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A- Optimal Slope Design for Second Degree Kronecker Model Mixture Experiment With Four Ingredients With Application in Selected Fruits Blending

Ngigi Peter Kung'u[1], J. K. Arap Koske[2], Josphat K. Kinyanjui[1]

[1] Department of mathematics, statistics and actuarial science, Karatina University, Karatina, Kenya

[2] Department of mathematics & computer science, Moi University, Eldoret, Kenya

Correspondence: Ngigi Peter Kung'u, Department of mathematics, statistics and actuarial science, Karatina University, Karatina, Kenya

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Abstract

This study presents an investigation of an optimal slope design in the second degree Kronecker model for mixture experiments in four dimensions and its application in blending of selected fruits to prepare punch. The study centers around weighted centroid designs, with the second degree Kronecker model. This is guided by the fact that the class of weighted centroid designs is a complete class in the Kiefer Ordering. To overcome the problem of estimability, a concise coefficient matrix is defined that aid in selecting a maximal parameter subsystem for the Kronecker model. The information matrix of the design is obtained using a linear function of the moment matrices for the centroids and directly linked to the slope matrix. The discussion is based on Kronecker product algebra which clearly reflects the symmetries of the simplex experimental region. From the family of matrix means, a well-defined function is used to determine optimal values of the efficient developed design. Finally, a demonstration is provided for the case where the design is applied in fruit blending.

Keywords: information matrix, Kiefer ordering, moment matrix, optimal design, response surface methodology, slope, weighted centroid design

1. Introduction

This study explores the response surface with the intent of obtaining the optimal response. The response of interest is considered as a function of a set of independent factors. In this response surface methodology (RSM) problem we assume a response of interest is influenced by four factors with the intent of optimizing (obtaining maximal value of) this response. The response in linked to the factors through a second degree polynomial model.

In this mixture experiment the response is a function of the proportions of each ingredient. Let x_i represent the proportion of the ith ingredient in the mixture. Then, factors involved are subject to two conditions, $x_i \geq 0,\ i=1, 2, 3, 4$ and $\sum_{i=1}^{4} x_i = 1$. The second constraint clearly shows that the levels of the four factors are interdependent. It is therefore easy to write a regression model without an intercept. The experimental region for this mixture problem is a three dimensional simplex.

2. Materials and Methods

Let $1_m=(1, \ldots, 1)' \in \Re^m$ be a unity vector. The experimental conditions $t=(t_1, t_2, \ldots, t_m)$ with $t_i \geq 0$ of a mixture experiment are points in the probability simplex,

$$T_m = \{t = (t_1, \quad t_2, \quad \ldots, \quad t_m)' \in [0, \quad 1]^m : 1_m' t = 1\}.$$

Under experimental conditions, $t \in T_m$, the response Y_t is taken to be a quantitative random variable. The responses are assumed to be uncorrelated with equal but unknown finite variance say $\sigma^2 \in (0, \infty)$. The design considered in this study has fifteen support points.

This study adopts Kronecker's second degree polynomial regression function with the expected response:

$$E(Y_t) = \sum_{i=1}^{m} \theta_{ii} t_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{m} (\theta_{ij} + \theta_{ji}) t_i t_j \quad (1)$$

where Y_t , is the response under experimental condition $t \in T_m$, and $\theta = (\theta_{11}, \ \theta_{12}, \ ..., \ \theta_{mm}) \in \Re^{m^2}$ an unknown parameter. (Draper, N. R. and Pukelsheim, F., 1998)

(Pukelsheim, 1993), gives a general review of the design environment. (Klein, 2004) and (Draper, N. R., Heiligers, B. and Pukelsheim, F., 2000), showed that the class of weighted centroid designs is a complete class for the Kiefer ordering.

2.1 General Design Problem

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

$$\text{Maximize } \varphi_p(C_k(M(\tau))) \text{ with } \tau \in T \quad (2)$$

$$\text{Subject to } C_k(M(\tau)) \in PD(s), \ \tau \in T$$

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, (Pukelsheim, 1993). In which case, the design τ is called feasible for $K'\theta$. Any design solving problem (2) above for a fixed p∈ (-∞, 1] is said to be $\phi_p - optimal$ for $K'\theta$ in T. For all p∈ (-∞, 1], (Pukelsheim, 1993) shows that $\phi_p - optimal$ design for $K'\theta$ exists.

2.2 Moment Matrix

An experimental design τ is a probability measure on the experimental domain with a finite number of support points. Each support point $s \in \sup p(\tau)$ directs the experimenter to take a proportion T({t}) of all observations under experimental condition T. The statistical properties of a design are reflected by its moment matrix:

$$M(\tau) = \int_{\tau} f(t) f(t)' d\tau \in NND(m^2) \quad (3)$$

where, NND(m^2) denotes the cone of nonnegative definite $m^2 \times m^2$ matrices. The entries of M(τ) are fourth moments of τ, since the regression function $f(t)$ is purely quadratic.

2.3 Information Matrix

We use unit vectors e_1, e_2, e_3, e_4 and set $e_{ij} = e_i \otimes e_j$ for i<j i,j={1, 2, 3, 4} and define the coefficient matrix

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

where

$$K_1 = \sum_{i=1}^{m} e_{ii} e_i' \quad \text{and} \quad K_2 = \tfrac{1}{m} \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E_{ij}' \quad (4)$$

Obtainable as follows:

From, $e_1 = (1\ 0\ 0\ 0)'$, $e_2 = (0\ 1\ 0\ 0)'$ $e_3 = (0\ 0\ 1\ 0)'$ and $e_4 = (0\ 0\ 0\ 0\ 1)'$ we have:

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

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

$$e_{44} = e_4 \otimes e_4 = (0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 1)',$$

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

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

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

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

$$e_{14} = e_1 \otimes e_4 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}'$$
$$e_{41} = e_4 \otimes e_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}'$$
$$e_{23} = e_2 \otimes e_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$
$$e_{32} = e_3 \otimes e_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$
$$e_{24} = e_2 \otimes e_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}',$$
$$e_{42} = e_4 \otimes e_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}',$$
$$e_{34} = e_3 \otimes e_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}' \text{ and}$$
$$e_{43} = e_4 \otimes e_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}'$$

The vectors forming the standard basis of $\Re^6$ in a lexicographic order are:

$$E_{12} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}', \quad E_{13} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}', \quad E_{14} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}',$$

$$E_{23} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}', \quad E_{24} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}' \text{ and } E_{34} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}'$$

Therefore, we obtain using (4);

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

and

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

$$= \frac{1}{4}[(e_{12} + e_{21})E_{12}' + (e_{13} + e_{31})E_{13}' + (e_{14} + e_{41})E_{14}' + (e_{23} + e_{32})E_{23}' + (e_{24} + e_{42})E_{24}' + (e_{34} + e_{43})E_{34}']$$

$$K_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 0 & 0 & 0 \\ 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Thus

$$K = (K_1, K_2) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The full parameter vector $\theta \in \Re^{16}$ for model equation (1) is not estimable since the design matrix is column deficient. We select a maximal sub parameter vector:

$$K'\theta = \begin{Bmatrix} (\theta_{ii})_{1\le i\le 4} \\ \frac{1}{4}(\theta_{ij} + \theta_{ji}),_{1\le i<j\le 4} \end{Bmatrix} \in \Re^{10} \quad \text{for all} \quad \theta \in \Re^{10} \tag{5}$$

To optimize the response, we focus on the movement of the design center along the direction of the instantaneous slope of the response function, that is, $\frac{\partial Y_t}{\partial t}$. Designs attain certain properties in Y (estimated response) that do not coincide with the similar properties for the estimated slopes. Therefore, our focus is in experimental designs that are constructed based on derivatives (instantaneous changes), (Murty N. N. and Studden W. J., 1972) and (Ott L. S. and Mendenhall W., 1972).

(Aggarwal, M. L., Singh, P., Sarin, V. and Husain, B., 2013) obtained D-, A- and E-optimal orthogonal block designs for four mixture components in two blocks for Becker's models and K-model. This study investigates the slope of the response surface at a point t, over any specified direction. We develop the concept of robust slope over all directions. Define D, a matrix arising from the differentiation of $f(t)'\theta$ with respect to each of the four independent factors, (Sung H. Park, Hyang S. Jung and Rabindra Nath Das, 2009). That is;

$$D = \left(\frac{\partial f'(t)}{\partial t_1} \frac{\partial f'(t)}{\partial t_2}, \frac{\partial f'(t)}{\partial t_3} \frac{\partial f'(t)}{\partial t_4} \right)', \quad \text{where; } f(t) = t \otimes t \text{ and } t = (t_1 \ t_2 \ t_3 \ t_4)' \tag{6}$$

An important matrix for the design with four ingredients is the adjusted 4×10 slope matrix $H_0 = DK$.

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

$$C_k(M(\tau)) = \min\{LM(\tau)L' \quad L \in \Re^{10\times16};\ LK = I_{10}\} \tag{7}$$

where I_{10} denotes the 10×10 identity matrix and L is the left inverse of K derived from the computation, $L = (K'K)^{-1}K'$. The information matrix for K'θ which is a linear transformation of the moment matrix, takes the form:

$$C_0 = LM(\tau)L' \in NND(10) \tag{8}$$

We then consider optimizing the information matrix for K'θ of the form:

$$C = H_0 C_0 H_0' \in NNND(4) \tag{9}$$

2.4 Optimality Criteria

We will compute optimal design for the Kronecker model using matrix mean ϕ_p which is an information function (Pukelsheim, 1993). For an information matrix $C_k(M(\tau)) \in$ PD(m) the kiefers ϕ_p -criteria are defined by:

$$\phi_p(C) = \begin{cases} \lambda_{\min}(C) & if \quad p = -\infty \\ \det(C)^{\frac{1}{\binom{m+1}{2}}} & if \quad p = 0 \\ \left[\frac{1}{\binom{m+1}{2}} traceC^p \right]^p & if \quad p \in [-\infty;1] \setminus \{0\} \end{cases} \tag{10}$$

where $\lambda_{\min}$(C) refers to the smallest eigenvalue of C. By definition ϕ_p (C) is a scalar measure which is a function of the eigenvalues of C for all $p \in [-\infty, 1]$. (Pukelsheim, 1993).

Consequently a design with maximum information on the parameter subsystem $K'\theta$ solves the problem;

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

$$\text{Subject to } C_k(M(\tau)) \in PD(m) \tag{11}$$

Suppose $\eta(\alpha)$ satisfies the side condition $C_k(M(\tau)) \in$ PD(m) and write $C_j = C_k(M(\eta_j))$ for j=(1, 2, 3, 4). For all $p \in (-\infty, 1]$, $\eta(\alpha)$ solves problem (11) if and only if it satisfies the equivalence theorem;

$$traceH_0 C_j C^{p-1} H_0' \begin{cases} = traceH_0 C^p H_0' & for\ all\ \ j \in \partial(\alpha) \\ \leq traceH_0 C^p H_0' & otherwise \end{cases} \tag{12}$$

(Klein, 2004).

3. Construction of the Design

We consider the weighted centroid design $\eta(\alpha) = \sum_{j=1}^{4} \alpha_j \eta_j = \alpha_1\eta_1 + \alpha_2\eta_2 + \alpha_3\eta_3 + \alpha_4\eta_4$ with four elementary centroids derived from support points:

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

$$\eta_4 = \left\{ \begin{pmatrix}1/4\\1/4\\1/4\\1/4\end{pmatrix} \right\}.$$

These weighted centroid designs discovered by (Sceffe', 1958) and (Sheffe'., 1963), are exchangeable and invariant under permutations, (Klein T. , 2004).

Thus the moment matrices for the two centroid designs 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}$$

Defining the left inverse $\tilde{L} = (K'K)^{-1}K'$ where K is the coefficient matrix defined equation (4),

$$\widetilde{L} = (K'K)^{-1}K' = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 \end{pmatrix}$$

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

$$C_1 = C_k(M(\eta_1)) = \widetilde{L}(M(\eta_1))\widetilde{L}' = \begin{pmatrix} 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad (13)$$

and

$$C_2 = C_k(M(\eta_2)) = \widetilde{L}(M(\eta_2))\widetilde{L}' = \begin{pmatrix} \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{24} & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 \\ \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{24} & 0 & 0 & \frac{1}{24} & \frac{1}{24} & 0 \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & 0 & \frac{1}{24} & 0 & \frac{1}{24} & 0 & \frac{1}{24} \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & 0 & 0 & \frac{1}{24} & 0 & \frac{1}{24} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{24} & 0 & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 \\ \frac{1}{24} & 0 & 0 & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 \\ 0 & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 & 0 & \frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{24} & 0 & \frac{1}{24} & 0 & 0 & 0 & 0 & \frac{1}{6} & 0 \\ 0 & 0 & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 & 0 & 0 & \frac{1}{6} \end{pmatrix} \qquad (14)$$

Using equations (13) and (14), we obtain the information matrix for the design $\eta(\alpha)$ from; $C_k(M(\eta(\alpha))) = \alpha_1 C(M(\eta_1)) + \alpha_2 C(M(\eta_2))$, as

$$C_0=\begin{pmatrix}
\frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0\\
\frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0\\
\frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24}\\
\frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24}\\
\frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 & 0 & 0 & 0\\
\frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 & 0 & 0\\
\frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha}{6} & 0 & 0 & 0\\
0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0\\
0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} & 0\\
0 & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6}
\end{pmatrix}$$

This matrix has an inverse,

$$C_0^{-1}=\begin{pmatrix}
\frac{4}{\alpha_1} & 0 & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & 0 & 0\\
0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0\\
0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1}\\
0 & 0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1}\\
\frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & 0 & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0\\
\frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{1}{4\alpha_1}\\
\frac{-1}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1}\\
0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1}\\
0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1}\\
0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2}
\end{pmatrix} \quad (15)$$

which on squaring yields,

$$C_0^{-2}=\begin{pmatrix}
a & b & b & b & c & c & c & d & d & d\\
b & a & b & b & c & d & d & c & c & d\\
b & b & a & b & d & c & d & c & d & c\\
b & b & b & a & d & d & c & d & c & c\\
c & c & d & d & e & f & f & f & f & g\\
c & d & c & d & f & e & f & f & g & f\\
c & d & d & c & f & f & e & g & f & f\\
d & c & c & d & f & f & g & e & f & f\\
d & c & d & c & f & g & f & f & e & f\\
d & d & c & c & g & f & f & f & f & e
\end{pmatrix} \quad (16)$$

where:

$$a=\frac{19}{\alpha_1^2},\ b=\frac{1}{\alpha_1^2},\ c=\frac{-(6\alpha_1+5\alpha_2)}{\alpha_1^2\alpha_2},\ d=\frac{-1}{2\alpha_1^2},\ e=\frac{65\alpha_1^2+2\alpha_1+5}{2\alpha_1^2\alpha_2^2},$$

$$f=\frac{24\alpha_1+11\alpha_2}{8\alpha_1^2\alpha_2}\ \text{ and }\ g=\frac{1}{4\alpha_1^2}$$

The slope matrix D as defined by equation (6) is obtained as

$$D=\begin{pmatrix} 2t_1 & t_2 & t_3 & t_4 & t_2 & 0 & 0 & 0 & t_3 & 0 & 0 & 0 & t_4 & 0 & 0 & 0 \\ 0 & t_1 & 0 & 0 & t_1 & 2t_2 & t_3 & t_4 & 0 & t_3 & 0 & 0 & 0 & t_4 & 0 & 0 \\ 0 & 0 & t_1 & 0 & 0 & 0 & t_2 & 0 & t_1 & t_2 & 2t_3 & t_4 & 0 & 0 & t_4 & 0 \\ 0 & 0 & 0 & t_4 & 0 & 0 & 0 & t_2 & 0 & 0 & 0 & t_3 & t_1 & t_2 & t_3 & 2t_4 \end{pmatrix}$$

A corresponding adjusted slope matrix $H_0=DK$ is thus given by;

$$H_0=\begin{pmatrix} 2t_1 & 0 & 0 & 0 & \frac{1}{2}t_2 & \frac{1}{2}t_3 & \frac{1}{2}t_4 & 0 & 0 & 0 \\ 0 & 2t_2 & 0 & 0 & \frac{1}{2}t_1 & 0 & 0 & \frac{1}{2}t_3 & \frac{1}{2}t_4 & 0 \\ 0 & 0 & 2t_3 & 0 & 0 & \frac{1}{2}t_1 & 0 & \frac{1}{2}t_2 & 0 & \frac{1}{2}t_4 \\ 0 & 0 & 0 & 2t_4 & 0 & 0 & \frac{1}{2}t_1 & 0 & \frac{1}{2}t_2 & \frac{1}{2}t_3 \end{pmatrix}$$

To get the A-optimal design we invoke the equivalence theorem, that $\eta(\alpha)$ is $\phi_p-optimal$ for $K'\theta$ in T if and only if;

$$trace\,H_0C_jC^{p-1}H_0'\begin{cases} =traceH_0C^pH_0' & for\ \ j=1,2 \\ <traceH_0C^pH'_0 & otherwise \end{cases}$$

From which, the unique A-optimal design for $K'\theta$ is arrived at when we substitute putting p=-1.

$$traceH_0C_jC_k^{-2}H_0'=traceH_0C_k^{-1}H_0' \qquad (17)$$

The following results were a consequence of using condition (17):

For j=1 we have:

$$H_0C_1C_o^{-2}H_0'=\frac{1}{4\alpha_1^2}\begin{bmatrix} 76t_1^2+A(t_1t_2+t_1t_3+t_1t_4) & 4t_1t_2+At_1^2-\frac{1}{2}(t_1t_3+t_1t_4) & 4t_1t_3+At_1^2-\frac{1}{2}(t_1t_2+t_1t_4) \\ 4t_1t_2+At_2^2-\frac{1}{2}(t_2t_3+t_2t_4) & 76t_2^2+A(t_1t_2+t_2t_3+t_2t_4) & 4t_2t_3+At_2^2-\frac{1}{2}(t_1t_2+t_2t_4) \\ 4t_1t_3+At_3^2-\frac{1}{2}(t_2t_3+t_3t_4) & 4t_2t_3+At_3^2-\frac{1}{2}(t_1t_3+t_3t_4) & 76t_3^2+A(t_1t_3+t_2t_3+t_3t_4) \\ 4t_1t_4+At_4^2-\frac{1}{2}(t_2t_4+t_3t_4) & 4t_2t_4+At_4^2-\frac{1}{2}(t_1t_4+t_3t_4) & 4t_3t_4+At_4^2-\frac{1}{2}(t_1t_4+t_2t_4) \end{bmatrix}$$

$$\begin{bmatrix} 4t_1t_4+At_1^2-\frac{1}{2}(t_1t_2+t_1t_3) \\ 4t_2t_4+At_2^2-\frac{1}{2}(t_1t_2+t_2t_3) \\ 4t_3t_4+At_3^2-\frac{1}{2}(t_1t_3+t_2t_3) \\ 76t_4^2+A(t_1t_4+t_2t_4+t_3t_4) \end{bmatrix}$$

where:

$$A=\frac{-(6\alpha_1+5\alpha_2)}{\alpha_2},\ \ t_i^2=\frac{103}{48}, i=1,2,3,4 \text{ and } \ t_it_j=\frac{77}{144},\ i\neq j=1,2,3,4$$

The trace being;

$$traceH_0C_1C_0^{-2}H_0'=\frac{1}{4\alpha_1^2}\left[76(t_1^2+t_2^2+t_3^2+t_4^2)-\frac{2(6\alpha_1+5\alpha_2)}{\alpha_2}(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4)\right]$$
$$=\frac{7443\alpha_2-462\alpha_1}{48\alpha_1^2\alpha_2} \qquad \text{…. (18)}$$

and

$$H_0C_0^{-1}H_0' = \frac{-1}{\alpha_1}\begin{bmatrix} -16t_1^2+\frac{a}{4}(t_2^2+t_3^2+t_4^2)+2(t_1t_2+t_1t_3+t_1t_4)-\frac{1}{8}(t_2t_3+t_2t_4+t_3t_4) \\ t_2^2+t_1^2-\frac{1}{16}(t_3^2+t_4^2+t_1t_3+t_1t_4+t_2t_3+t_3t_4)+\frac{a}{4}t_1t_2 \\ t_3^2+t_1^2-\frac{1}{16}(t_2^2+t_4^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\frac{a}{4}t_1t_3 \\ t_4^2+t_1^2-\frac{1}{16}(t_2^2+t_3^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\frac{a}{4}t_1t_4 \end{bmatrix.$$

$$\begin{vmatrix} t_1^2+t_2^2-\frac{1}{16}(t_3^2+t_4^2+t_1t_3+t_1t_4+t_2t_3+t_2t_4)+\frac{a}{4}t_1t_2 \\ -16t_2^2+\frac{a}{4}(t_1^2+t_3^2+t_4^2)+2(t_1t_2+t_2t_3+t_2t_4)-\frac{1}{8}(t_1t_3+t_1t_4+t_3t_4) \\ t_3^2+t_2^2-\frac{1}{16}(t_1^2+t_4^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\frac{a}{4}t_2t_3 \\ t_4^2+t_2^2-\frac{1}{16}(t_1^2+t_3^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\frac{a}{4}t_2t_4 \end{vmatrix.$$

$$\begin{vmatrix} t_1^2+t_3^2-\frac{1}{16}(t_2^2+t_4^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\frac{a}{4}t_1t_3 \\ t_2^2+t_3^2-\frac{1}{16}(t_1^2+t_4^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\frac{a}{4}t_2t_3 \\ -16t_3^2+\frac{a}{4}(t_1^2+t_2^2+t_4^2)+2(t_1t_3+t_2t_3+t_3t_4)-\frac{1}{8}(t_1t_2+t_1t_4+t_2t_4) \\ t_4^2+t_3^2-\frac{1}{16}(t_1^2+t_2^2+t_1t_3+t_1t_4+t_2t_3+t_2t_4)+\frac{a}{4}t_3t_4 \end{vmatrix.$$

$$\left|\begin{matrix} t_1^2+t_4^2-\frac{1}{16}(t_2^2+t_3^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\frac{a}{4}t_1t_4 \\ t_2^2+t_4^2-\frac{1}{16}(t_1^2+t_3^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\frac{a}{4}t_2t_4 \\ t_3^2+t_4^2-\frac{1}{16}(t_1^2+t_2^2+t_1t_3+t_1t_4+t_2t_3+t_2t_4)+\frac{a}{4}t_3t_4 \\ -16t_4^2+\frac{a}{4}(t_1^2+t_2^2+t_3^2)+2(t_1t_4+t_2t_4+t_3t_4)-\frac{1}{8}(t_1t_2+t_1t_3+t_2t_3) \end{matrix}\right]$$

where:

$$a=\frac{-(12\alpha_1+\alpha_2)}{2\alpha_2},\quad t_i^2=\frac{103}{48}, i=1,2,3,4 \text{ and } t_it_j=\frac{77}{144},\ i\neq j=1,2,3,4$$

Trace of this matrix is;

$$\begin{aligned} traceH_0C_k^{-1}H_0' &= \frac{-1}{\alpha_1}\left[(-16+\tfrac{3}{4}a)(t_1^2+t_2^2+t_3^2+t_4^2)+\tfrac{15}{4}(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4)\right] \\ &= \frac{1854\alpha_1+6169\alpha_2}{48\alpha_1\alpha_2} \end{aligned} \tag{19}$$

From condition (17) using the values from (19) and (20) we have;

$$\frac{7443\alpha_2-462\alpha_1}{48\alpha_1^2\alpha_2}=\frac{1854\alpha_1+6169\alpha_2}{48\alpha_1\alpha_2}$$

giving a plausible value $\alpha_1=0.664039581$.

For j=2;

The following elementary evaluation are realized:

$$H_0C_2C_0^{-1}H_0' = \frac{-1}{4\alpha_1\alpha_2}\begin{bmatrix} 12t_1^2+\frac{1}{4}d(t_2^2+t_3^2+t_4^2)+(4+a)t_1(t_2+t_3+t_4)-\frac{1}{2}(t_2t_3+t_2t_4+t_3t_4) & 4t_2(t_2+t_1)+2t_1(2at_1-t_3-t_4)+\frac{1}{4}t_2(dt_1-t_3-t_4)-\frac{1}{4}t_3(t_1+t_3)-\frac{1}{4}t_4(t_1+t_4) & 4t_3(t_3+t_1)+2t_1(2at_1-t_2-t_4)+\frac{1}{4}t_3(dt_1-t_2-t_4)-\frac{1}{4}t_2(t_1+t_2)-\frac{1}{4}t_4(t_1+t_4) & 4t_4(t_4+t_1)+2t_1(2at_1-t_2-t_3)+\frac{1}{4}t_4(dt_1-t_2-t_3)-\frac{1}{4}t_2(t_1+t_2)-\frac{1}{4}t_3(t_1+t_3) \\ 4t_1(t_1+t_2)+2t_2(2at_2-t_3-t_4)+\frac{1}{4}t_1(dt_2-t_3-t_4)-\frac{1}{4}t_3(t_2+t_3)-\frac{1}{4}t_4(t_2+t_4) & 12t_2^2+\frac{1}{4}d(t_1^2+t_3^2+t_4^2)+(4+a)t_2(t_1+t_3+t_4)-\frac{1}{2}(t_1t_3+t_1t_4+t_3t_4) & 4t_3(t_3+t_2)+2t_2(2at_2-t_1-t_4)+\frac{1}{4}t_3(dt_2-t_1-t_4)-\frac{1}{4}t_1(t_1+t_2)-\frac{1}{4}t_4(t_2+t_4) & 4t_4(t_4+t_2)+2t_2(2at_2-t_1-t_3)+\frac{1}{4}t_4(dt_2-t_1-t_3)-\frac{1}{4}t_1(t_1+t_2)-\frac{1}{4}t_3(t_2+t_3) \\ 4t_1(t_1+t_3)+2t_3(2at_3-t_2-t_4)+\frac{1}{4}t_1(dt_3-t_2-t_4)-\frac{1}{4}t_2(t_2+t_3)-\frac{1}{4}t_4(t_3+t_4) & 4t_2(t_2+t_3)+2t_3(2at_3-t_1-t_4)+\frac{1}{4}t_2(dt_3-t_1-t_4)-\frac{1}{4}t_1(t_1+t_3)-\frac{1}{4}t_4(t_3+t_4) & 12t_3^2+\frac{1}{4}d(t_1^2+t_2^2+t_4^2)+(4+a)t_3(t_1+t_2+t_4)-\frac{1}{2}(t_1t_2+t_1t_4+t_2t_4) & 4t_4(t_4+t_3)+2t_3(2at_3-t_1-t_2)+\frac{1}{4}t_4(dt_3-t_1-t_2)-\frac{1}{4}t_1(t_1+t_3)-\frac{1}{4}t_2(t_2+t_3) \\ 4t_1(t_1+t_4)+2t_4(2at_4-t_2-t_3)+\frac{1}{4}t_1(dt_4-t_2-t_3)-\frac{1}{4}t_2(t_2+t_4)-\frac{1}{4}t_3(t_3+t_4) & 4t_2(t_2+t_4)+2t_4(2at_4-t_1-t_3)+\frac{1}{4}t_2(dt_4-t_1-t_3)-\frac{1}{4}t_1(t_1+t_4)-\frac{1}{4}t_3(t_3+t_4) & 4t_3(t_3+t_4)+2t_4(2at_4-t_1-t_2)+\frac{1}{4}t_3(dt_4-t_1-t_2)-\frac{1}{4}t_1(t_1+t_4)-\frac{1}{4}t_2(t_2+t_4) & 12t_4^2+\frac{1}{4}d(t_1^2+t_2^2+t_3^2)+(4+a)t_4(t_1+t_2+t_3)-\frac{1}{2}(t_1t_2+t_1t_3+t_2t_3) \end{bmatrix}$$

where:

$$a=\frac{-(5\alpha_1+1)}{\alpha_2},\quad d=\frac{-2(11\alpha_1+1)}{\alpha_2},\quad t_i^2=\frac{103}{48}, i=1,2,3,4 \text{ and } t_it_j=\frac{77}{144}, i\neq j=1,2,3,4$$

The trace of matrix being,

$$\begin{aligned} traceH_0C_2C_0^{-2}H' &= \frac{-1}{4\alpha_1\alpha_2}\left[(12+\tfrac{3}{4}d)(t_1^2+t_2^2+t_3^2+t_4^2)+(7+2a)(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4)\right] \\ &= \frac{463+4169\alpha_1-3011\alpha_2}{96\alpha_1\alpha_2^2} \end{aligned} \tag{20}$$

From condition (17) and the values in (19) and (20) we have;

$$\frac{1854\alpha_1+6169\alpha_2}{48\alpha_1\alpha_2}=\frac{463+4169\alpha_1-3011\alpha_2}{96\alpha_1\alpha_2^2},$$

with the unique solution $\alpha_2 = 0.335960419$.

Therefore the unique A-slope optimal design for $K'\theta$ is

$$\eta(\alpha^A)=\alpha_1\eta_1+\alpha_2\eta_2=0.664039581\eta_1+0.335960419\eta_2.$$

The information matrix after employing the ordinates of the support points and the optimal vector becomes:

$$H_0C_0^{-1}H_0'=\begin{bmatrix} 77.1282 & -3.3696 & -3.3696 & -3.3696 \\ -3.3696 & 77.1282 & -3.3696 & -3.3696 \\ -3.3696 & -3.3696 & 77.1282 & -3.3696 \\ -3.3696 & -3.3696 & -3.3696 & 77.1282 \end{bmatrix}$$

The maximum of the A-criterion using (10) is given by;

$$v(\phi_{-1}) = \left(\frac{1}{4} trace H_0 C_0^{-1} H_0'\right)^{-1} = (77.1282)^{-1} = 0.012965426\,.$$

4. Fruit Blending Experiment

Four fruits (pine apple, pawpaw, banana and coconut) were involved in the experiment. The response on a scale 1-15 was taken as the average score for the four attributes considered: taste, colour, texture and smell. The sixty data values are from fifteen support points for the weighted centroid design each replicated four times. The points comprised the four pure blends, six binary blends, four ternary blend and the four fruits together in the mixture.

4.1 Sample Data: For Four Replicates

Combinations (support points)				**ATTRIBUTES**				TOTAL	MEAN
pina apple	paw paw	banana	coconut	texture	colour	taste	smell		
1	0	0	0	10	8	10	12	40	10.00
1	0	0	0	12	15	11	9	47	11.75
1	0	0	0	8	9	11	11	39	9.75
1	0	0	0	14	14	14	15	57	14.25
. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .
0.25	0.25	0.25	0.25	11	13	10	15	49	12.25
0.25	0.25	0.25	0.25	9	8	11	10	38	9.50
0.25	0.25	0.25	0.25	10	13	12	14	49	12.25
0.25	0.25	0.25	0.25	9	7	10	13	39	9.75

4.2 Fitted Model

The estimates of the coefficients for the Kronecker model were obtained using SAS software package. The model from equation (4) with m=4 is;

$$\begin{aligned}\hat{y} = E(y) = 11.17(pineapple)^2 + 10.50(pawpaw)^2 + 10.12(banana)^2 + 9.31(coconut)^2 + \\ 24.68\,peneapple * pawpaw + 21.54\,pineapple * banana + 16.40\,pineapple * coconut + \\ 19.25\,pawpaw * banana + 10.86\,pawpaw * coconut + 16.72 banana * coconut\end{aligned}$$

4.3 Model Validity

We performed the analysis on the model validity to examine the fitted model if it provides a good approximation of the true response surface. Analysis of variance (ANOVA) was used to examine the Kronecker model. As is evident from the output table 1 below, 96.67% of the variation in the response is accounted for by the purposeful changes made on the amounts of each fruit in the mixture. The overall model is highly significant with an estimated probability value less than 0.0001, much lower than the 0.05 and 0.01 levels of significance.

Table 1. ANOVA for the four ingredients Kronecker model

The GLM Procedure

Dependent Variable: yield

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	10	5794.907380	579.490738	145.17	<.0001
Error	50	199.592620	3.991852		
Uncorrected Total	60	5994.500000			

R-Square	Coeff Var	Root MSE	yield Mean
0.966704	20.43951	1.997962	9.775000

NOTE: No intercept term is used: R-square is not corrected for the mean.

We also used the t-test values to test for the significance of the individual coefficients (hence fruits) in the model. The test is, we test the null hypothesis $H_o : \beta_{ij} = 0$ against the alternative hypothesis $H_1 : \beta_{ij} \neq 0$. From the information below (in table 2), all the coefficients are significant with small estimated probability (Pr > |t|) values at the 0.05 level of significance. The interaction between pawpaw and coconut, compared to the other coefficients, is the least significant at the 0.01 level of significance.

Table 2. T-test Values for coefficients of the four ingredients Kronecker model

The GLM Procedure

Dependent Variable: yield

Parameter	Estimate	Standard Error	t Value	Pr > |t|
pine*pine	11.16953443	0.98751632	11.31	<.0001
paw*paw	10.49541136	0.98751632	10.63	<.0001
ban*ban	10.12119869	0.98751632	10.25	<.0001
coco*coco	9.30566494	0.98751632	9.42	<.0001
pine*paw	24.67598681	3.63911375	6.78	<.0001
pine*ban	21.53760215	3.63911375	5.92	<.0001
pine*coco	16.40167588	3.63911375	4.51	<.0001
paw*ban	19.24769445	3.63911375	5.29	<.0001
paw*coco	10.86176818	3.63911375	2.98	0.0044
ban*coco	16.72338352	3.63911375	4.60	<.0001

The assumption of normality on the errors, clearly points to a similar distribution on the observations. By examination of the P-P and Q-Q plots in figure 1 below, there is no indication of any serious deviation from normality.

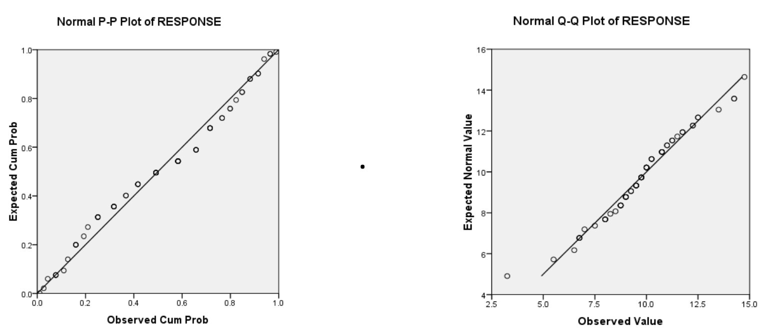

Figure 1.

4.4 Slope Information for the A-optimal Criterion

To get the A-optimal slope value for the design with the four ingredients, we first pre- and post-multiplied the inverse of information matrix (15) with the adjusted slope matrix (H_0), to get the necessary slope information matrix;

$$C=\begin{pmatrix}
\frac{16a^2}{\alpha_1}t_1^2+\frac{(12\alpha_1+\alpha_2)(e^2t_2^2+f^2t_3^2+g^2t_4^2)}{32\alpha_1\alpha_2}-\frac{at_1(et_2+ft_3+gt_4)}{\alpha_1}+\frac{eft_2t_3+egt_2t_4+fgt_3t_4}{32\alpha_1} &
-\frac{be}{2\alpha_1}t_2^2-\frac{ae}{2\alpha_1}t_1^2+\frac{fh}{64\alpha_1}t_3^2+\frac{gk}{64\alpha_1}t_4^2+\frac{e(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)e^2t_1t_2}{32\alpha_1\alpha_2} &
-\frac{cf}{2\alpha_1}t_3^2-\frac{af}{2\alpha_1}t_1^2+\frac{eh}{64\alpha_1}t_2^2+\frac{gm}{64\alpha_1}t_4^2+\frac{f(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)f^2t_1t_3}{32\alpha_1\alpha_2} &
-\frac{dg}{2\alpha_1}t_4^2-\frac{ag}{2\alpha_1}t_1^2+\frac{ek}{64\alpha_1}t_2^2+\frac{fm}{64\alpha_1}t_3^2+\frac{g(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)g^2t_1t_4}{32\alpha_1\alpha_2} \\
-\frac{be}{2\alpha_1}t_2^2-\frac{ae}{2\alpha_1}t_1^2+\frac{fh}{64\alpha_1}t_3^2+\frac{gk}{64\alpha_1}t_4^2+\frac{e(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)e^2t_1t_2}{32\alpha_1\alpha_2} &
\frac{16b^2}{\alpha_1}t_2^2+\frac{(12\alpha_1+\alpha_2)(e^2t_1^2+h^2t_3^2+k^2t_4^2)}{32\alpha_1\alpha_2}-\frac{bt_2(et_1+ht_3+kt_4)}{\alpha_1}+\frac{eht_1t_3+ekt_1t_4+hkt_3t_4}{32\alpha_1} &
-\frac{ch}{2\alpha_1}t_3^2-\frac{bh}{2\alpha_1}t_2^2+\frac{ef}{64\alpha_1}t_1^2+\frac{km}{64\alpha_1}t_4^2+\frac{h(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)h^2t_2t_3}{32\alpha_1\alpha_2} &
-\frac{dk}{2\alpha_1}t_4^2-\frac{bk}{2\alpha_1}t_2^2+\frac{eg}{64\alpha_1}t_1^2+\frac{hm}{64\alpha_1}t_3^2+\frac{k(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)k^2t_2t_4}{32\alpha_1\alpha_2} \\
-\frac{cf}{2\alpha_1}t_3^2-\frac{af}{2\alpha_1}t_1^2+\frac{eh}{64\alpha_1}t_2^2+\frac{gm}{64\alpha_1}t_4^2+\frac{f(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)f^2t_1t_3}{32\alpha_1\alpha_2} &
-\frac{ch}{2\alpha_1}t_3^2-\frac{bh}{2\alpha_1}t_2^2+\frac{ef}{64\alpha_1}t_1^2+\frac{km}{64\alpha_1}t_4^2+\frac{h(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)h^2t_2t_3}{32\alpha_1\alpha_2} &
\frac{16c^2}{\alpha_1}t_3^2+\frac{(12\alpha_1+\alpha_2)(f^2t_1^2+h^2t_2^2+m^2t_4^2)}{32\alpha_1\alpha_2}-\frac{ct_3(ft_1+ht_2+mt_4)}{\alpha_1}+\frac{fht_1t_2+fmt_1t_4+hmt_2t_4}{32\alpha_1} &
-\frac{dm}{2\alpha_1}t_4^2-\frac{cm}{2\alpha_1}t_3^2+\frac{fg}{64\alpha_1}t_1^2+\frac{hk}{64\alpha_1}t_2^2+\frac{m(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)m^2t_3t_4}{32\alpha_1\alpha_2} \\
-\frac{dg}{2\alpha_1}t_4^2-\frac{ag}{2\alpha_1}t_1^2+\frac{ek}{64\alpha_1}t_2^2+\frac{fm}{64\alpha_1}t_3^2+\frac{g(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)g^2t_1t_4}{32\alpha_1\alpha_2} &
-\frac{dk}{2\alpha_1}t_4^2-\frac{bk}{2\alpha_1}t_2^2+\frac{eg}{64\alpha_1}t_1^2+\frac{hm}{64\alpha_1}t_3^2+\frac{k(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)k^2t_2t_4}{32\alpha_1\alpha_2} &
-\frac{dm}{2\alpha_1}t_4^2-\frac{cm}{2\alpha_1}t_3^2+\frac{fg}{64\alpha_1}t_1^2+\frac{hk}{64\alpha_1}t_2^2+\frac{m(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1}+\frac{(12\alpha_1+\alpha_2)m^2t_3t_4}{32\alpha_1\alpha_2} &
\frac{16d^2}{\alpha_1}t_4^2+\frac{(12\alpha_1+\alpha_2)(g^2t_1^2+k^2t_2^2+m^2t_3^2)}{32\alpha_1\alpha_2}-\frac{dt_4(gt_1+kt_2+mt_3)}{\alpha_1}+\frac{gkt_1t_2+gmt_1t_3+kmt_2t_3}{32\alpha_1}
\end{pmatrix} \tag{21}$$

which after using the coordinates of the support points for the four ingredients design simplified to the matrix;

$$C=\begin{pmatrix}
\frac{103a^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(e^2+f^2+g^2)}{1536}-\frac{77a(e+f+g)}{144\alpha_1}+\frac{77(ef+eg+fg)}{4608\alpha_1} &
-\frac{103e(b+a)}{972\alpha_1}+\frac{103(fh+gk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)e^2}{4608\alpha_1\alpha_2}+\frac{77e(f+g+h+k)}{9216\alpha_1} &
-\frac{103f(c+a)}{972\alpha_1}+\frac{103(eh+gm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)f^2}{4608\alpha_1\alpha_2}+\frac{77f(e+g+h+m)}{9216\alpha_1} &
-\frac{103g(d+a)}{972\alpha_1}+\frac{103(ek+fm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)g^2}{4608\alpha_1\alpha_2}+\frac{77g(e+f+k+m)}{9216\alpha_1} \\
-\frac{103e(b+a)}{972\alpha_1}+\frac{103(fh+gk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)e^2}{4608\alpha_1\alpha_2}+\frac{77e(f+g+h+k)}{9216\alpha_1} &
\frac{103b^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(e^2+h^2+k^2)}{1536}-\frac{77b(e+h+k)}{144\alpha_1}+\frac{77(eh+kg+hk)}{4608\alpha_1} &
-\frac{103h(c+b)}{972\alpha_1}+\frac{103(ef+km)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)h^2}{4608\alpha_1\alpha_2}+\frac{77h(e+f+k+m)}{9216\alpha_1} &
-\frac{103k(d+b)}{972\alpha_1}+\frac{103(eg+hm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)k^2}{4608\alpha_1\alpha_2}+\frac{77k(e+g+h+m)}{9216\alpha_1} \\
-\frac{103f(c+a)}{972\alpha_1}+\frac{103(eh+gm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)f^2}{4608\alpha_1\alpha_2}+\frac{77f(e+g+h+m)}{9216\alpha_1} &
-\frac{103h(c+b)}{972\alpha_1}+\frac{103(ef+km)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)h^2}{4608\alpha_1\alpha_2}+\frac{77h(e+f+k+m)}{9216\alpha_1} &
\frac{103c^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(f^2+h^2+m^2)}{1536}-\frac{77c(f+h+m)}{144\alpha_1}+\frac{77(fh+fm+hm)}{4608\alpha_1} &
-\frac{103m(c+d)}{972\alpha_1}+\frac{103(fg+hk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)m^2}{4608\alpha_1\alpha_2}+\frac{77m(f+g+h+k)}{9216\alpha_1} \\
-\frac{103g(d+a)}{972\alpha_1}+\frac{103(ek+fm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)g^2}{4608\alpha_1\alpha_2}+\frac{77g(e+f+k+m)}{9216\alpha_1} &
-\frac{103k(d+b)}{972\alpha_1}+\frac{103(eg+hm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)k^2}{4608\alpha_1\alpha_2}+\frac{77k(e+g+h+m)}{9216\alpha_1} &
-\frac{103m(c+d)}{972\alpha_1}+\frac{103(fg+hk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)m^2}{4608\alpha_1\alpha_2}+\frac{77m(f+g+h+k)}{9216\alpha_1} &
\frac{103d^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(g^2+k^2+m^2)}{1536}-\frac{77d(g+k+m)}{144\alpha_1}+\frac{77(gk+gm+km)}{4608\alpha_1}
\end{pmatrix} \tag{22}$$

With

$$\begin{aligned} traceC &= \frac{103(a^2+b^2+c^2+d^2)}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(e^2+f^2+g^2+h^2+k^2+m^2)}{768} \\ &\quad -\frac{77(ae+af+ag+be+bh+bk+cf+ch+cm+dg+dk+dm)}{486\alpha_1} \\ &\quad +\frac{77(ef+eg+fg+eh+ek+hk+fh+fm+hm+gk+gm+km)}{243\alpha_1\alpha_2} \\ &= 2.2545\times10^4 \end{aligned} \tag{23}$$

where the A-optimal slope weight vector entries were employed and coefficient values from the fitted model.

The A-optimal slope information was gotten by using equation (10) with $p=-1,\ m=4$ and the trace value from (23) as;

$$v(\phi_{-1})=\left(\frac{1}{4}traceC\right)^{-1}=\left(\frac{2.2545\times10^4}{4}\right)^{-1}=1.7742\times10^{-4}.$$

5. Conclusion

The design presented is highly efficient for designs with fixed sample size. As is clear from the fruit blending experiment, the designs describe the response surface involved very well. However, the experimenter is mandated to ensure accuracy in the measurement of ingredient amounts and to determine the necessary number of replications required to achieve the desired precision levels.

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