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# D-Optimal Slope Design for Second Degree Kronecker Model Mixture Experiment With Three Ingredients

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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 three dimensions. The study is restricted to weighted centroid designs, with the second degree Kronecker model. A well-defined coefficient matrix is used to select a maximal parameter subsystem for the model since its full parameter space is inestimable. 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. Eventually the matrix means are used in determining optimal values of the efficient developed design.

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

## 1. Introduction

This study deals with the exploration and optimization of response surface. This is a problem faced by experimenters in many technical fields, where in general the response of interest is affected by a set of independent factors. In this response surface methodology (RSM) problem we assume a response of interest is influenced by three factors with the intent of optimizing 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, we have two conditions, $x_i \geq 0, i=1,2,3$ and $\sum_{i=1}^{3} x_i = 1$. Evidently the levels of the factors $x_i$ are interdependent. The experimental region for the mixture problem is a two 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 in point has finite number of support points.

This study adopts a second degree polynomial regression function with the expected response:

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

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. (see (Draper & Pukelsheim, 1998)).

A general review of design environment is done by (Pukelsheim, 1993) while (Klein, 2004) showed that the class of weighted centroid designs with at least two ingredients is essentially complete for the Kiefer ordering, (Draper, Heilijers, & Pukelsheim, 2000). As a consequence, we restrict the study to weighted centroid design.

***General Design Problem***

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

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

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

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 $\tau$, Pukelsheim (1993). In which case, the design $\tau$ is called feasible for $K'\theta$. Any design solving problem (2) above for a fixed p∈ (-∞, 1] is called $\phi_p - optimal$for $K'\theta$ in T. For all p∈ (-∞, 1], the existence of $\phi_p - optimal$design for $K'\theta$ is certain, (Pukelsheim, 1993).

***Moment Matrix***

An experimental design $\tau$ is a probability measure on the experimental domain with a finite number of support points. Each support point s ∈ supp(τ) 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:

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

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.

***Information matrix***

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

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

where

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

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

Obtainable as follows:

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

$$e_{11} = e_1 \otimes e_1 = (1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0)', \ e_{22} = e_1 \otimes e_1 = (0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0)',$$

$$e_{33} = e_3 \otimes e_3 = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1)', \ e_{12} = e_1 \otimes e_2 = (0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0)',$$

$$e_{21} = e_2 \otimes e_1 = (0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0)', \ e_{13} = e_1 \otimes e_3 = (0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0)',$$

$$e_{31} = e_3 \otimes e_1 = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0)', \ e_{23} = e_2 \otimes e_3 = (0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0)',$$

$$e_{32} = e_3 \otimes e_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}', \ E_{12} = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}', \ E_{13} = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}' \text{ and}$$

$$E_{23} = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}'$$

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

$$K_2 = (e_{12} + e_{21})E'_{12} + (e_{13} + e_{31})E'_{13} + (e_{23} + e_{32})E'_{23} = \begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 \end{pmatrix}$$

Thus

$$K = \begin{pmatrix} K_1 & K_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

The full parameter vector $\theta \in \Re^{m^2}$ for model equation (1) is not estimable. We select a maximal sub parameter vector:

$$K'\theta = \begin{Bmatrix} (\theta_{ii})_{1 \le i \le m} \\ \frac{1}{m}(\theta_{ij} + \theta_{ji}),_{1 \le i < j \le m} \end{Bmatrix} \in \Re^{\binom{m+1}{2}}$$

for all

$$\theta \in \Re^{m^2} \tag{5}$$

To optimize the response, we focus on the movement of the design center along the direction of the directional derivatives of the response function, that is, $\frac{\partial Y_t}{\partial t}$. Since the designs that attain certain properties in Y (estimated response) do not enjoy the same properties for the estimated derivatives (slopes), we consider experimental designs that are constructed with derivatives in mind, (Murty & Studden, 1972) and (Ott & Mendenhall, 1972).

In practice, it is often of interest to investigate the slope of the response surface at a point $t$, not only over the axial directions, but also 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 m independent factors, (see (Sung, Hyang, & Rabindra, 2009)). That is;

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

An important matrix for the design with three ingredients is the adjusted $3\times 6$ slope matrix $H_0 = DK$.

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

$$C_k(M(\tau))=\min\{LM(\tau)L' \quad L \in \Re^{\binom{m+1}{2}\times m^2};\ LK=I_{\binom{m+1}{2}}\} \tag{7}$$

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 derived from the linear relation, $L=(K'K)^{-1}K'$. The information matrices for K'θ takes the form:

$$C_0 = LM(\tau)L' \in NND\left(\binom{m+1}{2}\right) \tag{8}$$

Thus the information matrices for K'θ are linear transformations of the moment matrices.

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

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

***Optimality Criteria***

We will compute optimal design for the polynomial fit model using matrix mean $\phi_p$ which is an information function (Pukelsheim, 1993). For an information matrix $C_k(M(\tau))\in$ PD(m) the kiefers $\phi_p$-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 $\phi_p$(C) is a scalar measure which is a function of the eigenvalues of C for all p∈[-∞;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). For all p∈(-∞;1], $\eta(\alpha)$ solves problem (11) if and only if;

$$traceH_0C_jC^{p-1}H_0'\begin{cases}=traceH_0C^pH_0' & for\ all\ j\in\partial(\alpha)\\ \le traceH_0C^pH_0' & otherwise\end{cases} \tag{12}$$

(T. K. , 2004).

**3. Construction of the design**

We consider the weighted centroid design $\eta(\alpha)=\sum_{j=1}^{3}\alpha_j\eta_j=\alpha_1\eta_1+\alpha_2\eta_2+\alpha_3\eta_3$ with three elementary centroids (captured from the support points):

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

These designs discovered by ( (Scheffe', 1958) and (H., 1963)), are exchangeable and invariant under permutations, (T. K. , 2002). Weighted centroid designs are exchangeable.

The moment matrices for $\eta_1$ and $\eta_2$ 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

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

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

$$\tilde{L}=(K'K)^{-1}K'=\begin{pmatrix}1&0&0&0&0&0&0&0&0\\0&0&0&0&1&0&0&0&0\\0&0&0&0&0&0&0&0&1\\0&3/2&0&3/2&0&0&0&0&0\\0&0&3/2&0&0&0&3/2&0&0\\0&0&0&0&0&3/2&0&3/2&0\end{pmatrix}$$

The information matrices for the designs $\eta_1$ and $\eta_2$ are obtained as follows:

$$C_1 = C_k(M(\eta_1)) = \tilde{L}(M(\eta_1))\tilde{L}' = \begin{pmatrix} 1/3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{13}$$

and

$$C_2 = C_k(M(\eta_2)) = \tilde{L}(M(\eta_2))\tilde{L}' = \begin{pmatrix} 1/24 & 1/48 & 1/48 & 1/16 & 1/16 & 0 \\ 1/48 & 1/24 & 1/48 & 1/16 & 0 & 1/16 \\ 1/48 & 1/48 & 1/24 & 0 & 1/16 & 1/16 \\ 1/16 & 1/16 & 0 & 3/16 & 0 & 0 \\ 1/16 & 0 & 1/16 & 0 & 3/16 & 0 \\ 0 & 1/16 & 1/16 & 0 & 0 & 3/16 \end{pmatrix} \tag{14}$$

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

$$C_k = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{16} & 0 & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 & \frac{3\alpha_2}{16} & 0 & 0 \\ \frac{\alpha_2}{16} & 0 & \frac{\alpha_2}{16} & 0 & \frac{3\alpha_2}{16} & 0 \\ 0 & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 & 0 & \frac{3\alpha_2}{16} \end{pmatrix}$$

This matrix has a regular inverse,

$$[C(M(\eta(\alpha)))]^{-1} = \begin{pmatrix} \frac{3}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 \\ 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} & \frac{1}{3\alpha_1} & \frac{1}{3\alpha_1} \\ \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{1}{3\alpha_1} & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} & \frac{1}{3\alpha_1} \\ 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{1}{3\alpha_1} & \frac{1}{3\alpha_1} & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} \end{pmatrix} \tag{15}$$

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

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

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

$$H_0 = \begin{pmatrix} 2t_1 & 0 & 0 & \frac{2}{3}t_2 & \frac{2}{3}t_3 & 0 \\ 0 & 2t_2 & 0 & \frac{2}{3}t_1 & 0 & \frac{2}{3}t_3 \\ 0 & 0 & 2t_3 & 0 & \frac{2}{3}t_1 & \frac{2}{3}t_2 \end{pmatrix}$$

To get the D-optimal design we employ the relation, that $\eta(\alpha)$ is $\phi_p - optimal$ for $K'\theta$ in T if and only if;

$$trace\, H_0 C_j C^{p-1} H_0' \begin{cases} = trace H_0 C^p H_0' & for \quad j = 1,2 \\ < trace C^p & otherwise \end{cases}$$

From which, the unique D-optimal design for $K'\theta$ is derived using the equation (putting p=0)

$$trace\, H_0 C_j C^{-1} H_0' = trace H_0 C^0 H_0' = trace H_0 H_0' \quad for \quad j = 1,2 \tag{16}$$

The following results can be easily demonstrated using condition (16):

- For j=1

$$H_0 C_1 C^{-1} H_0' = \frac{1}{3\alpha_1} \begin{pmatrix} 12t_1^2 - \frac{4}{3}(t_1t_2 + t_1t_3) & -\frac{4}{3}t_1^2 & -\frac{4}{3}t_1^2 \\ -\frac{4}{3}t_2^2 & 12t_2^2 - \frac{4}{3}(t_1t_2 + t_2t_3) & -\frac{4}{3}t_2^2 \\ -\frac{4}{3}t_3^2 & -\frac{4}{3}t_3^2 & 12t_3^2 - \frac{4}{3}(t_1t_3 + t_2t_3) \end{pmatrix}, \text{ with}$$

$$trace\, H_0 C_1 C^{-1} H_0' = \frac{1}{3\alpha_1}\left[12(t_1^2 + t_2^2 + t_3^2) - \frac{8}{3}(t_1t_2 + t_1t_3 + t_2t_3)\right] = \frac{496}{27\alpha_1} \text{ and}$$

$$H_0 H_0' = \begin{pmatrix} 4t_1^2 + \frac{4}{9}(t_2^2 + t_3^2) & \frac{4}{9}t_1t_2 & \frac{4}{9}t_1t_3 \\ \frac{4}{9}t_1t_2 & 4t_2^2 + \frac{4}{9}(t_1^2 + t_3^2) & \frac{4}{9}t_2t_3 \\ \frac{4}{9}t_1t_3 & \frac{4}{9}t_2t_3 & 4t_3^2 + \frac{4}{9}(t_1^2 + t_2^2) \end{pmatrix}, \text{ with}$$

$$trace H_0 H_0' = \frac{44}{9}(t_1^2 + t_2^2 + t_3^2) = \frac{638}{27}$$

The condition, $trace H_0 C_1 C^{-1} H_0' = trace H_0 H_0'$ implies that $\frac{496}{27\alpha_1} = \frac{638}{27}$, giving $\alpha_1 = \frac{248}{319}$

- For j=2;

$$H_0 C_2 C^{-1} H_0' = \frac{4}{9\alpha_2} \begin{pmatrix} t_2^2 + t_3^2 + t_1t_2 + t_1t_3 & t_1^2 + t_1t_2 & t_1^2 + t_1t_3 \\ t_2^2 + t_1t_2 & t_1^2 + t_3^2 + t_1t_2 + t_2t_3 & t_2^2 + t_2t_3 \\ t_3^2 + t_1t_3 & t_3^2 + t_2t_3 & t_2^2 + t_2^2 + t_1t_3 + t_2t_3 \end{pmatrix}$$

with $trace H_0 C_2 C^{-1} H_0' = \frac{8}{9\alpha_2}\left(t_1^2 + t_2^2 + t_3^2 + t_1t_2 + t_1t_3 + t_2t_3\right) = \frac{142}{27\alpha_2}$

The equation, $trace H_0 C_2 C^{-1} H_0' = trace H_0 H_0'$ implies that $\frac{142}{27\alpha_2} = \frac{638}{27}$, giving $\alpha_2 = \frac{71}{319}$

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

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{248}{319}\eta_1 + \frac{71}{319}\eta_2 .$$

The information matrix:

$$H_0CH_0' = \begin{pmatrix} 4at_1^2 + 4b(t_2^2 + t_3^2 + 2t_1t_2 + 2t_1t_3) & 4b(t_1^2 + t_2^2 + 2t_1t_2) & 4b(t_1^2 + t_3^2 + 2t_1t_3) \\ 4b(t_1^2 + t_2^2 + 2t_1t_2) & 4at_2^2 + 4b(t_1^2 + t_3^2 + 2t_1t_2 + 2t_2t_3) & 4b(t_2^2 + t_3^2 + 2t_2t_3) \\ 4b(t_1^2 + t_3^2 + 2t_1t_3) & 4b(t_2^2 + t_3^2 + 2t_2t_3) & 4at_3^2 + 4b(t_1^2 + t_2^2 + 2t_1t_3 + 2t_2t_3) \end{pmatrix}$$

Where $a = \frac{8\alpha_1 + \alpha_2}{24}, b = \frac{\alpha_2}{48}, \; t_1^2 = \frac{29}{18} \; and \; t_it_j = \frac{13}{36}$

The maximum of the D-criterion is $v(\phi_0) = \left(\frac{1}{5.964}\right)^{\frac{1}{3}} = 0.5514 \cdot$

## 4. Conclusion

The design presented is highly efficient and can be employed as a design for a finite sample size. Of importance is to relate the weights to the number of support points for each centroid. However, the experimenter is cautioned to ensure high accuracy levels in the measurement of ingredient levels.

## References

Draper, N. R., & Pukelsheim, F. (1998). Mixture Models Based on Homogeneous Polynomials. *Journal of Statistical Planning and Inference, 71*, 303-311. https://doi.org/10.1016/S0378-3758(98)00012-3

Draper, N. R., Heilijers, B., & Pukelsheim, F. (2000). Kiefer Orderinf of Simplex Designs for Mixture Models with Four Ingredients. *Annals of Statistics, 28,* 578-590. https://doi.org/10.1214/aos/1016218231

Henry, S. (1963). The Simplex-Centroid Design for Experiments with Mixtures. *J. Roy. Statist. Soc. Ser., 25*, 235-257. https://doi.org/10.1111/j.2517-6161.1963.tb00506.x

Klein, T. (2004). Optimal Designs for Second-Degree Kronecker Model Mixture Experiments. *Journal of Statistical Planing and Inference, 123*, 117-131. https://doi.org/10.1016/S0378-3758(03)00145-9

Murty, V. N., & Studden, W. J. (1972). Optimal Designs for Estimating the Slope of a Polynomial Regression. *Journal of America Statistics Association, 67*, 869-873. https://doi.org/10.1080/01621459.1972.10481308

Ott, L., & Mendenhall, W. (1972). Designs for Estimating the Slope of a Second Order Linear Model. *Technometrics, 14*, 341-353. https://doi.org/10.1080/00401706.1972.10488920

Pukelsheim, F. (1993). *Optimal Designs of Experiments.* New York: wiley.

Scheffe, H. (1958). Experiments with Mixtures. *J. Roy. Statist. Ser, B20*, 344-360. https://doi.org/10.1111/j.2517-6161.1958.tb00299.x

Sung, H. P., Hyang, S. J., & Rabindra, D. (2009). Rotatability of Second Order Response Surface Regression Models with Corrected Error. *Quality Technology & Quantitative Management, 6*(4), 471-492. https://doi.org/10.1080/16843703.2009.11673211

T., K. (2002). Invariant Symmetric Block Matices for Design of Mixture Experiments. *Journal of Statistical Planning and Inference*, 178-196.

T., K. (2004). Optimal Designs for Second-Degree Kronecker Model ixture Experiments. *Journal of Statistical Planning and Inference, 123*, 117-131. https://doi.org/10.1016/S0378-3758(03)00145-9