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D-Optimal Designs for Third-Degree Kronecker Model Mixture Experiments with an Application to Artificial Sweetener Experiment

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Abstract: *This study investigates some optimal designs in the third degree Kronecker model mixture experiments for non-maximal subsystem of parameters, where Kiefer's functions serve as optimality criteria. Based on the completeness result, the considerations are restricted to weighted centroid designs. First, the coefficient matrix and the associated parameter subsystem of interest using the unit vectors and a characterization of the feasible weighted centroid design for a maximal parameter subsystem is obtained. Once the coefficient matrix is obtained, the information matrices associated with the parameter subsystem of interest are generated for the corresponding factors. We apply the optimality criteria to evaluate the designs.*
Key words: *Mixture experiments, Kronecker product, Optimal designs, Weighted centroid designs, Optimality criteria, Moment and information matrices, Efficiency.*

I. Introduction

Many practical problems are associated with investigation of a mixture of m factors, assumed to influence the response only through the proportions in which they are blended together. The m factors, $t_1, t_2, \dots,$ t_m are such that $t_i \geq 0$ and subject to the simplex restriction $\sum_{i=1}^{m} t_i = 1$.

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

Let $1_m=(1, \dots, 1)' \in \Re^m$ be the unity vector. Thus the experimental conditions $t=(t_1, t_2, \dots, t_m)$ with $t_i \geq 0$ of a mixture experiments are points in the probability simplex $T_m = \{t = (t_1, \ t_2, \ \dots, \ t_m)' \in [0, \ 1]^m : 1_m' t = 1\}$.

Under experimental conditions $t \in \tau$, the experimental response Y_t is taken to be a scalar random variable. Replications under identical experimental conditions or responses from distinct experimental conditions are assumed to be of equal (unknown) variance σ^2 and uncorrelated. The work done by Draper and Pukelsheim (1998) is being extended to polynomial regression model for third-degree mixture model, whereby the S-polynomial and the expected response takes the form

$$E[Y_t] = f(t)'\theta = \sum_{i=1}^{m} t_i\theta_i + \sum\sum_{i<j}^{m} t_i t_j \theta_{ij} + \sum\sum\sum_{i<j<k}^{m} \theta_{ijk}\, t_i t_j t_k \quad \text{......................................} \ \textbf{(1)}$$

and when the regression function is the homogeneous third-degree K-polynomial, the expected response takes the form

$$E[Y_t] = f(t)'\theta = \sum_{i=1}^{m}\sum_{j=1}^{m}\sum_{k=1}^{m} t_i t_j t_k \theta_{ijk} = (t \otimes t \otimes t)'\theta \quad \text{...} \ \textbf{(2)}$$

in which the Kronecker powers $t^{\otimes^3} = (t \otimes t \otimes t)$, $(m^3 \times 1)$ vectors, consists of pure cubic and three-way interactions of components of t in lexicographic order of the subscripts and with evident that third-degree restrictions are $\theta_{ijk} = \theta_{ikj} = \theta_{jik} = \theta_{jki} = \theta_{kij} = \theta_{kji}$ for all i, j, and k.

All observations taken in an experiment are assumed to be uncorrelated and to have common variance $\sigma^2 \in (0, \infty)$.

Draper and Pukelsheim (1998) put forward several advantages of the Kronecker model, for example, a more compact notation, more convenient invariance properties and the homogeneity of regression terms.

The moment matrix $M(\tau) = \int_\tau f(t)f(t)'d\tau$ for the Kronecker model of degree three has all entries homogeneous of degree six. This matrix reflects the statistical properties of a design τ.

Pukelsheim (1993) gives a review of the general design environment. Klein (2002) showed that the class of weighted centroid designs is essentially complete for m≥2 for the Kiefer ordering Cheng, S. C. (1995). As a consequence the search for optimal designs may be restricted to weighted centroid designs for most criteria. For particular criteria applied to mixture experiments Kiefer (1959, 1975, and 1978) and Galil and Kiefer (1977).All these authors have concentrated their work on the second degree Kronecker model. Korir et al (2009) extended the work to Third degree Kronecker model simple designs .The present work now determines optimal designs for a maximal subsystem of parameters in the third degree Kronecker model. TheKeifer's ϕ_p functions will serve as optimality criteria.

1.1Design problem

Considercanonical unit vectors in $\Re$ i.e. $e_1, e_2, \ldots, e_m$ and set $e_{iij} = e_i \otimes e_i \otimes e_j$, $e_{ijk} = e_i \otimes e_j \otimes e_k$ for i<j<k, i,j,k={1 2, …, m}.

Defining the matrix

$$K = (K_1; K_2) \in \Re^{m^3 \times (m+1)}$$

Where,

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

and

$$K_2 = \frac{1}{(m^3 - m)} \left\{ \sum_{\substack{i,j=1 \\ i \neq j}}^{m} \left(e_{iij} + e_{iji} + e_{jii}\right) + \sum_{\substack{i,j,k=1 \\ i \neq j \neq k}}^{m} \left(e_{ijk}\right) \right\}$$

Further define

$$L = (K'K)^{-1}K'$$

So that

$$C_k(M(\tau)) = LM(\tau)L'$$

As is evident from model equation (2), the Kronecker model's full parameter vector $\theta \in \Re^{m^3}$ is not estimable. When fitting this model, the parameter subsystem considered in this study can be written as

$$K'\theta = \left\{ \begin{matrix} (\theta_{iii})_{1 \le i \le m} \\ \dfrac{1}{m^3 - m} \left\{ \sum\limits_{\substack{i,j=1 \\ i \neq j}}^{m} (\theta_{iij} + \theta_{iji} + \theta_{jii}) + \sum\limits_{\substack{i,j,k=1 \\ i \neq j \neq k}}^{m} (\theta_{ijk}) \right\} \end{matrix} \right\} \in \Re^{(m+1)} \text{ for all } \theta \in \Re^{m^3}$$

where $K \in \Re^{m^3 \times (m+1)}$

The parameter subsystem $K'\theta$ of interest is a non-maximal parameter system in model (2).

The amount of information a design t contains on K' θ is captured by the information matrix $C_k(M(\tau)) = \min\{LM(\tau)L'\}; \Re^{(m+1)\times(m+1)}$

The information matrix $C_k(M(\tau))$ is the precision matrix of the best linear unbiased estimator for $K'\theta$ under design τ, Pukelsheim (1993, chapter 3). In the present case information matrices for $K'\theta$ takes a particular simple form:

$$\mathrm{C_k(M(\tau)) = (K'K)^{-1}K'M(\tau)K(K'K)^{-1} \in NND(m+1)}$$

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

1.2 Optimality Criteria

The most prominent optimality criteria in the design of experiments are the determinant criterion, ϕ_0, the average-variance criterion, ϕ_{-1}, the smallest eigenvalue criterion, $\phi_{-\infty}$ and the trace criterion, ϕ_1. These are a particular cases of the matrix means ϕ_p with parameter $p \in [-\infty;1]$.

The optimality properties of designs are determined by their moment matrices (Pukelsheim 1993, chapter 5). We compute optimal design for the polynomial fit model, the third degree Kronecker model. This involves searching for the optimum in a set of competing moment matrices. The matrix means ϕ_p which are information functions (Pukelsheim (1993)) we utilized in this study.

The amount of information inherent to $C_k(M(\tau))$ is provided by Kiefers ϕ_p-criteria with $C_k(M(\tau)) \in$ PD (m+1).

These are defined by:

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

for all C in PD$(m+1)$, the set of positive definite $(m+1)\times(m+1)$ matrices, 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 2006, chapter 6). The class of ϕ_p-criteria includes the prominently used T-, D-, A- and E-criteria corresponding to parameter values 1, 0, -1 and -∞ respectively.

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

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

Subject to $C_k(M(\tau)) \in$ PD$(m+1)$

Theorem 1.0

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

$$traceC_jC_k(M(\eta(\alpha)))^{p-1} \begin{cases} = traceC_k(M(\eta(\alpha)))^p & for \quad all \quad j \in \partial(\alpha) \\ \leq traceC_k(M(\eta(\alpha)))^p & otherwise \end{cases}$$

Klein (2002).

Weighted centroid designs are exchangeable, that is, they are invariant under permutations of ingredients.

1.3 Optimal Weighted Centroid Designs

A convex combination, $\eta(\alpha) = \sum_{j=1}^{m} \alpha_j \eta_j$, with $\alpha = (\alpha_1, ..., \alpha_m)' \in T_m$, is called a weighted centroid design with weight vector α restricted by $\sum_{i=1}^{m} \alpha_i = 1$. These designs were introduced by Scheffe' (1963). Weighted centroid designs are exchangeable, that is they are invariant under permutations Klein (2002).

Klein (2002) summarized the work by Draper and Heiligers (1999) and Draper, Heiligers and Pukelsheim (2000) by putting forward an idea that affirms the importance of weighted centroid design for the Kronecker model. The researcher proved that, in the second degree Kronecker model for mixture experiments with m $\geq$ 2 ingredients, the set of weighted centroid designs is an essentially complete class. That is, for every p $\in$ [- ∞ ;1] and for every design $\tau \in \mathrm{T}$ there exists a weighted centroid design η with

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

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

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

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

For the information matrix obtained, we show that the matrix is an improvement of a given design in terms of increasing symmetry, as well as obtaining a larger moment matrix under the Loewner ordering. These two criteria show that the information matrix obtained is Kiefer optimal for K' θ, the parameter subsystem of interest.

1.4 Information Matrices

Information matrices for subsystems of mean parameters in a classical linear model are derived. First,the coefficient matrix, K,is obtained, which will be used to identify the linear parameter subsystems $K'\theta$ of interest .Hence this will be utilized in generating the associated information matrices C_k for m factors. The information matrices so obtained will be useful in obtaining the optimality criteria. As an illustration the information matrices for three factors can be derived as follows:

1.4.1Information matrices for three ingredients

The information matrix for three ingredients for a mixture experiment is given by

$$C_k = C_k(M(n(\alpha))) = \begin{bmatrix} \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{9\alpha_2}{16} \end{bmatrix}$$

Proof

First the coefficient matrix, K, for m=3 is derived as follows

$$K_1 = \sum_{i=1}^{3} e_{iii}e_i' = e_{111}e_1' + e_{222}e_2' + e_{333}e_3', \text{ and}$$

$$K_2 = \frac{1}{(3^3-3)}\left\{ \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \left(e_{iij} + e_{iji} + e_{jii}\right) + \sum_{\substack{i,j,k=1 \\ i \neq j \neq k}}^{3} \left(e_{ijk}\right) \right\} = e_{112} + e_{121} + e_{211} + e_{113} + e_{131} + e_{311}$$

$$+e_{221} + e_{212} + e_{122} + e_{223} + e_{232} + e_{322}$$

$$+e_{331} + e_{313} + e_{133} + e_{332} + e_{323} + e_{233}$$

$$+e_{123} + e_{132} + e_{213} + e_{231} + e_{312} + e_{321}$$

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

$$L = (K'K)^{-1}K'$$

$$= \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1 \\ 0&1&1&1&1&1&1&1&1&1&1&1&1&0&1&1&1&1&1&1&1&1&1&1&1&1&0 \end{bmatrix}.$$

For the design η_1 , the information matrix is given by

$$C_1 = LM(n_1)L' = \begin{bmatrix} \frac{1}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = C_k(M(n_1))$$

While that of design η_2 is given by

$$C_2 = LM(n_2)L' = \begin{bmatrix} \frac{1}{96} & \frac{1}{192} & \frac{1}{192} & \frac{1}{16} \\ \frac{1}{192} & \frac{1}{96} & \frac{1}{192} & \frac{1}{16} \\ \frac{1}{192} & \frac{1}{192} & \frac{1}{96} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{9}{16} \end{bmatrix} = C_k(M(n_2))$$

$$C_k = C_k(M(n(\alpha))) = \begin{bmatrix} \frac{32\alpha_1 + \alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{192} & \frac{32\alpha_1 + \alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{32\alpha_1 + \alpha_2}{96} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{9\alpha_2}{16} \end{bmatrix}$$

This is the desired information matrix for three ingredients.

1.6 D-optimal weighted centroid designs

We derive optimal weighted centroid designs for the determinant criterion, ϕ_0 , that is, D-optimality criteria. The D-criterion has an important property in optimal designs because it minimizes the variance and the covariance of the parameters estimates.

1.6.1D-optimal design for m=3 ingredients

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

$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.7474373094\eta_1 + 0.252626906\eta_2$.

The maximum value of the D-criterion for $K'\theta$ in three ingredients is

$v(\phi_0) = 0.216665662$.

Proof

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

$trace C_j C(\alpha)^{-1} = trace C(\alpha)^0 = trace I_s \;\; for \; all \;\; j \in \{1,2\}$.

Therefore for j=1

$$C_1C_k^{-1}=\begin{pmatrix} \frac{192\alpha_1+\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{-1}{9\alpha_1} \\ \frac{\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{192\alpha_1+\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{-1}{9\alpha_1} \\ \frac{\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{192\alpha_1+\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)} & \frac{-1}{9\alpha_1} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$trace\,C_1C(\alpha)^{-1}=\frac{192\alpha_1+\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)}+\frac{192\alpha_1+\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)}+\frac{192\alpha_1+\alpha_2}{3\alpha_1(64\alpha_1+\alpha_2)}+0=\frac{192\alpha_1+\alpha_2}{\alpha_1(64\alpha_1+\alpha_2)}$$ and

$traceC_k^0=traceI_4=4$.

Thus

$$trace\,C_1C(\alpha)^{-1}=traceI_4\Leftrightarrow\frac{192\alpha_1+\alpha_2}{\alpha_1(64\alpha_1+\alpha_2)}=4,$$

which reduces to

$$252\alpha_1^2-187\alpha_1-1=0$$

Solving this polynomial together with $\alpha_1+\alpha_2=1$ yields

$\alpha_1=-0.005309602$ or $\alpha_1=0.747373094$

We take $\alpha_1=0.747373094$ since $\alpha_1\in(0,1)$.

For j=2

$$C_2C_k^{-1}=\begin{pmatrix} \frac{a}{96}+\frac{b}{96}+\frac{c}{16} & \frac{a}{192}+\frac{3b}{192}+\frac{c}{16} & \frac{a}{192}+\frac{3b}{192}+\frac{c}{16} & \frac{c}{48}+\frac{d}{16} \\ \frac{a}{192}+\frac{3b}{192}+\frac{c}{16} & \frac{a}{96}+\frac{b}{96}+\frac{c}{16} & \frac{a}{192}+\frac{3b}{192}+\frac{c}{16} & \frac{c}{48}+\frac{d}{16} \\ \frac{a}{192}+\frac{3b}{192}+\frac{c}{16} & \frac{a}{192}+\frac{3b}{192}+\frac{c}{16} & \frac{a}{96}+\frac{b}{96}+\frac{c}{16} & \frac{c}{48}+\frac{d}{16} \\ \frac{a}{16}+\frac{2b}{16}+\frac{9c}{16} & \frac{a}{16}+\frac{2b}{16}+\frac{9c}{16} & \frac{a}{16}+\frac{2b}{16}+\frac{9c}{16} & \frac{3c}{16}+\frac{9d}{16} \end{pmatrix}$$

$a=\dfrac{192\alpha_1+\alpha_2}{\alpha_1(64\alpha_1+\alpha_2)}$, $b=\dfrac{\alpha_2}{\alpha_1(64\alpha_1+\alpha_2)}$, $c=\dfrac{-1}{3\alpha_1}$, and $d=\dfrac{16\alpha_1+\alpha_2}{9\alpha_1\alpha_2}$.

and

$$\begin{aligned} traceC_2C(\alpha)^{-1} &= \frac{a}{96}+\frac{b}{96}+\frac{c}{16}+\frac{a}{96}+\frac{b}{96}+\frac{c}{16}+\frac{a}{96}+\frac{b}{96}+\frac{c}{16}+\frac{3c}{16}+\frac{9d}{16} \\ &= \frac{a}{32}+\frac{b}{32}+\frac{6c}{16}+\frac{9d}{16} \\ &= \frac{192\alpha_1+\alpha_2}{32\alpha_1(64\alpha_1+\alpha_2)}+\frac{\alpha_2}{32\alpha_1(64\alpha_1+\alpha_2)}-\frac{6}{48\alpha_1}+\frac{9(16\alpha_1+\alpha_2)}{16\times 9\alpha_1\alpha_2} \\ &= \frac{1024\alpha_1+48\alpha_2}{16\alpha_2(64\alpha_1+\alpha_2)} \end{aligned}$$

Thus

$$trace\,C_2C(\alpha)^{-1}=trace\,I_4\Leftrightarrow\frac{1024\alpha_1+48\alpha_2}{16\alpha_2(64\alpha_1+\alpha_2)}=4,$$ which reduces to

$$252\alpha_2^2-317\alpha_2+64=0$$

Solving this polynomial together with $\alpha_1+\alpha_2=1$ yields

$\alpha_2=1.005309602$ or $\alpha_2=0.252626906$

We take $\alpha_2 = 0.252626906$ since $\alpha_2 \in (0,1)$.

Implying that, the unique D-optimal weighted centroid design for $K'\theta$ in m=3 ingredients is $\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.747373094\eta_1 + 0.252626906\eta_2$ as required.

From Pukelsheim (1993), the maximum value of the D-criterion is obtained as

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

For $m = 3$, we have $v(\phi_0) = (\det[C(\alpha)])^{\frac{1}{4}}$.

the information matrix for a design with three ingredients is given by

$$C_k = C_k(M(n(\alpha))) = \begin{bmatrix} \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{192} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{192} & \frac{\alpha_2}{192} & \frac{32\alpha_1+\alpha_2}{96} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{9\alpha_2}{16} \end{bmatrix}.$$

Substituting for the values of α_1 and α_2 we get

$$C_k = \begin{bmatrix} 0.251755894 & 0.001315765 & 0.001315765 & 0.015789181 \\ 0.001315765 & 0.251755894 & 0.001315765 & 0.015789181 \\ 0.001315765 & 0.001315765 & 0.251755894 & 0.015789181 \\ 0.015789181 & 0.015789181 & 0.015789181 & 0.142102634 \end{bmatrix}$$

and $Det[C_k] = 0.002220374$.

Hence the optimal value of the D-criterion for $K'\theta$ in three ingredients is $v(\phi_0) = (\det[C(\alpha)])^{\frac{1}{4}} = (0.002220374)^{\frac{1}{4}} = 0.216665662$

1.8 D-optimal design for m ingredients
Theorem 1.2

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

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

where,

$$\alpha_1 = \frac{(31m^2 - 32m + 4) + \sqrt{(961m^4 - 1860m^3 + 1028m^2 - 384m + 256)}}{2(m+1)(31m-30)},$$

$$\alpha_2 = \frac{(31m^2 + 34m - 64) - \sqrt{(961m^4 - 1860m^3 + 1028m^2 - 384m + 256)}}{2(m+1)(31m-30)}.$$

The optimal value of the D-criterion for $K'\theta$ in $m \geq 2$ ingredients is

$$v(\phi_0) = (\det C(\alpha))^{\frac{1}{s}} = \left\{ \frac{9\alpha_1\alpha_2}{16m} \left(\frac{32(m-1)\alpha_1 + (m-2)\alpha_2}{32m(m-1)} \right)^{m-1} \right\}^{\frac{1}{m+1}}$$

Proof

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

Equation implies that for p=0,

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

From equation (4), any matrix $C \in Sym(s,H)$ can be uniquely represented in the form

$$C = \begin{pmatrix} aU_1 + bU_2 & cV \\ cV' & d\frac{V'V}{m} \end{pmatrix},$$

with coefficients $a,b,c,d \in \Re$.

Furthermore, any given symmetric matrix $C \in Sym(s)$, can be partitioned according to the block structure of matrices in H, that is

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C'_{12} & C_{22} \end{pmatrix},$$

with $C_{11} \in sym(m)$, $C_{12} \in \Re^{m\times 1}$ and $C_{22} \in \Re^1$ Klein (2004).

For $j = 1$, we have

$$traceC_1C_k(\alpha)^{-1} = traceC(\alpha)^0 = trace\,I_s$$

where

$$C_1C_k(\alpha)^{-1} = \begin{pmatrix} \frac{a}{m}U_1 + \frac{b}{m}U_2 & \frac{c}{m}V \\ 0 & 0 \end{pmatrix},$$

where, $a = \dfrac{32m(m-1)\alpha_1 + (m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}$, $b = \dfrac{(m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}$, and $c = \dfrac{-1}{3\alpha_1}$

giving,

$trace(C_1C_k(\alpha)^{-1}) = trace\left(\frac{a}{m}U_1 + \frac{b}{m}U_2\right) + 0 = trace\frac{a}{m}U_1$, since $trace(U_1) = m$ and $trace(U_2) = 0$

Therefore,

$$trace(C_1C_k(\alpha)^{-1}) = \left\{ m\frac{32m(m-1)\alpha_1 + (m-2)\alpha_2}{m\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} \right\}$$

$$= \frac{32m(m-1)\alpha_1 + (m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]}$$

Also for m factors, $trace\,I_s = (m+1)$, where $s = (m+1)$.

Thus

$$traceC_1C_k(\alpha)^{-1} = traceC(\alpha)^0 = trace\,I_s,$$

$$\Leftrightarrow \frac{32m(m-1)\alpha_1 + (m-2)\alpha_2}{\alpha_1[32(m-1)\alpha_1 + (m-2)\alpha_2]} = (m+1).$$

This reduces to

$$(m+1)(31m-30)\alpha_1^2 - (31m^2 - 32m + 4)\alpha_1 - (m-2) = 0$$

Solving this polynomial together with $\alpha_1 + \alpha_2 = 1$ yields

$$\alpha_1 = \frac{(31m^2 - 32m + 4) + \sqrt{(961m^4 - 1860m^3 + 1028m^2 - 384m + 256)}}{2(m+1)(31m-30)} \quad \alpha_1 \in (0,1).$$

Similarly,

$$C_2 C_k(\alpha)^{-1} = \begin{pmatrix} a'''U_1 + b'''U_2 & c'''V \\ c'''V' & d'''\frac{V'V}{m} \end{pmatrix}$$

where, $a''' = \frac{(m-1)(m-2)}{m[32(m-1)\alpha_1 + (m-2)\alpha_2]}$, $b''' = \frac{-(m-2)}{m[32(m-1)\alpha_1 + (m-2)\alpha_2]}$, $c''' = \frac{1}{3m\alpha_2}$

and $d''' = \frac{1}{\alpha_2}$

Hence

$$trace(C_2 C_k(\alpha)^{-1}) = \left\{ m\left(\frac{(m-1)(m-2)}{m[32(m-1)\alpha_1 + (m-2)\alpha_2]} \right) + \frac{1}{\alpha_2} \right\}$$

$$= \frac{(m-1)(m-2)}{[32(m-1)\alpha_1 + (m-2)\alpha_2]} + \frac{1}{\alpha_1}$$

Therefore,

$$traceC_2 C_k(\alpha)^{-1} = traceC(\alpha)^0 = traceI_s, \Leftrightarrow \frac{(m-1)(m-2)}{[32(m-1)\alpha_1 + (m-2)\alpha_2]} + \frac{1}{\alpha_1} = (m+1),$$

which reduces to

$$(m+1)(31m-30)\alpha_2^2 - (31m^2 + 34m - 64)\alpha_2 + 32(m-1) = 0$$

Solving this polynomial together with $\alpha_1 + \alpha_2 = 1$ yields

$$\alpha_2 = \frac{(31m^2 + 34m - 64) - \sqrt{(961m^4 - 1860m^3 + 1028m^2 - 384m + 256)}}{2(m+1)(31m-30)} \quad \alpha_2 \in (0,1).$$

the information matrix for a design with m factors is given by

$$C_k(\alpha) = \alpha_1 C_1 + \alpha_2 C_2 = \begin{pmatrix} \frac{32\alpha_1 + \alpha_2}{32m} U_1 + \frac{\alpha_2}{32m(m-1)} U_2 & \frac{3\alpha_2}{16m} V \\ \frac{3\alpha_2}{16m} V' & \frac{9\alpha_2}{16} \frac{V'V}{m} \end{pmatrix}$$

Hence the optimal value of the D-criterion for $K'\theta$ in $m \geq 2$ ingredients is

$$v(\phi_0) = (\det C(\alpha))^{\frac{1}{s}} = \left\{ \frac{9\alpha_1\alpha_2}{16m} \left(\frac{32(m-1)\alpha_1 + (m-2)\alpha_2}{32m(m-1)} \right)^{m-1} \right\}^{\frac{1}{m+1}}$$

where,

$$\alpha_1 = \frac{(31m^2 - 32m + 4) + \sqrt{(961m^4 - 1860m^3 + 1028m^2 - 384m + 256)}}{2(m+1)(31m-30)},$$

$$\alpha_2 = \frac{(31m^2 + 34m - 64) - \sqrt{(961m^4 - 1860m^3 + 1028m^2 - 384m + 256)}}{2(m+1)(31m-30)}$$

and $s = (m+1)$.

A. Numerical Example Using Artificial Sweetener Experiment Of Three Components Mixture Experiment

The D optimal design for three factors can now be applied to three factor numerical example .In these study only pure blends and binary blends are considered where the average score is the response.

Consider the following simplex centroid design for three ingredients as the initial design.

Design points	t_1	t_2	t_3	average score
1	1	0	0	10.40
2	0	1	0	6.16
3	0	0	1	3.90
4	$\frac{1}{2}$	$\frac{1}{2}$	0	14.97
5	$\frac{1}{2}$	0	$\frac{1}{2}$	12.17
6	0	$\frac{1}{2}$	$\frac{1}{2}$	12.27

Where t_1=glycine,t_2=saccharin and t_3=enhancer

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

Implying that, the unique D-optimal weighted centroid design for $K'\theta$ in m=3 ingredients is $\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.747373094\eta_1 + 0.252626906\eta_2$ as shown above. Therefore the corresponding D-optimal for the above designs is as follows.

Design points	t_1	t_2	t_3
1	0.747373094	0	0
2	0	0.747373094	0
3	0	0	0.747373094
4	0.126313453	0.126313453	0
5	0.126313453	0	0.126313453
6	0	0.126313453	0.126313453

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