E-Optimal Designs For Maximal Parameter Subsystem Second-Degree Kronecker Model Mixture Experiments

Koech Eliud[1*], Koech Milton[1], Koske Joseph[2], Kerich Gregory[2], Argwings Otieno[1],
1. Department of Mathematics and Computer Science,
University of Eldoret, P.o Box 1125, Eldoret, (Kenya)
E-mail: elkoech4@gmail.com
2. Department of Mathematics and Computer Science,
Moi University, P.o Box 3900, Eldoret (Kenya),
E-mail:josephkoske@yahoo.com

ABSTRACT
Many products are formed by mixing together two or more ingredients, for example, in building construction; concrete is formed by mixing sand, water and cement. Many practical problems are associated with investigation of mixture of m ingredients which are assumed to influence the response through the proportions in which they are blended together. Second degree Kronecker model put forward by Draper and Pukelsheim is applied in the study. This study investigates E-optimal designs, second degree Kronecker model, maximal parameter subsystem for two, three and four ingredients, where Kiefer's function serves as optimality criteria. The consideration was restricted to weighted centroid design for completeness results. By employing the Kronecker model approach, coefficient matrices and a set of feasible weighted centroid designs for maximal parameters subsystem is obtained. Once the coefficient matrix is developed, information matrices associated to the parameter subsystem of interest for two, three, and four is then obtained. E-optimal weighted centroid designs based on maximal parameter subsystem for the corresponding two, three, four ingredients is derived. Also optimal weights and values for the weighted centroid designs were numerically obtained using Matlab software. Results based on maximal parameter subsystem, second degree mixture model with two, three and four ingredient for E-optimal weighted centroid design for information matrix ($K'\theta$) therefore exist.

Keywords: Mixture experiments, Kronecker product, Moment matrices, Weighted Centroid Designs, Information matrices.

1.0 Introduction

There are many problems that deal with investigation of mixtures of m factors or ingredients which they influence the response through the ratios or proportions which are mixed together. The response is a measurable quality or property of interest on the product. In this study 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;

- To determine whether some combination of the factors can be considered best in some sense.
- To gain a better understanding of the overall system by studying the roles played by the different ingredients.

Cornel (1990) lists numerous examples of applications of mixture experiments and provides a thorough discussion of both theory and practice. Early work done by Scheffe' (1958, 1963) suggested and analyzed canonical model forms when the regression function for the expected response is a polynomial of degree one, two or three.

The mixture ingredients are such that $t_1, t_2, ..., t_m$, where $t_i \geq 0$ and further restricted by $\sum_{i=1}^{m} = 1$. Creation of controlled conditions is the main characteristic feature of experimentation. Thus the experimental domain is the probability simplex $T_m = \left\{ t = (t_1,..,t_m)' \in [0,1]^n : \sum_{i=1}^{m} = 1 \right\}$ under experimental condition $t \in T_m$, where the response Y_t is taken to be a real valued random variable. In a polynomial regression model the expected value $E(Y_t)$ is a polynomial function of t.

Draper and Pukelsheim (1998) suggested the second degree Kronecker model as;

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

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

The Kronecker representation has several advantages, this include; a more compact notations, more convenient invariance properties, and the homogeneity of the regression terms Draper and Pukelsheim (1998) and Prescott, et al (2002). The moment matrix $M(\tau) = \int_{\mathrm{T}} f(t) f(t)' d\tau$ for the second-degree Kronecker-model has all entries homogeneous in degree four and reflects the statistical properties of a design τ. Graffke and Heilingers (1996) and Pukelsheim (1993) gave a review of the general design environment. Klein (2004) showed that the class of weighted centroid designs is essentially complete for m≥2 ingredients for Kiefer ordering. As a consequence, the search for optimal designs may be restricted to weighted centroid designs for most criteria. Kinyanjui (2007) and Ngigi (2009) showed that second degree mixture experiments for maximal parameter subsystem with m≥2 ingredients, unique D-and A-optimal weighted centroid designs for *K'θ* exist. In the same study E-optimal weighted centroid design mixture experiment with two ingredients only was derived. This study extends the work by deriving E-optimal weighted centroid designs for three and four ingredients.

2.0 Design problem

The main design problem here is to obtain a design with maximum information for the maximal parameter subsystem $K'\theta$, subject to the side's conditions. The maximum is accomplished through the application of E-optimality criteria of weighted centroid design which follows the Kiefer-Wolfowitz equivalence theorem.

More often, the primary concern of the experimenter is to learn more about the subsystems of interest. This situation, therefor, allows the designer to evaluate the performance of a design relative to the subsystems of interest only. The parameter system of the mixture experiments contains a lot of repeated terms making it rank deficient hence not all the parameters can be estimated efficiently. The parameter subsystem with $\binom{m+1}{2}$ parameters has been shown to have properties similar to those of the full parameter system.

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 **(2)**

(ii) $rank\, K = r_M$. **(3)**

In this case, we have $r_M = \binom{m+1}{2}$ and K is called a maximal coefficient matrix for M. In this study we define the matrix $K = (K_1, K_2) \in \Re^{m^2 \times \binom{m+1}{2}}$ under maximal parameter subsystem. The coefficient matrix $K \in \Re^{k \times \binom{m+1}{2}}$ is assumed to have full column rank. Where;

$K_2 = \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E'_{ij}$ and $K_1 = \sum_{i=1}^{m} e_{ii} e'_i$

3.0 E-Optimal Weighted Centroid Design

We now derive optimal weighted centroid designs for the smallest eigenvalue criterion, $\phi_{-\infty}$, that is, E-optimality criteria. To forge our way forward, we adopt two theorems in Pukelsheim (1993), which specifically focuses on E-optimality.

(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 $traceE = 1$

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, which is the information matrix.

(ii) Suppose $\eta(\alpha)$ is E-optimal for $K'\theta$ in T and E is a matrix satisfying the optimality condition for $\eta(\alpha)$ given in (i), furthermore, let $\eta(\beta)$ be a weighted centroid 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 information matrices involved in our designs can be uniquely partitioned as follows, Klein (2004).

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

For $\lambda \in \Re$, let

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

Furthermore,

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

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

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

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

$$\lambda_{2,3} = \frac{1}{2}\left[a + (m-1)b + e + 2(m-3)f + \binom{m-2}{2} g \pm \sqrt{D_1} \right] \qquad \textbf{(4)}$$

and

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

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>2 there are four eigenvalues $\lambda_2, \lambda_3, \lambda_4$ *and* λ_5.

4.0 E-optimal weighted centroid design for Maximal parameter subsystem

The derivation of weighted centroid designs for two, three and four ingredients respectively is illustrated below. An information matrix from Kinyanjui (2007) is used in the three derivations of the weighted centroid designs.

4.0.1 E-optimal weighted centroid design for two ingredient

The information matrix $C_k(M(\eta(\alpha)))$ is given as;

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \end{pmatrix} \qquad \textbf{(6)}$$

Any matrix $C \in sym(s, H)$, Klein (2004) can uniquely be represented in the form

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

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

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

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

We then compute the eigenvalues of the above matrix as follows;

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

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

using equation (4), we obtain

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

again, using equation (5) 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;

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

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

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

From Pukelsheim (1993), if the smallest eigenvalue for $C_k(M(\eta(\alpha)))$ 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 $C_k(M(\eta(\alpha)))$. In our case m=2, the smallest eigenvalue is;

$$\lambda_{\min} C = \lambda_3 = \frac{1}{32}\left[(5\alpha_1 + 3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] \quad \textbf{(7)}$$

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

Thus, from equation (6) and equation (7), we have

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

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

If we let

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

We obtain the equations

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

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

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

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

$$\vec{z} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \frac{-4q}{r} \end{pmatrix} \tag{8}$$

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;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{2r^2+16q^2} & \frac{r^2}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} \\ \frac{r^2}{2r^2+16q^2} & \frac{r^2}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} \\ \frac{-4qr}{2r^2+16q^2} & \frac{-4qr}{2r^2+16q^2} & \frac{16q^2}{2r^2+16q^2} \end{pmatrix} \tag{9}$$

From Kinyanjui (2007) we have C_1 as;

$$C_1 = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$, multiplying with equation (9), we obtain C_1E as;

$$C_1E = \begin{pmatrix} \frac{r^2}{2(2r^2+16q^2)} & \frac{r^2}{2(2r^2+16q^2)} & \frac{-4qr}{2(2r^2+16q^2)} \\ \frac{r^2}{2(2r^2+16q^2)} & \frac{r^2}{2(2r^2+16q^2)} & \frac{-4qr}{2(2r^2+16q^2)} \\ 0 & 0 & 0 \end{pmatrix} \quad \textbf{(10)}$$

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

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

$$\frac{r^2}{2r^2+16q^2} = \frac{1}{32}\left[(5\alpha_1+3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] \quad \textbf{(11)}$$

Substituting the values of q and r, this simplifies to;

$$-39914624\alpha_1^6 - 373568\alpha_1^5 - 283059600\alpha_1^4 + 121760\alpha_1^3 - 11152\alpha_1^2 - 26048\alpha_1 + 7168 = 0 \quad \textbf{(12)}$$

The root of polynomial (12) is 0.0662 since it satisfy $\alpha_1 \in (0,1)$, then it implies that $\alpha_1 = 0.0661$ and $\alpha_2 = 1 - \alpha_1 = 0.9339$. The smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$, Pukelsheim (1993), hence substituting the value of $\alpha_1 = 0.0661$ in equation (7), we get the smallest eigenvalue as;

$$\lambda_{\min} = \frac{1}{32}\left[(5\alpha_1+3) - \sqrt{57\alpha_1^2 - 2\alpha_1 + 9}\right] = 0.026314645 \quad \textbf{(13)}$$

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

$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.0662\eta_1 + 0.9338\eta_2$ is E-optimal for $K'\theta$ in T and the maximum value for E-criterion is $v(\phi_{-\infty}) = 0.026314645$.

4.0.2 E-optimal weighted centroid design for three ingredients

The information matrix, $C_k(M(\eta(\alpha)))$, for three ingredients is given as;

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & 0 \\ \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 \\ 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{48} \end{pmatrix} \quad \textbf{(14)}$$

Any matrix $C \in sym(s, H)$ Klein (2004) can uniquely be represented as;

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

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

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

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

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

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

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

Using equation (4), we obtain $\lambda_{2,3}$ for m=3

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

(15)

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

Similarly, using equation (7) we get

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

$$= \frac{1}{48}\left[(7\alpha_1 + 1) \pm \sqrt{65\alpha_1^2 - 2\alpha_1 + 1}\right] \quad \textbf{(16)}$$

From Pukelsheim (1993) eigenvalues $\lambda_2, \lambda_3, \lambda_4$ *and* λ_5 occur for the case m=3. These are

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

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

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

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

From Pukelsheim (1993), if the smallest eigenvector for $C_k(M(\eta(\alpha)))$ 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 $C_k(M(\eta(\alpha)))$. In our case for m=3, the smallest eigenvalue is;

$$\lambda_3 = \frac{1}{96}\left[(11\alpha_1 + 5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right] \qquad \textbf{(17)}$$

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

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, $(\vec{z} = u \quad v \quad w \quad x \quad y \quad z)$, is an eigenvector of C corresponding to λ. Thus, from equation (14) and equation (17), $(C - \lambda_{\min} I)\vec{z} = \vec{0}$, implies that;

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

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

We obtain the equations as;

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

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

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

$$2qu + 2qw + ry = 0$$

$$2qv + 2qw + rz = 0$$

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

$$\vec{z} = \begin{pmatrix} u \\ v \\ w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \frac{-4q}{r} \\ \frac{-4q}{r} \\ \frac{-4q}{r} \end{pmatrix} \quad \textbf{(18)}$$

Then the matrix

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

Thus the matrix E is given as;

$$E = \frac{zz'}{\|z\|^2} = \begin{pmatrix} \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{r^2}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} \\ \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} \\ \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} & \frac{16q^2}{3r^2+48q^2} \end{pmatrix} \quad \textbf{(19)}$$

From Kinyanjui (2007) we obtain matrix C_1 as;

$$C_1 = \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$, multiplying with equation (19), we have

$$C_1E = \begin{pmatrix} \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{r^2}{3(3r^2+12q^2)} & \frac{r^2}{3(3r^2+12q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{r^2}{3(3r^2+48q^2)} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} & \frac{-4qr}{3r^2+48q^2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \textbf{(20)}$$

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

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

$$\frac{r^2}{3r^2+48q^2} = \frac{1}{96}\left[(11\alpha_1+5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right] \quad \textbf{(21)}$$

Substituting the values of q and r .This simplifies to

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

(22)

The root of polynomial (22) is 0.1012 hence $\alpha_1 = 0.1012$.

Then it implies that when, $\alpha_1 = 0.1012$, $\alpha_2 = 1 - \alpha_1 = 0.8988$.

Again in Pukelsheim (1993), the smallest eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$. Hence from equation (17), the smallest eigenvalue is,

$$\lambda_{\min} = \frac{1}{96}\left[(11\alpha_1+5) - \sqrt{185\alpha_1^2 - 46\alpha_1 + 25}\right] = 0.01455548 \quad \textbf{(23)}$$

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

$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.1012\eta_1 + 0.8988\eta_2$ is E-optimal for $K'\theta$ in T and the maximum value for E-criterion when m=3 ingredients is $v(\phi_{-\infty}) = 0.01455548$.

4.0.3 E-optimal weighted centroid design for four ingredients

The Information matrix $C_k(M(\eta(\alpha)))$, when m=4 ingredients is given as;

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & 0 \\ \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{48} & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{96} & 0 & 0 \\ 0 & \frac{\alpha_2}{48} & 0 & \frac{\alpha_2}{48} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{96} & 0 \\ 0 & 0 & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha_2}{96} \end{pmatrix} \quad \textbf{(24)}$$

Any matrix $C \in sym(s, H)$, Klein (2004) can be represented as:

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix}$$ with coefficients $a, \ldots, g \in \Re$.

The terms containing V_2, W_2 and W_3 occur for $m \geq 3$ or $m \geq 4$ respectively.

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

From Pukelsheim (1993) we compute the eigenvalues of the above matrix as follows

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

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

Using equation (4) we obtain

$$\lambda_{2,3} = \frac{1}{2}\left[a + 3b + e \pm \sqrt{D_1}\right] = \frac{1}{2}\left[\frac{8\alpha_1 + \alpha_2}{32} + 3\left[\frac{\alpha_2}{96}\right] + \left[\frac{\alpha_2}{96}\right] \pm \sqrt{\frac{385\alpha_1^2 + 142\alpha_1 + 49}{96^2}}\right] \quad \textbf{(25)}$$

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

Similarly, using equation (5) we get

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

$$=\frac{1}{96}\left[21\alpha_1+3\pm\sqrt{561\alpha_1^2-156\alpha_1+36}\right],\ \text{with multiplicity 2} \qquad \textbf{(26)}$$

The smallest eigenvalue is;

$$\lambda_{2,3}=\frac{1}{192}\left[17\alpha_1+7\pm\sqrt{385\alpha_1^2-142\alpha_1+49}\right] \qquad \textbf{(27)}$$

The eigenvalues, $\lambda_2, \lambda_3, \lambda_4$ *and* λ_5 occur for the case m=4. These are

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

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

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

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

If the smallest eigenvector of $C_k(M)$ has multiplicity 1, Pukelsheim (1993), then the only choice for the matrix E is, $E=\frac{zz'}{\|z\|^2}$, where $z\in\Re^s$ is an eigenvector corresponding to the smallest eigenvalue of the information matrix $C_k(M)$. In our case, the smallest eigenvalue is;

$$\lambda_{\min}=\frac{1}{192}\left[17\alpha_1+7-\sqrt{385\alpha_1^2+142\alpha_1+49}\right], \qquad \textbf{(28)}$$

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

Thus, from equation (24) and equation (28) we have $(C-\lambda_{\min}I)\vec{z}=\vec{0}$,

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

where, $p = 25\alpha_1 + 13 + \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}$, $q = \alpha_2 = 1 - \alpha_1$ and $r = 19\alpha_1 - 5 + \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}$

we obtain the equations as;

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

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

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

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

$$4qg + 4qh + ru = 0$$

$$4qg + 4qs + rv = 0$$

$$4qg + 4qt + rw = 0$$

$$4qh + 4qs + rx = 0$$

$$4qh + 4qt + ry = 0$$

$$4qs + 4qt + rz = 0$$

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

$$\vec{z} = \begin{pmatrix} g \\ h \\ s \\ t \\ u \\ v \\ w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \\ \frac{-8q}{r} \end{pmatrix} \tag{29}$$

Then the matrix zz' is;

$$zz' = \begin{pmatrix} 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ 1 & 1 & 1 & 1 & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \\ \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{-8q}{r} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} & \frac{64q^2}{r^2} \end{pmatrix} \tag{30}$$

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

Thus the matrix E is given as;

$$E=\frac{zz'}{\|z\|^2}=\begin{pmatrix}
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} \\
\frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2} & \frac{64q^2}{4r^2+384q^2}
\end{pmatrix} \quad \textbf{(31)}$$

From Kinyanjui (2007), we have C_1 as;

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

Multiplying C_1 with equation (31), we obtain;

$$\begin{pmatrix} \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\ \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\ \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\ \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{r^2}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} & \frac{-8qr}{4r^2+384q^2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \textbf{(32)}$$

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

Now $traceC_1E = \lambda_{\min}(C)$,we have;

$$\frac{r^2}{4r^2+384q^2} = \frac{1}{192}\left[17\alpha_1 + 7 - \sqrt{385\alpha_1^2 - 142\alpha_1 + 49}\right] \quad \textbf{(33)}$$

Substituting the values of q and r , this simplifies to;

$$-5512679936\alpha_1^6 - 30324736\alpha_1^5 - 2271901952\alpha_1^4 + 2900480\alpha_1^3 + 10876672\alpha_1^2 - 4265984\alpha_1 + 897024 = 0 \quad \textbf{(34)}$$

The root of polynomial (34) is $\alpha_1 = 0.1231$ since, $\alpha_1 \in (0,1)$, then $\alpha_2 = 1 - \alpha_1 = 0.8769$.

The smallest-eigenvalue criterion $v(\phi_{-\infty}) = \lambda_{\min}(C)$, Pukelsheim (1993), hence from equation (28), the smallest eigenvalue is;

$$\lambda_{\min} = \frac{1}{192}\left[17\alpha_1 + 7 - \sqrt{385\alpha_1^2 + 142\alpha_1 + 49}\right] = 0.015525588 \quad \textbf{(35)}$$

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

$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.1231\eta_1 + 0.8769\eta_2$, is E-optimal for $K'\theta$ in T.

The maximum value for E-criterion when m=4 ingredients is $v(\phi_{-\infty}) = 0.015525588$.

Results and conclusion

E-optimal weighted centroid designs for maximal parameter subsystem for the corresponding two, three and four ingredients is derived. Optimal weights and values for the corresponding weighted centroid designs were numerically obtained using Matlab software. In conclusion results based on maximal parameter subsystem, second degree Kronecker mixture model with two, three and four ingredient, E-optimal weighted centroid design for $K'\theta$ (information matrix) therefore exist for the specific design points.

Recommendation

In line with the study it could be interesting to see practical results for the implementation of the designs suggested in this study.

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