where; $a = \dfrac{8\alpha_1 + \alpha_2}{32}$, $b = \dfrac{\alpha_2}{96}$, $c = \dfrac{\alpha_2}{8}$, and $d = 0$ $e = \dfrac{3\alpha_2}{2}$ $f = 0$ $g = 0$

From lemma (3.1), we compute the eigenvalues of the above matrix as follows

$$D_1 = [a + 3b - e - 4f - g]^2 + 6[2c - 2d]^2$$

$$= \left[\frac{8\alpha_1 + \alpha_2}{32} + \frac{\alpha_2}{32} - \frac{3\alpha_2}{2}\right]^2 + 6\left[\frac{\alpha_2}{4}\right]^2 = \frac{825\alpha_1^2 - 1434\alpha_1 + 625}{256} \quad \text{.........................} \quad (4.57)$$

$$D_2 = [a - b - e + g]^2 + 8(c-d)^2 = \left[\frac{8\alpha_1 + \alpha_2}{32} - \frac{\alpha_2}{96} - \frac{3\alpha_2}{2}\right]^2 + 8\left[\frac{\alpha_2}{8}\right]^2 \quad \text{................} \quad (4.58)$$

$$= \frac{7177\alpha_1^2 - 12362\alpha_1 + 5329}{2304}$$

From lemma (4.2), for m=4,

$$\lambda_1 = e - 2f + g = \frac{3\alpha_2}{2} - 0 + 0 = \frac{3\alpha_2}{2} = \frac{3 - 3\alpha_1}{2}$$

Using equation (4.57) and equation (4.40) in lemma (4.2), we obtain for m=4

$$\lambda_{2,3} = \frac{1}{2}\left[a + 3b + e + 4f + g \pm \sqrt{D_1}\right] = \frac{1}{32}\left[-21\alpha_1 + 25 \pm \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right]$$

Similarly, using equation (4.58) and equation (4.41) in lemma (4.2) we get

$$\lambda_{4,5} = \frac{1}{2}\left[a - b + e - g \pm \sqrt{D_2}\right] = \frac{1}{96}\left[-61\alpha_1 + 73 \pm \sqrt{7177\alpha_1^2 - 12362\alpha_1 + 5329}\right]$$

From lemma (4.2) the eigenvalues $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ *and* λ_5 occur for the case m=4. These are

$\lambda_1 = e - 2f + g = \frac{3\alpha_2}{2} = \frac{3 - 3\alpha_1}{2}$, with multiplicity 2,

$\lambda_2 = \frac{1}{32}\left[-21\alpha_1 + 25 + \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right]$, with multiplicity 1,

$\lambda_3 = \frac{1}{32}\left[-21\alpha_1 + 25 - \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right]$, with multiplicity 1,

$\lambda_4 = \frac{1}{96}\left[-61\alpha_1 + 73 + \sqrt{7177\alpha_1^2 - 12362\alpha_1 + 5329}\right]$, with multiplicity 3 and

$\lambda_5 = \frac{1}{96}\left[-61\alpha_1 + 73 - \sqrt{7177\alpha_1^2 - 12362\alpha_1 + 5329}\right]$, with multiplicity 3

From theorem (4.18), 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

$$\lambda_{\min} = \frac{1}{32}\left[-21\alpha_1 + 25 - \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right], \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4.59)$$

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, $\vec{z} = \begin{pmatrix} y_1 & y_2 & y_3 & y_4 & y_5 & y_6 & y_7 & y_8 & y_9 & y_{10} \end{pmatrix}'$,

is an eigenvector of C corresponding to λ.

Thus, from equation (4.56) and equation (4.59)

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

$$\begin{pmatrix} 3p & q & q & q & 12q & 12q & 12q & 0 & 0 & 0 \\ q & 3p & q & q & 12q & 0 & 0 & 12q & 12q & 0 \\ q & q & 3p & q & 0 & 12q & 0 & 12q & 0 & 12q \\ q & q & q & 3p & o & o & 12q & 0 & 12q & 12q \\ 12q & 12q & 0 & 0 & 3r & 0 & 0 & 0 & 0 & 0 \\ 12q & 0 & 12q & 0 & 0 & 3r & 0 & 0 & 0 & 0 \\ 12q & 0 & 0 & 12q & 0 & 0 & 3r & 0 & 0 & 0 \\ 0 & 12q & 12q & 0 & 0 & 0 & 0 & 3r & 0 & 0 \\ 0 & 12q & 0 & 12q & 0 & 0 & 0 & 0 & 3r & 0 \\ 0 & 0 & 12q & 12q & 0 & 0 & 0 & 0 & 0 & 3r \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

where

$p = \frac{1}{32}\left[28\alpha_1 - 24 + \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right]$, $q = \alpha_2 = 1 - \alpha_1$ and

$r = \frac{1}{32}\left[-27\alpha_1 + 23 + \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right]$.

$$3py_1 + qy_2 + qy_3 + qy_4 + 12qy_5 + 12qy_6 + 12qy_7 = 0$$

$$qy_1 + 3py_2 + qy_3 + qy_4 + 12qy_5 + 12qy_8 + 12qy_9 = 0$$

$$qy_1 + qy_2 + 3py_3 + qy_4 + 12qy_6 + 12qy_8 + 12qy_{10} = 0$$

$$qy_1 + qy_2 + qy_3 + 3py_4 + 12qy_7 + 12qy_9 + 12qy_{10} = 0$$

$$12qy_1 + 12qy_2 + 3ry_5 = 0$$

$$12qy_1 + 12qy_3 + 3ry_6 = 0$$

$$12qy_1 + 12qy_4 + 3ry_7 = 0$$

$$12qy_2 + 12qy_3 + 3ry_8 = 0$$

$$12qy_2 + 12qy_4 + 3ry_9 = 0$$

$$12qy_3 + 12qy_4 + 3ry_{10} = 0$$

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

$$\vec{z} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \end{pmatrix}$$

Then the matrix

$$zz' = \begin{pmatrix} 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \end{pmatrix} \quad \ldots\ldots (4.60)$$

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

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \\ b & b & b & b & c & c & c & c & c & c \end{pmatrix}$$

where a= $\dfrac{r^2}{4r^2 + 384q^2}$, b= $\dfrac{-8qr}{4r^2 + 384q^2}$, c= $\dfrac{64q^2}{4r^2 + 384q^2}$ …..…………………… (4.61)

From equation (4.10)

$$C_1 = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$ and equation (4.61), we have

$$\begin{pmatrix} a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ a & a & a & a & b & b & b & b & b & b \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \ldots\ldots\ldots\ldots (4.62)$$

Where $a = \frac{r^2}{4(4r^2 + 384q^2)}$ and $b = \frac{-8qr}{4(4r^2 + 384q^2)}$

Thus $traceC_1E = 4a = 4\left[\frac{r^2}{4(4r^2 + 384q^2)}\right]$

Now

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

$$\frac{r^2}{4r^2 + 384q^2} = \frac{1}{32}\left[-21\alpha_1 + 25 - \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right]$$

This simplifies to

$$-1946419200\alpha_1^6 + 11168907260\alpha_1^5 - 26676559870\alpha_1^4 + 33945550850\alpha_1^3$$
$$- 24270077960\alpha_1^2 + 9243721732\alpha_1 - 1465122816 = 0 \quad \text{...... (4.63)}$$

Upon substituting the values of q and r.

The roots of polynomial (4.63) are $\alpha_1 = 0.91966779 and 0.81818901$

Since, $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.91966779$ or $\alpha_1 = 0.81818901$.

When, $\alpha_1 = 0.91966779$, $\alpha_2 = 1 - \alpha_1 = 0.08033221$ and

$$\lambda_{\min} = \frac{1}{32}\left[-21\alpha_1 + 25 - \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right] = 0.115435693$$

When, $\alpha_1 = 0.81818901$, $\alpha_2 = 1 - \alpha_1 = 0.18181099$ and

$$\lambda_{\min} = \frac{1}{32}\left[-21\alpha_1 + 25 - \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right] = 0.18181818$$

We observe that $\lambda_{\min}$ is maximum When $\alpha_1 = 0.81818901$, $\alpha_2 = 1 - \alpha_1 = 0.18181099$.

Thus for m=4 ingredients we have, $\alpha_1 = 0.81818901$ and $\alpha_2 = 0.18181099$

From Pukelsheim (1993), the smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$.

From equation (4.59), the smallest eigenvalue is

$$\lambda_{\min} = \frac{1}{32}\left[-21\alpha_1 + 25 - \sqrt{825\alpha_1^2 - 1434\alpha_1 + 625}\right] = 0.18181818$$

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

$v(\phi_{-\infty}) = \lambda_{\min}(C) = 0.18181818$ ▪

4.5.4 E-optimal design for $m \geq 2$ ingredients

Theorem 4.21

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.

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

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{16m}\left[\left(-m^3 + m^2 + 6\right)\alpha_1 + m^3 - m^2 + 2 \pm \sqrt{D}\right]$$

Where

$$D = \left(m^6 - 2m^5 + m^4 + 20m^3 - 20m^2 + 36\right)\alpha_1{}^2 - \left(2m^6 - 4m^5 + 2m^4 + 24m^3 - 24m^2 - 24\right)\alpha_1 + \left(m^6 - 2m^5 + m^4 + 4m^3 - 4m^2 + 4\right)$$

Proof

From equation (3.3) 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 caseof 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 $\mathrm{a, b, c, d} \in \Re$, Form lemma (3.2) we get

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

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

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

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

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

$$= \begin{pmatrix} \dfrac{8\alpha_1 + \alpha_2}{8m} U_1 + \dfrac{\alpha_2}{8m(m-1)} U_2 & \dfrac{\alpha_2}{8} V \\ \dfrac{\alpha_2}{8} V' & \dfrac{m(m-1)\alpha_2}{8} \dfrac{V'V}{m} \end{pmatrix} \quad \text{............ (4.64)}$$

From lemma (4.2) for m ingredients we have

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

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

$$= \frac{\left(m^6-2m^5+m^4+20m^3-20m^2+36\right)\alpha_1^{\ 2} - \left(2m^6-4m^5+2m^4+24m^3-24m^2-24\right)\alpha_1 + \left(m^6-2m^5+m^4+4m^3-4m^2+4\right)}{64m^2}$$

The eigenvalues are;

$$\lambda_{2,3} = \frac{1}{2}\left[a+(m-1)b+c\pm\sqrt{D_1}\right] = \frac{1}{2}\left[\frac{8\alpha_1+\alpha_2}{8m} + \frac{(m-1)\alpha_2}{8m(m-1)} + \frac{m(m-1)\alpha_2}{8} \pm\sqrt{D_1}\right]$$

$$= \frac{1}{16m}\left[\left(-m^3+m^2+6\right)\alpha_1 + m^3 - m^2 + 2 \pm\sqrt{D}\right]$$

Where

$$D = \left(m^6-2m^5+m^4+20m^3-20m^2+36\right)\alpha_1^{\ 2} - \left(2m^6-4m^5+2m^4+24m^3-24m^2-24\right)\alpha_1$$
$$+\left(m^6-2m^5+m^4+4m^3-4m^2+4\right)$$

with multiplicity 1

Hence the smallest eigenvalue is $\lambda_3 = \frac{1}{16m}\left[\left(-m^3+m^2+6\right)\alpha_1 + m^3 - m^2 + 2 \pm\sqrt{D}\right]$

Now let $\lambda_{\min} = \frac{1}{16m}\left[\left(-m^3+m^2+6\right)\alpha_1 + m^3 - m^2 + 2 \pm\sqrt{D}\right]$ 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

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

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

Let $p_1 = m^3\alpha_1 - m^2\alpha_1 + \alpha_1 - m^3 + m^2 - 1 + \sqrt{D}$,

$q_1 = \alpha_2$, $r_1 = -6\alpha_1 - 2 + \sqrt{D}$

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

$$\frac{1}{8m} \begin{pmatrix} (p_1 U_1 + \frac{q_1}{m-1} U_2 & m q_1 V \\ m q_1 V' & r_1 \frac{V'V}{m} \end{pmatrix} \qquad \ldots\ldots (4.65)$$

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

$$E = \frac{\bar{z}\bar{z}'}{\|z\|^2} = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} U_1 + U_2 & -cmqV \\ \frac{cmq}{r}V' & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix} \qquad \text{(4.66)}$$

And from equation (4.15) and equation (4.66)

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

From theorem (4.17) a weighted centroid design $\eta(\alpha)$ is E-optimal for $K'\theta$ in T if and only if t $traceC_jE = \lambda_{\min}(C)$.

For j=1

$$traceC_1E = \frac{r^2}{m(mr^2 + c^2m^2q^2)} + ... + .\frac{r^2}{m(mr^2 + c^2m^2q^2)} = \frac{r^2}{(mr^2 + c^2m^2q^2)}$$

Hence

$$traceC_j E = \lambda_{\min}(C) \Leftrightarrow \frac{r^2}{(mr^2 + c^2 m^2 q^2)} = \frac{1}{16m}\left[\left(-m^3 + m^2 + 6\right)\alpha_1 + m^3 - m^2 + 2 \pm \sqrt{D}\right]$$

Putting $q = \alpha_2$, $r_1 = -6\alpha_1 - 2 + \sqrt{D}$ and

$$D = \left(m^6 - 2m^5 + m^4 + 20m^3 - 20m^2 + 36\right)\alpha_1{}^2 - \left(2m^6 - 4m^5 + 2m^4 + 24m^3 - 24m^2 - 24\right)\alpha_1 + \left(m^6 - 2m^5 + m^4 + 4m^3 - 4m^2 + 4\right)$$

Then solving the polynomial using Matlab, the value of α_1 is chosen such that $\alpha_1 \in (0,1)$; substitute this values to $\lambda_{\min}$ and take the values that miximizes the $\lambda_{\min}$, hence the optimal E-criterion is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{16m}\left[\left(-m^3 + m^2 + 6\right)\alpha_1 + m^3 - m^2 + 2 \pm \sqrt{D}\right]$$

4.6 Numerical example

The following is a numerical example using Response (% Dead Insect) Data from applications of 4 chemical compounds in a mixture experiment. The assumption is that a researcher wishes to examine 4 chemical compounds (X1, X2, X3, and X4) for their effectiveness (independently or in combinations) for insect control. The % dead insect is determined as a response to these chemicals in this numerical example (Bondari, K., 2005).

Table 4.4: Numerical example

Run	Blend	Type	X1	X2	X3	X4	Resp
			Components				
1	Pure	Vertex	1	0	0	0	4.6
2	Pure	Vertex	0	1	0	0	51.8
3	Pure	Vertex	0	0	1	0	58.2
4	Pure	Vertex	0	0	0	1	78.0
5	Binary	Edge Centroid	0	0	0.5	0.5	10.8
6	Binary	Edge Centroid	0	0.5	0	0.5	7.2
7	Binary	Edge Centroid	0	0.5	0.5	0	58.4
8	Binary	Edge Centroid	0.5	0	0	0.5	7.8
9	Binary	Edge Centroid	0.5	0	0.5	0	75.8
10	Binary	Edge Centroid	0.5	0.5	0	0	22.4
11	Ternary	Face Centroid	0	1/3	1/3	1/3	45.0
12	Ternary	Face Centroid	1/3	0	1/3	1/3	6.2
13	Ternary	Face Centroid	1/3	1/3	0	1/3	5.8
14	Ternary	Face Centroid	1/3	1/3	1/3	0	23.2
15	All	Overall Centroid	1/4	1/4	1/4	1/4	2.6

4.6.1 Application of A-optimal Weighted Centroid Design

Consider the simplex centroid design for four ingredients in the above design. The A-optimal design for four factors can now be applied to four factor numerical example. In this study only pure blends and binary blends are considered.

From A-optimal for four ingridients, we have;

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

Implying that, the unique A-optimal weighted centroid design for $K'\theta$ in m=4 ingredients is $\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.668953748\eta_1 + 0.331046251\eta_2$.

Therefore the corresponding A-optimal for the above design is as follows.

Table 4.5: Application of A-optimal Weighted Centroid Design

Run	Blend	Type	X1	X2	X3	X4
			Components			
1	Pure	Vertex	0.668953748	0	0	0
2	Pure	Vertex	0	0.668953748	0	0
3	Pure	Vertex	0	0	0.668953748	0
4	Pure	Vertex	0	0	0	0.668953748
5	Binary	Edge Centroid	0	0	0.165523125	0.165523125
6	Binary	Edge Centroid	0	0.165523125	0	0.165523125
7	Binary	Edge Centroid	0	0.165523125	0.165523125	0
8	Binary	Edge Centroid	0.165523125	0	0	0.165523125
9	Binary	Edge Centroid	0.165523125	0	0.165523125	0
10	Binary	Edge Centroid	0.165523125	0.165523125	0	0

4.6.2 Application of D-optimal Weighted Centroid Design

The unique D-optimal weighted centroid design for $K'\theta$ in m=4 ingredients is

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.4\eta_1 + 0.6\eta_2 \ .$$

Therefore the corresponding D-optimal Design for the above experiment is as follows.

Table 4.6: Application of D-optimal Weighted Centroid Design

Run	Blend	Type	X1	X2	X3	X4
			Components			
1	Pure	Vertex	0.4	0	0	0
2	Pure	Vertex	0	0.4	0	0
3	Pure	Vertex	0	0	0.4	0
4	Pure	Vertex	0	0	0	0.4
5	Binary	Edge Centroid	0	0	0.3	0.3
6	Binary	Edge Centroid	0	0.3	0	0.3
7	Binary	Edge Centroid	0	0.3	0.3	0
8	Binary	Edge Centroid	0.3	0	0	0.3
9	Binary	Edge Centroid	0.3	0	0.3	0
10	Binary	Edge Centroid	0.3	0.3	0	0

4.6.3 Application of E-optimal Weighted Centroid Design

The unique E-optimal weighted centroid design for $K'\theta$ in m=4 ingredients is

$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = ,0.81818901\eta_1 + 0.18181099\eta_2$.

Therefore the corresponding E-optimal Design for the above experiment is as follows.

Table 4.7: Application of E-optimal Weighted Centroid Design

			Components			
Run	Blend	Type	X1	X2	X3	X4
1	Pure	Vertex	0.81818901	0	0	0
2	Pure	Vertex	0	0.81818901	0	0
3	Pure	Vertex	0	0	0.81818901	0
4	Pure	Vertex	0	0	0	0.81818901
5	Binary	Edge Centroid	0	0	0.090905495	0.090905495
6	Binary	Edge Centroid	0	0.090905495	0	0.090905495
7	Binary	Edge Centroid	0	0.090905495	0.090905495	0
8	Binary	Edge Centroid	0.090905495	0	0	0.090905495
9	Binary	Edge Centroid	0.090905495	0	0.090905495	0
10	Binary	Edge Centroid	0.090905495	0.090905495	0	0

The above numerical example illustration demonstrates the applicability of the weighted values of the designs in this study. It is clearly seen that the number of runs is reduced and only pure and binary blend are considered in this case. Thus this cut on the cost which is always the goal of every experimentor.

CHAPTER FIVE

CONCLUSION AND RECOMMENDATIONS

5.1 Conclusion

Investigations were done based on the selected optimality criteria and each design was subjected to the Kiefer-Wolfowitz equivalence Theorem. The optimal moment and information matrices were obtained based on the choice of the coefficient matrix $K'\theta$ of interest. It was found that for second-degree model with $m \geq 2$ ingredients the unique D-, A- and E- optimal weighted centroid designs for $K'\theta$, exist for the choice of the coefficient matrix specifically in this study.

The study indicates that for the average-variance criterion (A- criterion), as the number of ingredients m increase, $\alpha_1^{(p)}$ increases while $\alpha_2^{(p)}$ decreases. The value of the maximum criterion increases. For the determinant criterion (D-criterion), as the number of ingredients m increase, $\alpha_1^{(p)}$ decreases while $\alpha_2^{(p)}$ increases. The value of the maximum criterion also increases. Also for the smallest eigenvalue criterion (E-criterion), as the number of ingredients m increase, $\alpha_1^{(p)}$ increases while $\alpha_2^{(p)}$ decreases. The value of the maximum criterion increases.

In summary, the optimal values obtained have been found to be larger than those obtained in the previous studies. These large values indicate that the information matrices of these designs carry large information. Thus the model is more informative. This is always the goal of every experimenter and it is the main result of this study.

Table 4.8: $\phi_p - optimal$ **weights for** $K'\theta$**,** $m = 2,3,4$

m	p	$\alpha_1^{(p)}$	$\alpha_2^{(p)}$	v_p
2	$-\infty$	0.45454545	0.54545455	0.09090909
	-1	0.52786405	0.47213595	0.16718427
	0	0.66666667	0.33333333	0.20998684
3	$-\infty$	0.66666667	0.33333332	0.16666667
	-1	0.60647018	0.39352982	0.23229856
	0	0.50000000	0.50000000	0.25000000
4	$-\infty$	0.81818901	0.18181099	0.18181818
	-1	0.66895375	0.33104625	0.27397905
	0	0.40000000	0.60000000	0.373719282

5.1 Recommendations

The regression function considered in this study is the Kronecker square, $f(t) = t \otimes t$.

Since the computation of the matrices with unknows is done by hand, it would therefore be very interesting to develop a programm that can compute the optimal values.

The hypothetical example clearly indicates that the designs in this study meet the goal of every experimenter since the cost of the experiment is reduced. Considering the simplex centroid design for four ingredients in the above designs, the number of runs is reduced. Therefore it can be clearly seen that the design in the study is practically applicable, hence it is recommented that such design can be used in mixture experiments to cut on cost.

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