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Extensions of D-optimal Minimal Designs for Symmetric Mixture Models

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Abstract

The purpose of mixture experiments is to explore the optimum blends of mixture components, which will provide desirable response characteristics in finished products. D-optimal minimal designs have been considered for a variety of mixture models, including Scheffé's linear, quadratic, and cubic models. Usually, these D-optimal designs are minimally supported since they have just as many design points as the number of parameters. Thus, they lack the degrees of freedom to perform the Lack of Fit tests. Also, the majority of the design points in D-optimal minimal designs are on the boundary: vertices, edges, or faces of the design simplex.

In This Paper, Extensions Of The D-Optimal Minimal Designs Are Developed For A General Mixture Model To Allow Additional Interior Points In The Design Space To Enable Prediction Of The Entire Response Surface—Also a new strategy for adding multiple interior points for symmetric mixture models is proposed. We compare the proposed designs with Cornell (1986) two ten-point designs for the Lack of Fit test by simulations.

Keywords

Mixture models; Interior design points; D-optimal minimal design; Lack of Fit

1 Introduction

Mixture experiments, where the predictor variables are proportions of the non-negative components adding to 1, are increasingly used in chemical, pharmaceutical, biomedical and epidemiological research. The cost restrictions often seek as few design points as possible in order to address a particular problem efficiently. Then the standard approach is to construct a D-optimal minimal design that maximizes the determinant of the Fisher information matrix. D-optimal designs are known for a variety of mixture models, including Scheffé's linear, quadratic and special cubic models. Chan (2000) summarized known optimal designs for various mixture models. These designs usually contain the same number of design points as the number of parameters in the models. Therefore, minimal supported designs do not allow

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for performing the Lack of Fit (LOF) test. Most of their design points are on the boundary (vertices, edges, faces) of the design space. As many mixture models aim to predict the entire response surface, it would be preferable to include some additional interior design points to test the adequacy of model by means of the LOF test.

For mixture models, commonly used designs include the simplex lattice design (Scheffé, 1958), the simplex centroid (Scheffé, 1963), the symmetric simplex design (Murty and Das, 1968) and the axial designs (Cornell, 1975). Their design points are mainly on the boundary: vertices, edges, or faces of design simplex. Optimum designs (optimum of D-, A-, and E-optimality criteria) for estimation of parameters of the response functions have also been studied (Galil and Kiefer, 1977; Liu and Neudecker, 1997; Pal and Mandal, 2006, 2007; Mandal and Pal, 2008, 2013). But the question of extending D-optimal minimal designs has not been addressed for mixture models. In this paper, we investigate an approach for adding interior design points to known D-optimal minimal designs for general mixture models including a wide subclass of symmetric mixture models. In section 2, we consider adding one interior design point for general mixture models and investigate adding multiple interior points for symmetric mixture models. In sections 3 to 5, we apply the proposed methodology to commonly used mixture models: Scheffé's quadratic, special cubic model and additive quadratic models. In section 6, we consider the LOF test for various mixture models and compare the proposed designs with two ten-points designs (Cornell, 1986) by simulation. Section 7 presents the conclusions.

2 Extensions of D-optimal Minimal Designs

2.1 One Additional Interior Point for General Mixture Models

A general nth order q-factor mixture model is defined as

$$y=\sum_{1\le i\le q}\beta_i x_i+\sum_{1\le i,j\le q}\beta_{ij}h_2(x_i,x_j)+\ldots+\sum_{1\le i_1,\ldots,i_n\le q}\beta_{i_1,\ldots,i_n}h_n(x_{i_1},\ldots,x_{i_n})+\varepsilon. \tag{1}$$

where $\sum_{i=1}^{q}x_i=1$, $x_i \ge 0$ for all i, **and each function** $h_k(x_{i_1}, \ldots, x_{i_k})$ **is a twice differentiable function of** k **arguments,** $k = 2, \ldots, n$. **For most commonly used mixture models,** $h_k(x_{i_1}, \ldots, x_{i_k})$ **are polynomial functions**. For any q nonnegative components $(x_1, x_2, \ldots, x_q)$, we use $x \leftrightarrow (x_1, x_2, \ldots, x_q)$ to denote any permutation of $(x_1, x_2, \ldots, x_q)$. In addition, we use $C(n, k)$ to denote $n!/[k!(n-k)!]$, when $n \ge k \ge 0$ are integers. The most common particular case of model (1) is the Scheffé's q-factor polynomial model of order n,

$$y=\sum_{1\le i\le q}\beta_i x_i+\sum_{1\le i<j\le q}\beta_{ij}x_i x_j+\ldots+\sum_{1\le i_1<\ldots<i_n\le q}\beta_{i_1,\ldots,i_n}x_{i_1},\ldots,x_{i_n}+\varepsilon. \tag{2}$$

Also, if $\Sigma_{1\le i_1,\ldots,i_n\le q}\beta_{i_1,\ldots,i_k}x_{i_1}\ldots x_{i_k}$ reduces to $\sum_{1\le i\le q}\beta_{i,\ldots,i}x_i^k$ for $1 \le k \le n$, then model (1) becomes the q-factor additive polynomial model of order n,

$$y=\sum_{1\leq i\leq q}\beta_i x_i+\sum_{1\leq i\leq q}\beta_{ii}x_i^2+\ldots+\sum_{1\leq i\leq q}\beta_{i,\ldots,i}x_i^n+\varepsilon, \quad (3)$$

Polynomial mixture models are most common, but other mixture models have been also studied and employed (Becker, 1968, 1978; Zhang and Wong, 2013).

The D-optimal minimal designs are known for a variety of mixture models. Let **X** be the given $M_n \times M_n$ D-optimal minimal design matrix for model (1). For example, for general polynomial mixture model, $M_n = C(q + n - 1, n)$, and for general additive polynomial model, $M_n = nq$. Without loss of generality, we assume $\sigma^2 = 1$. Then the corresponding nonsingular information matrix $(\mathbf{X}'\mathbf{X})$ is also known. The design matrix is constructed as

$$\mathbf{X}=\begin{bmatrix} x_{11} & \cdots & x_{1q} & h_2(x_{11},x_{12}) & \cdots & h_n(x_{11},\ldots,x_{1q}) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{M_n1} & \cdots & x_{M_nq} & h_2(x_{M_n1},x_{M_n2}) & \cdots & h_n(x_{M_n1},\ldots,x_{M_nq}) \end{bmatrix}$$

and is partitioned as $\mathbf{X}=\begin{bmatrix}\mathbf{V} & \mathbf{U}\end{bmatrix}$, with $M_n \times q$ matrix $\mathbf{V}=\begin{bmatrix}\mathbf{v_1} & \cdots & \mathbf{v_{M_n}}\end{bmatrix}'$, where $\mathbf{v}_i'=[x_{i1},\ldots,x_{iq}]$, and $M_n \times (M_n - q)$ matrix $\mathbf{U}=\begin{bmatrix}\mathbf{u_1} & \cdots & \mathbf{u_{M_n}}\end{bmatrix}'$, where $\mathbf{u_i}'=[h_2(x_{i1},x_{i2}),\ldots,h_n(x_{i1},\ldots,x_{iq})]$. Respectively,

$$\mathbf{X}'\mathbf{X}=\begin{bmatrix}\mathbf{V}'\\ \mathbf{U}'\end{bmatrix}\begin{bmatrix}\mathbf{V} & \mathbf{U}\end{bmatrix}=\begin{bmatrix}\mathbf{V}'\mathbf{U} & \mathbf{V}'\mathbf{U}\\ \mathbf{U}'\mathbf{V} & \mathbf{U}'\mathbf{U}\end{bmatrix}, \quad (4)$$

where $\mathbf{V}'\mathbf{V}$ is a $q \times q$ matrix and $\mathbf{U}'\mathbf{U}$ is a $(M_n - q) \times (M_n - q)$ matrix. Let us further denote

$$(X'X)^{-1}=\begin{bmatrix}\mathbf{A} & \mathbf{B}'\\ \mathbf{B} & \mathbf{D}\end{bmatrix} \quad (5)$$

Using the Schur Complement,

$$\begin{aligned}\mathbf{A}&=\left(\mathbf{V}'\mathbf{V}-\mathbf{V}'\mathbf{U}(\mathbf{U}'\mathbf{U})^{-1}\mathbf{U}'\mathbf{V}\right)^{-1}\\ \mathbf{D}&=\left(\mathbf{U}'\mathbf{U}-\mathbf{U}'\mathbf{V}(\mathbf{V}'\mathbf{V})^{-1}\mathbf{V}'\mathbf{U}\right)^{-1}\\ \mathbf{B}&=-\left[\mathbf{U}'\mathbf{U}-\mathbf{U}'\mathbf{V}(\mathbf{V}'\mathbf{V})^{-1}\mathbf{V}'\mathbf{U}\right]^{-1}\mathbf{U}'\mathbf{V}(\mathbf{V}'\mathbf{V})^{-1}.\end{aligned}$$

First, consider the problem of adding one interior design point to the known D-optimal minimal design. Let $\mathbf{z}_1' = (\mathbf{v}_1', \mathbf{u}_1')$ be the new interior design point to be added, where

$$\mathbf{v}_1' = (x_1^z, \ldots, x_q^z), \quad (6)$$

$$\mathbf{u}_1' = \mathbf{u}_1'(\mathbf{v}_1) = (h_2(x_1^z, x_2^z), \ldots, h_n(x_1^z, \ldots, x_q^z)), \quad (7)$$

with $0 < x_1^z, \ldots, x_q^z < 1$ and $\mathbf{v}_1' 1 = 1$. Further denote by $\mathbf{X_1}$ the new design matrix, $\mathbf{X_1} = \begin{bmatrix} \mathbf{X} \\ \mathbf{z}_1' \end{bmatrix}$.

Theorem 1 For the extended design $\mathbf{X_1}$, $|\mathbf{X}_1' \mathbf{X_1}|$ has a local maximum with respect to additional interior design point $\mathbf{z}_1' = (\mathbf{v}_1', \mathbf{u}_1')$ (with $0 < x_1^z, \ldots, x_q^z < 1$ and $\mathbf{v}_1' \mathbf{1} = 1$) if and only if $\mathbf{v}_1$ is a solution of the equations

$$\begin{bmatrix} -\mathbf{1_{q-1}} & \mathbf{I_{q-1}} \end{bmatrix} \begin{bmatrix} \mathbf{I_q} & \mathbf{K} \end{bmatrix} (\mathbf{X}'\mathbf{X})^{-1} \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{u}_1 \end{bmatrix} = \mathbf{0} \quad (8)$$

where $\mathbf{K} = \frac{\partial \mathbf{u}'}{\partial \mathbf{v}}$ and $\mathbf{1_{q-1}}$ is a column vector of $(q-1)$ ones. The Hessian matrix

$$\mathbf{A} + \frac{\partial \mathbf{u}'}{\partial \mathbf{v}} \mathbf{B} + \mathbf{B}' \frac{\partial \mathbf{u}'}{\partial \mathbf{v}} + \frac{\partial \mathbf{u}'}{\partial \mathbf{v}} \mathbf{D} \frac{\partial \mathbf{u}}{\partial \mathbf{v}'} + \begin{bmatrix} (\mathbf{v}'\mathbf{B}' + \mathbf{u}'\mathbf{D}) \frac{\partial^2 \mathbf{u}}{\partial v_1 \partial v_1} & \cdots & (\mathbf{v}'\mathbf{B}' + \mathbf{u}'\mathbf{D}) \frac{\partial^2 \mathbf{u}}{\partial v_1 \partial v_q} \\ \cdots & \cdots & \cdots \\ (\mathbf{v}'\mathbf{B}' + \mathbf{u}'\mathbf{D}) \frac{\partial^2 \mathbf{u}}{\partial v_q \partial v_1} & \cdots & (\mathbf{v}'\mathbf{B}' + \mathbf{u}'\mathbf{D}) \frac{\partial^2 \mathbf{u}}{\partial v_q \partial v_q} \end{bmatrix} \quad (9)$$

is negative definite.

The proof of Theorem 1 is given in the Appendix 1.

2.2 Symmetric Mixture Models

We consider model (1) to be a symmetric mixture model if all functions

$$H_k(x_1, x_2, \ldots x_q) = \sum_{1 \le i_1 \le, \cdots \le, i_k \le q} h_k(x_{i_1}, \ldots, x_{i_k}), \quad 1 \le k \le n, \quad (10)$$

with $\sum_{1\le i\le q} h_1(x_{i_1},\ldots,x_{i_k}) \stackrel{\text{def}}{=} \sum_{1\le i\le q} x_i$, are symmetric functions of q arguments $x_1, \ldots, x_q$. Most of the commonly used mixture models are symmetric, including the Scheffé's quadratic, special cubic, full cubic, and additive mixture models. From the proof of Theorem 1, it is straightforward to obtain the Proposition 1 below:

Proposition 1 Let model (1) be symmetric and $f(\mathbf{v}){=}\mathbf{z}_1^{'}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1$ be a symmetric function of q variables $x_1^z,\ldots,x_q^z$. The extended minimal design with one added point $\mathbf{v}_1$ has the same D-efficiency as the extended minimal design with one added point $\mathbf{v}_2$ if $\mathbf{v}_2 \leftrightarrow \mathbf{v}_1$.

Thus, for symmetric mixture models, each stationary point, except for the overall centroid, provides at least q distinct additional design points. The following proposition gives a sufficient condition for $f(\mathbf{v})$ to be a symmetric function.

Proposition 2 Let $(\mathbf{X}'\mathbf{X})^{-1}$ be partitioned as in (5). If matrices **A**, **B** and **D** are such that functions $\mathbf{v}_1^{'}\mathbf{A}\mathbf{v}_1, \mathbf{u}_1^{'}\mathbf{B}\mathbf{v}_1$, and $\mathbf{u}_1^{'}\mathbf{D}\mathbf{u}_1$ are invariant with respect to a transposition of any i^{th} and j^{th} coordinates of vector $\mathbf{v}_1$ ($1 \le i \le j \le q$), then $f(\mathbf{v}_1){=}\mathbf{z}_1^{'}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1$ is a symmetric function of q arguments

Proof: Since any permutation can be expressed as a composition of a sequence of transpositions, it is sufficient to show that function $f(\mathbf{v}_1){=}\mathbf{z}_1^{'}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1$ is invariant with respect to any transposition of arguments (a permutation of any two coordinates x_i^z and x_j^z in the independent subvector $\mathbf{v}_1^{'}{=}(x_1^z,\ldots,x_q^z)$). Using (5), $f(\mathbf{v}_1){=}\mathbf{z}_1^{'}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1{=}\mathbf{v}_1^{'}\mathbf{A}\mathbf{v}_1{+}2\mathbf{u}_1^{'}\mathbf{B}\mathbf{v}_1{+}\mathbf{u}_1^{'}\mathbf{D}\mathbf{u}_1$. Then $f(\mathbf{v}_1)$ is invariant with respect to a permutation of any two coordinates x_i^z and x_j^z by the assumptions.

3 Scheffé's Quadratic Mixture Model

3.1 One Additional Point for Quadratic Mixture Model

Scheffé's quadratic mixture model is defined as

$$y{=}\sum_{1\le i\le q}\beta_i x_i{+}\sum_{1\le i<j\le q}\beta_{ij}x_i x_j{+}\varepsilon. \quad (11)$$

There are $\frac{q(q+1)}{2}$ parameters in the model and, hence at least $\frac{q(q+1)}{2}$ design points are needed to estimate all parameters. For practical applications, it is sufficient to consider models with 3 or more factors. Kiefer (1961) proved that the $\{q, 2\}$ simplex-lattice design is D-optimal. This minimal design contains q vertices $\leftrightarrow$ (1, 0, …, 0) and $C(q, 2)$ midpoints $\leftrightarrow$ (2, 2, 0, …, 0), and the blocks in $\mathbf{X}'\mathbf{X}$ are given by $\mathbf{V}'\mathbf{V}{=}\frac{q+2}{4}\mathbf{I}_q{+}\frac{1}{4}\mathbf{J}_q, \mathbf{U}'\mathbf{U}{=}\frac{1}{16}\mathbf{I}_{\frac{q(q-1)}{2}},$

where $\mathbf{I_q}$ is the identity matrix and $\mathbf{J_q}$ is the matrix of ones of order q, $\mathbf{U}'\mathbf{V} = (a_{ij,k})$ is $\frac{q(q-1)}{2} \times q$ matrix with

$$(a_{ij,k})=\begin{cases} \frac{1}{8} & \text{when} k=i \text{or} k=j, \\ 0 & \text{otherwise,} \end{cases}$$

where i, j, k = 1, 2, …, q and $i < j$ and the rows of $\mathbf{U}'\mathbf{V}$ are labeled ij representing all interaction terms. Then as shown in the Appendix 2, we have

$$(\mathbf{X}'\mathbf{X})^{-1}=\begin{bmatrix} \mathbf{I_q} & -16\mathbf{V}'\mathbf{U} \\ -16\mathbf{U}'\mathbf{V} & 24\mathbf{B}_0+4\mathbf{B}_1 \end{bmatrix}, \quad (12)$$

where $\mathbf{B_0}$ and $\mathbf{B_1}$ are the association matrices of a triangular association scheme of order $\frac{q(q-1)}{2}$ defined in Appendix 2. Using the expression for $(\mathbf{X}'\mathbf{X})^{-1}$ provided in the Appendix 2, it is straightforward to show that conditions of Proposition 2 are satisfied. Hence, the conditions of Proposition 1 are satisfied, and all permutations of a stationary point result in the same determinant of the information matrix. Therefore, we can use the permutation of any stationary point except the overall centroid to get at least q additional distinct points. By solving equations (8), we get $(2q + 1)$ stationary points. We sort the stationary points to three solution groups according to their distance to the overall centroid points, calculated as $\sqrt{\sum_{i=1}^{q}(x_i-\frac{1}{q})^2}$.

Solution IQ: overall centroid $x=(\frac{1}{q},\ldots,\frac{1}{q})$,

Solution IIQ: $x \leftrightarrow (1-(q-1)\delta, \delta, \ldots, \delta)$, where $\delta=\frac{(5q+2+\sqrt{q^2-4q+76})}{8(q^2+q-3)}$,

Solution IIIQ: $x \leftrightarrow (1-(q-1)\delta, \delta, \ldots, \delta)$, where $\delta=\frac{(5q+2-\sqrt{q^2-4q+76})}{8(q^2+q-3)}$,

Let us denote $\mathbf{v}_1'\mathbf{B}'+\mathbf{u}_1'\mathbf{D}=\begin{bmatrix} w_{q+1} & w_{q+2} & \cdots & w_{\frac{q(q+1)}{2}} \end{bmatrix}$. Then the Hessian matrix is

$$\frac{\partial^2 f(\mathbf{v})}{\partial\mathbf{v}\partial\mathbf{v}'}=2\begin{bmatrix} \mathbf{I}_q & \mathbf{K} \end{bmatrix}(\mathbf{X}'\mathbf{X})^{-1}\begin{bmatrix} \mathbf{I}_q \\ \mathbf{K}' \end{bmatrix}+\mathbf{W},$$

where $\mathbf{K}=\frac{\partial\mathbf{u}'}{\partial\mathbf{v}}$ and

$$\mathbf{W}=2\begin{bmatrix} 0 & w_{q+1} & w_{q+2} & \cdots & w_{2q-1} \\ w_{q+1} & 0 & w_{2q} & \cdots & w_{3q-3} \\ w_{q+2} & w_{2q} & 0 & \cdots & w_{4q-6} \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ w_{2q-2} & w_{3q-4} & w_{4q-7} & \cdots & w_{\frac{q(q+1)}{2}} \\ w_{2q-1} & w_{3q-3} & w_{4q-6} & \cdots & 0 \end{bmatrix}. \quad (13)$$

The proof of Theorem 1 implies that the first part of this Hessian matrix is a non-negative definite matrix. The second part, matrix **W**, cannot be a negative definite matrix because $\mathbf{e}_{\mathbf{k}}'\mathbf{W}\mathbf{e}_{\mathbf{k}}=0$ for any canonical vector $\mathbf{e}_{\mathbf{k}}$. Hence the Hessian matrix cannot be a negative definite matrix, and none of the interior stationary points can be a local maximum of $\mathbf{z}_1'(\mathbf{X}'X)^{-1}\mathbf{z}_1$. In the absence of a local maximum, we select an additional design point among the stationary interior points so that the value of $\mathbf{z}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1$ is maximized. Among the stationary points, solution I obtains the maximum value of $\mathbf{z}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1$ when $q = 3$ and solution II has the maximum value of $\mathbf{z}_1'(\mathbf{X}'X)^{-1}\mathbf{z}_1$ when $q \geq 4$.

3.2 Multiple Design Points for Quadratic Mixture Model

Since the quadratic mixture model is a symmetric model, the multiple interior design points could be obtained as permutations of any stationary solutions except for the overall centroid. Thus, we consider the following Designs IIQ and IIIQ based on solutions IIQ and IIIQ:

Design IIQ: minimal design plus $x \leftrightarrow (1 - q - 1)\delta, \delta, \ldots, \delta)$, where $\delta=\frac{(5q+2+\sqrt{q^2-4q+76})}{8(q^2+q-3)}$.

Design IIIQ: minimal design plus $x \leftrightarrow (1 - q - 1)\delta, \delta, \ldots, \delta)$, where $\delta=\frac{(5q+2-\sqrt{q^2-4q+76})}{8(q^2+q-3)}$.

The new Designs IIQ and IIIQ are compared to the following commonly used designs:

Design IV: minimal design plus q midpoints between vertices and the overall centroid, i.e. $x \leftrightarrow \left(\frac{q+1}{2q}, \frac{1}{2q}, \ldots, \frac{1}{2q}\right)$.

Design V: minimal design plus q midpoints between vertices and (0, $\frac{1}{q-1}, \ldots, \frac{1}{q-1}$), i.e. $x \leftrightarrow \left(\frac{1}{2}, \frac{1}{2(q-1)}, \ldots, \frac{1}{2(q-1)}\right)$.

Design VI: minimal design plus q midpoints between the overall centroid and (0, $\frac{1}{q-1}, \ldots, \frac{1}{q-1}$), i.e. $x \leftrightarrow \left(\frac{1}{2q}, \frac{2q-1}{2q(q-1)}, \ldots, \frac{2q-1}{2q(q-1)}\right)$.

Usually Designs IV-VI are augmented with the overall centroid point, so we add the overall centroid to all considered designs, and compare designs with a total of $(q + 1)$ additional interior points. The D-efficiency is calculated as $100 \times |\mathbf{X}'\mathbf{X}|^{\mathbf{1/p}}/N$, where $p = C(q, 2)$ is the number of parameters in the mixture model, and N is the number of points used to fit the model. Here $N = C(q, 2) + q + 1$. Table 1 summarizes the D-efficiency (denoted as D_{q+1}) for all considered extended minimal plus $(q + 1)$ points designs. In summary, the proposed design has higher or comparable D-efficiencies when compared to standard designs. More specifically, Design IIIQ has the highest D-efficiency among all designs except for $q = 3$; Design VI has the highest D-efficiency when $q = 3$. However the difference is relatively small mainly because the determinant of the information matrix from D-optimal minimal design decreases when the number of factors increase.

4 Additive Quadratic Mixture Model

The additive quadratic mixture model is defined as

$$y=\sum_{i=1}^{q}\beta_i x_i+\sum_{i=1}^{q}\beta_{ii}x_i^2+\varepsilon. \qquad (14)$$

There are $2q$ parameters in the model and at least $2q$ design points are needed to estimate all parameters. Here, we consider additive quadratic models with $q \geq 3$. Chan et al (1995, 1998) proved that the D-optimal saturated axial design for model (14) contains the points $x \leftrightarrow (1, 0, \ldots, 0)$, and $x \leftrightarrow (1 - (q - 1)\delta, \delta, \ldots, \delta)$, where $\delta = 1/(q - 1)$ when $3 \leq q \leq 6$, and $\delta=((5q-1)-\sqrt{(9q^2-10q+1)})/(4q^2)$ when $q \geq 7$. The last expression for δ is asymptotically 1/2 when $q \to \infty$. As shown in the Appendix 3, the blocks of $(\mathbf{X}'\mathbf{X})^{-1}$ are given by $\mathbf{A} = a_1(q, \delta)\mathbf{I}_q + a_2(q, \delta)\mathbf{J}_q$, $\mathbf{B} = b_1(q, \delta)\mathbf{I}_q + b_2(q, \delta)\mathbf{J}_q$, $\mathbf{D} = d_1(q, \delta)\mathbf{I}_q + d_2(q, \delta)\mathbf{J}_q$.

Since the block of $(\mathbf{X}'\mathbf{X})^{-1}$ is the linear combination of $\mathbf{I_q}$ and $\mathbf{J_q}$, it is straightforward that conditions of Proposition 2 are satisfied. Thus, conditions of Proposition 1 are satisfied and we can use permutations of any stationary point except the overall centroid to obtain at least q additional interior points.

Denoting

$$\mathbf{v}'\mathbf{B}'+\mathbf{u}'\mathbf{D}=\begin{bmatrix} w_{q+1} & w_{q+2} & \cdots & w_{2q} \end{bmatrix},$$

the Hessian matrix can be expressed as

$$\frac{\partial^2 f(\mathbf{v})}{\partial\mathbf{v}\partial\mathbf{v}'}=2\begin{bmatrix} \mathbf{I}_q & \mathbf{K} \end{bmatrix}(\mathbf{X}'\mathbf{X})-1\begin{bmatrix} \mathbf{I}_q \\ \mathbf{K}' \end{bmatrix}+\mathbf{W},$$

where

$$\mathbf{W}=4\begin{bmatrix} w_{q+1} & 0 & \cdots & 0 \\ 0 & w_{q+2} & \cdots & 0 \\ \vdots & \cdots & \cdots & \vdots \\ 0 & 0 & \cdots & w_{2q} \end{bmatrix}. \quad (15)$$

For any canonical vector $\mathbf{e_k}$ = (1, 0, …, 0),

$\mathbf{e}_{\mathbf{k}}^{'}\mathbf{W}\mathbf{e}_{\mathbf{k}}=b_1+b_2+d_1+d_2=\frac{3+\delta+q^2\delta-2q(1+\delta)}{\delta(q-2)(q-1)(q\delta-2)}$ is greater than 0 for all q. Hence the Hessian matrix cannot be a negative definite matrix, and the stationary points for the additive quadratic model are either local minimal points or saddle points. Since the additive quadratic model is symmetric, we can add q additional distinct interior design points by permuting stationary solutions except for the overall centroid. Design IIA and IIIA are the proposed designs, which consist of $3q + 1$ points: q permuted stationary points, one overall centroid and $2q$ D-optimal minimal design points. Design IIA has a shorter distance to the overall centroid than Design IIIA. Table 2 summarizes the D-efficiencies for proposed Designs IIA and IIIA, and standard Designs IV-VI in section 3.2. Note that there is only one stationary solution (overall centroid point) when $q = 4$ and Designs IIA-IIIA are not available for $q = 4$. In summary, Design IIA has the highest efficiency among all designs when $q \geq 4$ and Design VI has the highest efficiency when $q = 3$.

5 Special Cubic Mixture Model

Another commonly used mixture model is the Scheffé's Special cubic model. It is defined as:

$$y=\sum_{1\le i\le q}\beta_i x_i+\sum_{1\le i<j\le q}\beta_{ij}x_i x_j+\sum_{1\le i<j<k\le q}\beta_{iijk}x_i x_j x_k+\varepsilon. \quad (16)$$

Lim (1990) proved that the D-optimal minimal design contains x ↔ (1, 0, …, 0), $x \leftrightarrow (\frac{1}{2},\frac{1}{2},0,\ldots,0)$ and $x \leftrightarrow (\frac{1}{3},\frac{1}{3},\frac{1}{3},0,\ldots,0)$. There is a total of $M=C(q,1)+C(q,2)+C(q,3)=\frac{q^3+5q}{6}$ parameters in the model. As shown in the Appendix 4, the blocks of $(\mathbf{X}'\mathbf{X})^{-1}$ are $\mathbf{A} = \mathbf{I}_q$, $\mathbf{B}=\begin{bmatrix} -16\mathbf{U}'\mathbf{V} \\ \mathbf{E}_1' \end{bmatrix}$ and $\mathbf{D}=\begin{bmatrix} 24\mathbf{B}_0+4\mathbf{B}_1 & \mathbf{E}_2 \\ \mathbf{E}_2' & \mathbf{D}_{22} \end{bmatrix}$, where $\mathbf{U}'\mathbf{V}$, $\mathbf{B_0}$ and $\mathbf{B_1}$ are the same as for the quadratic mixture model (12). Using the expression for $(\mathbf{X}'\mathbf{X})^{-1}$ provided in the Appendix 4, it is straightforward to show that function $f(\mathbf{v}_1)=\mathbf{z}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1$ is invariant with respect to any transposition of x_i^z and x_j^z. Therefore, we can use permutations of any stationary point to get multiple additional points using Propositions 1 and 2.

Let us denote $\mathbf{v}_1'\mathbf{B}'+\mathbf{u}_1'\mathbf{D}=\left[\begin{array}{cccc} w_{q+1} & w_{q+2} & \cdots & w_{\frac{q^3+5q}{6}}\end{array}\right]$. Then the Hessian matrix could be expressed as $\frac{\partial^2 f(\mathbf{v})}{\partial\mathbf{v}\partial\mathbf{v}'}=2\left[\begin{array}{cc}\mathbf{I}_q & \mathbf{K}\end{array}\right](\mathbf{X}'\mathbf{X})^{-1}\left[\begin{array}{c}\mathbf{I}_q\\ \mathbf{K}'\end{array}\right]+\mathbf{W}$,

where

$$\mathbf{W}=2\left[\begin{array}{ccc} 0 & \cdots & w_{2q-1}+x_2a_{l+q-2}+\ldots+x_qa_{l+C(q-1,2)} \\ w_{q+1}+\sum_{i=3}^{q}x_iw_{l+i-2} & \cdots & w_{3q-3}+x_1a_{l+q-2}+\ldots+x_{q-1}a_{M-C(q-2,3)} \\ \vdots & \cdots & \vdots \\ w_{2q-1}+x_2a_{l+q-2}+\ldots+x_qa_{l+C(q-1,2)} & \cdots & 0 \end{array}\right] \quad (17)$$

with $l = C(q + 1, 2)$, $M=\frac{q^3+5q}{6}$ and $C(q-2, 3) = 0$ when $q < 5$. Zero-diagonal symmetric matrix **W** cannot be negative definite, and the same arguments as in section 3 imply that the stationary points are either saddle points or points of local minimum. The multiple interior design points are added by permuting stationary points other than the overall centroid. The number of stationary solutions varies with the number of factors. We label the proposed design as Design IIC, IIIC,…, with lower design labels representing designs with shorter distances between the stationary solutions and the overall centroid. For stationary solutions containing more than q additional points, we choose q out of all permuted points for comparisons. We also include the overall centroid point in all designs. Table 3 summarizes the D-efficiencies for all designs. In general, the proposed designs have higher or similar D-efficiency when compared to the standard designs IV-VI.

6 Ten-points Designs for Three-Component Mixture Models

6.1 D-efficiency

Cornell (1986) considered two ten-point designs for the three-component quadratic mixture model. One is the {3, 3} simplex-lattice design, called as Design I. It contains 10 design points: 3 points of $x \leftrightarrow$ (1, 0, 0), 6 points of $x \leftrightarrow$ (1/3, 2/3, 0) and the overall centroid (1/3, 1/3, 1/3). Another design is the 3-component simplex centroid design, augmented with three interior points $x \leftrightarrow$ (2/3, 1/6, 1/6), which is Design IV in Section 3.2. We compare the proposed design with Design I and Design IV using three commonly used models: quadratic, additive quadratic and special cubic models. The design points for quadratic and additive quadratic models are the same, labeled as Design IIQ and IIIQ. The proposed designs for the special cubic model are labeled as Design IIC and IIIC.

Figure 1 sketches the ternary plots for all designs. Table 4 lists the D-efficiency for all designs. Note that the ratio of the boundary points and interior points for Design I is 9:1. Design I, which contains all boundary points except the overall centroid, has the highest D-efficiency among all designs. Yet the other designs (Design IIQ, IIIQ, IIC, IIIC and Design IV) provide a more uniform distribution of the information about the surface inside the triangle, as the ratio of the boundary points and interior points is 6:4. For the other designs, Design IIIQ has the highest D-efficiency for quadratic and additive quadratic models, and Design IIC has the highest D-efficiency for special cubic model. Next we will explore the power of the LOF test by simulation.

6.2 Power of the LOF test

LOF describes how the model fits a set of observations by summarizing the discrepancy between the observed values and the expected values under the fitted model. For testing the LOF, the residual sum of squares is partitioned into the sum of squares due to pure error (SSPE) and the sum of squares due to Lack of Fit (SSLF) as follows:

$$\sum_{j=1}^{c}\sum_{i=1}^{n_j}\hat{\varepsilon}_{ij}^2=\sum_{j=1}^{c}\sum_{i=1}^{n_j}\left(Y_{ij}-\hat{Y}_j\right)^2 \quad (18)$$

$$= \underbrace{\sum_{j=1}^{c}\sum_{i=1}^{n_j}(Y_{ij}-\overline{Y}_{j\bullet})^2}_{\text{(sum of squares due to pure error)}} + \underbrace{\sum_{j=1}^{c}n_j\left(Y_{ij}-\overline{Y}_{j\bullet}\right)^2,}_{\text{(sum of squares due to Lack of Fit)}} \quad (19)$$

where $i = 1, 2, 3, \dots, n_j$ and $j = 1, 2, \dots, c$. Y_{ij} denotes the ith observation at the jth design point, $\overline{Y}_{j\bullet}$ is the average of the n_j observations at the jth design point, and $\hat{Y}_j$ is the fitted value at jth design point. Under the assumptions of normally distributed errors, the sums of squares due to pure error and sum of squares due to LOF have chi-square distributions with corresponding degrees of freedom. The degree of freedom associated with SSPE is $N - c$, where N is the total number of observations and c is the number of the design points. The degree of freedom for SSE is $N - p$, where p is the number of parameters in the mixture model. The lack of fit sum squares (SSLF) is calculated as $SSLF = SSE - SSPE$ with the degree of freedom $c - p$.

F-statistics is used to test for LOF:

$$F* = \frac{\text{SSLF}/(c-p)}{\text{SSPE}/(N-c)} \quad (20)$$

In the simulation studies, we assume the true models are the commonly used mixture models, such as special cubic model, special quartic models etc. We also assume that the errors are independent and identically normally distributed with mean zero and a common variance $\sigma^2 = 0.1$, $\epsilon \sim N(0, 0.1)$. There are 2000 datasets simulated for each design, with 2 to 5 replicates for each design point. Table 5 lists the true models and the fitted models.

Under the assumption of the true models, the LOF is calculated by using the fitted models to detect the model inadequate at significant level 0.05. Figure 2 shows the LOF power for three mixture models. In summary, the proposed designs with the shortest distance to the overall centroid shows the highest LOF power among all designs, i.e. Design IIQ for quadratic and additive models, Design IIC for special cubic model.

7 Conclusion

We have investigated adding multiple interior points to the D-optimal minimal designs for a wide subclass of symmetric mixture models. The proposed designs address the interest of predicting the entire design surface and enabling testing the lack of fit. When compared to the standard designs, the proposed designs demonstrate higher or comparable D-efficiency. Additionally the proposed design with the shortest distance to the overall centroid shows the highest LOF power when the true models are the commonly used mixture models, such as special cubic, special quartic models, etc.

1. Proof of Theorem 1

The generalization of the Sylvester's determinant theorem (Harville (2008)) implies that

$$|\mathbf{X}_1'\mathbf{X}_1|=|\mathbf{X}'\mathbf{X}|[1+\mathbf{z}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1].$$

Since the determinant $|\mathbf{X}'\mathbf{X}|$ is already maximized by the definition of the D-optimal minimal design $\mathbf{X}$, maximizing $|\mathbf{X}_1'\mathbf{X}_1|$ is equivalent to maximizing $f(\mathbf{v})=\mathbf{z}_1'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}_1$ subject to constraint $\mathbf{v}_1'\mathbf{1}=1$. The general approach is to use Lagrange multipliers and maximize

$$L_1=[\ \mathbf{v}_1' \quad \mathbf{u}_1'\ ](\mathbf{X}'\mathbf{X})^{-1}\begin{bmatrix}\mathbf{v}_1\\ \mathbf{u}_1\end{bmatrix}-2\lambda(\mathbf{v}_1'\mathbf{1}-1).$$

where $(M_n - q) \times 1$ vector $\mathbf{u}_1'=[h_2(x_1^z,x_2^z),\dots,h_n(x_1^z,\dots,x_q^z)]$. Then $q \times 1$ vector

$$\frac{\partial}{\partial \mathbf{v}}L_1=2\begin{bmatrix}\mathbf{I_q} & \mathbf{K}\end{bmatrix}(\mathbf{X}'\mathbf{X})^{-1}\begin{bmatrix}\mathbf{v}_1\\ \mathbf{u}_1\end{bmatrix}-2\lambda\mathbf{1}, \qquad (21)$$

where $(M_n - q) \times q$ matrix $\mathbf{K}=\frac{\partial \mathbf{u}_1'}{\partial \mathbf{v}_1}$. Since $\left(\mathbf{I_{q-1}}\otimes\begin{bmatrix}1 & -1\end{bmatrix}\right)\mathbf{1}=\mathbf{0}$, (21) implies (8). Further,

$$\frac{\partial^2 L_1}{\partial \mathbf{v}' \partial \mathbf{v}} = \frac{\partial}{\partial \mathbf{v}'} \left[\frac{\partial}{\partial \mathbf{v}} L_1 \right] = \frac{\partial}{\partial \mathbf{v}'} \left(2 \left[\begin{array}{cc} \mathbf{I}_q & \mathbf{K} \end{array} \right] (\mathbf{X}'\mathbf{X})^{-1} \left[\begin{array}{c} \mathbf{v}_1 \\ \mathbf{u}_1 \end{array} \right] \right). \quad (22)$$

Let us denote $f_k'(\mathbf{v}) = \left[\begin{array}{cc} \mathbf{I_q} & \mathbf{K} \end{array} \right]_{k\cdot} = \left[\begin{array}{cc} \mathbf{e_k'} & [\mathbf{K}]_{k\cdot} \end{array} \right] = \left[\begin{array}{cc} \mathbf{e_k'} & \frac{\partial \mathbf{u}'}{\partial v_k} \end{array} \right]$, where $\mathbf{e_k}$ is $q \times 1$ k^{th} canonical vector, and $h(\mathbf{v}) = (\mathbf{X}'\mathbf{X})^{-1} \left[\begin{array}{c} \mathbf{v}_1 \\ \mathbf{u}_1 \end{array} \right]$. Then using (1.4.16) in Vonesh and Chinchilli (1997), the $1 \times q$ vector

$$\begin{aligned} &\frac{1}{2}\frac{\partial}{\partial \mathbf{v}'}\left[\frac{\partial}{\partial \mathbf{v}}L_1\right]_k\Big|_{\mathbf{v}=\mathbf{v}_1,\mathbf{u}=\mathbf{u}_1} = \frac{\partial}{\partial \mathbf{v}'}\left\{f_k'(\mathbf{v})h(\mathbf{v})\right\} \\ &= f_k'(\mathbf{v})(\mathbf{X}'\mathbf{X})^{-1}\left[\begin{array}{c}\mathbf{I_q} \\ \frac{\partial \mathbf{u}}{\partial \mathbf{v}'}\end{array}\right] + [\mathbf{v}'\mathbf{u}'](\mathbf{X}'\mathbf{X})^{-1}\frac{\partial}{\partial \mathbf{v}'}\left[\begin{array}{c}\mathbf{e}_k \\ \frac{\partial \mathbf{u}}{\partial v_k}\end{array}\right] \\ &= \left[\begin{array}{cc}\mathbf{e_k'} & [\mathbf{K}]_{k\cdot}\end{array}\right](\mathbf{X}'\mathbf{X})^{-1}\left[\begin{array}{c}\mathbf{I_q} \\ \mathbf{K}'\end{array}\right] + [\mathbf{v}'\mathbf{u}'](\mathbf{X}'\mathbf{X})^{-1}\left[\begin{array}{c}\mathbf{0_q} \\ \frac{\partial^2 \mathbf{u}}{\partial v_k \partial \mathbf{v}'}\end{array}\right], \end{aligned} \quad (23)$$

so that $\frac{1}{2}\frac{\partial}{\partial \mathbf{v}'}\left[\frac{\partial}{\partial \mathbf{v}}L_1\right]_k = \mathbf{a_k'} + \mathbf{b_k'}$,

where $a_k = \left[\begin{array}{cc}\mathbf{e_k'} & [\mathbf{K}]_{k\cdot}\end{array}\right](\mathbf{X}'\mathbf{X})^{-1}\left[\begin{array}{c}\mathbf{I_q} \\ \mathbf{K}'\end{array}\right]$ and $\mathbf{b_k'} = [\mathbf{v}'\mathbf{u}'](\mathbf{X}'\mathbf{X})^{-1}\left[\begin{array}{c}\mathbf{0}_q \\ \frac{\partial^2 u}{\partial v_k \partial v'}\end{array}\right]$.

Respectively, the Hessian is

$$\frac{\partial^2 L_1}{\partial \mathbf{v} \partial \mathbf{v}'} = \left[\begin{array}{c}\frac{\partial}{\partial \mathbf{v}'}\left[\frac{\partial}{\partial \mathbf{v}}L_1\right]_1 \\ \cdots \\ \frac{\partial}{\partial \mathbf{v}'}\left[\frac{\partial}{\partial \mathbf{v}}L_1\right]_q\end{array}\right] = 2\left[\begin{array}{c}\mathbf{a_1'} \\ \cdots \\ \mathbf{a_q'}\end{array}\right] + 2\left[\begin{array}{c}\mathbf{b_1'} \\ \cdots \\ \mathbf{b_q'}\end{array}\right].$$

It is straightforward that

$$\left[\begin{array}{c}\mathbf{a_1'} \\ \cdots \\ \mathbf{a_q'}\end{array}\right] = \left[\begin{array}{cc}\mathbf{I}_q & \mathbf{K}\end{array}\right](\mathbf{X}'\mathbf{X})^{-1}\left[\begin{array}{c}\mathbf{I}_q \\ \mathbf{K}'\end{array}\right].$$

Also, $\mathbf{b_K'} = \mathbf{h}(\mathbf{v})'\mathbf{C_k}$, where $\mathbf{C_k} = \left[\begin{array}{c}\mathbf{0}_q \\ \frac{\partial^2 \mathbf{u}}{\partial v_k \partial v'}\end{array}\right]$, and therefore,

$$\mathbf{b_k'} = [(\mathbf{I_q} \otimes \mathbf{h}(\mathbf{v})^{\mathbf{T}})\mathbf{Vec}(\mathbf{C_k})]^{\mathbf{T}} = \mathbf{Vec}(\mathbf{C_k})^{\mathbf{T}}(\mathbf{h}(\mathbf{v}) \otimes \mathbf{I_q}).$$

Let us denote $\mathbf{C}=\begin{bmatrix} \text{Vec}(C_1)^T \\ \cdots \\ \text{Vec}(C_q)^T \end{bmatrix}$, then

$$\begin{bmatrix} \mathbf{b}_1' \\ \cdots \\ \mathbf{b}_q' \end{bmatrix} = \begin{bmatrix} \text{Vec}(C_1)^T \\ \cdots \\ \text{Vec}(C_q)^T \end{bmatrix} (\mathbf{h}(\mathbf{v}) \otimes \mathbf{I_q}) = \mathbf{C}\left((\mathbf{X}'\mathbf{X})^{-1} \begin{bmatrix} \mathbf{v} \\ \mathbf{u} \end{bmatrix} \otimes \mathbf{I_q} \right). \tag{24}$$

Thus, the Hessian may be expressed as

$$\frac{\partial^2 L_1}{\partial \mathbf{v} \partial \mathbf{v}'}\Big|_{\mathbf{v}=\mathbf{v}_1} = 2[\ \mathbf{I_q} \quad \mathbf{K}\ ](\mathbf{X}'\mathbf{X})^{-1} \begin{bmatrix} \mathbf{I_q} \\ \mathbf{K}' \end{bmatrix} + 2\mathbf{C}\left((\mathbf{X}'\mathbf{X})^{-1} \begin{bmatrix} \mathbf{v} \\ \mathbf{u} \end{bmatrix} \otimes \mathbf{I_q} \right) \tag{25}$$

Using (5) we can write

$$[\ \mathbf{I_q} \quad \mathbf{K}\ ](\mathbf{X}'\mathbf{X})^{-1} \begin{bmatrix} \mathbf{I_q} \\ \mathbf{K}' \end{bmatrix} = \mathbf{A} + \frac{\partial \mathbf{u}'}{\partial \mathbf{v}}\mathbf{B} + \mathbf{B}'\frac{\partial \mathbf{u}}{\partial \mathbf{v}'} + \frac{\partial \mathbf{u}'}{\partial \mathbf{v}}\mathbf{D}\frac{\partial \mathbf{u}}{\partial \mathbf{v}'}. \tag{26}$$

Further, we have

$$\mathbf{b}_{\mathbf{K}}' = [\mathbf{v}'\mathbf{u}'](\mathbf{X}'\mathbf{X})^{-1} \begin{bmatrix} \mathbf{0}_q \\ \frac{\partial^2 \mathbf{u}}{\partial v_k \partial v'} \end{bmatrix} = [\mathbf{v}'\mathbf{u}'] \begin{bmatrix} \mathbf{A}_q & \mathbf{B}' \\ \mathbf{B} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{0}_q \\ \frac{\partial^2 \mathbf{u}}{\partial v_k \partial v'} \end{bmatrix} = (\mathbf{v}'\mathbf{B}' + \mathbf{u}'\mathbf{D})\frac{\partial^2 \mathbf{u}}{\partial \mathbf{v_k} \partial \mathbf{v}'} \tag{27}$$

and combining (26) and (27) we obtain (9).

2. Matrix (X′X)−1 for Quadratic Mixture Model

The blocks in $\mathbf{X}'\mathbf{X}$ are given by $\mathbf{V}'\mathbf{V} = \frac{q+2}{4}\mathbf{I_q} + \frac{1}{4}\mathbf{J_q}$, $\mathbf{U}'\mathbf{U} = \frac{1}{16}\frac{\mathbf{I_{q(q-1)}}}{\mathbf{2}}$, where $\mathbf{J_q}$ is the matrix of ones of order q, and $\mathbf{U}'\mathbf{V} = (a_{(i,j),k})$ is a $\frac{q(q-1)}{2} \times q$ matrix with

$$(a_{(i,j),k}) = \begin{cases} \frac{1}{8} & \text{when } k=i \text{ or } k=j, \\ 0 & \text{otherwise,} \end{cases}$$

where the rows of matrix $\mathbf{U}'\mathbf{V}$ are indexed by pairs (i, j), $1 \le j < l \le q$, and $k = 1, 2, \ldots, q$.

Denote $\mathbf{A_{11}} = \mathbf{V}'\mathbf{V}$, $\mathbf{A_{22}} = \mathbf{U}'\mathbf{U}$, $\mathbf{A_{21}} = \mathbf{U}'\mathbf{V}$ and $\mathbf{A_{12}}=\mathbf{A}'_{\mathbf{21}}$, then

$$(\mathbf{X}'\mathbf{X})^{-1}=\begin{bmatrix} \mathbf{A} & \mathbf{B}' \\ \mathbf{B} & \mathbf{D} \end{bmatrix}=\begin{bmatrix} \mathbf{A_{11}}^{-1}(\mathbf{I}+\mathbf{A_{12}}\mathbf{F}^{-1}\mathbf{A_{21}}\mathbf{A_{11}}^{-1}) & -\mathbf{A_{11}}^{-1}\mathbf{A_{12}}\mathbf{F}^{-1} \\ -\mathbf{F}^{-1}\mathbf{A_{21}}\mathbf{A_{11}}^{-1} & \mathbf{F}^{-1} \end{bmatrix},$$

where $\mathbf{F} = \mathbf{A_{22}} - \mathbf{A_{21}}\mathbf{A_{11}}^{-1}\,\mathbf{A_{12}}$ is non-singular. It is straightforward to verify that

$$\mathbf{A_{11}}^{-1}=\frac{4}{q+2}[\mathbf{I_q}-\frac{1}{2(q+1)}\mathbf{J_q}],\ \mathbf{A_{12}}\mathbf{A_{21}}=\frac{q-2}{64}\mathbf{I_q}+\frac{1}{64}\mathbf{J_q},\ \text{and}\ \mathbf{A_{21}}\mathbf{A_{12}}=\frac{1}{32}\mathbf{B_0}+\frac{1}{64}\mathbf{B_1},$$

where $\mathbf{B_0}=\frac{\mathbf{I_{q(q-1)}}}{2}$ and $\mathbf{B_1}$ is the association matrix of the first associates in a triangular association scheme of order $\frac{q(q-1)}{2}$ (Raghavarao, 1971). The association scheme is an array of q rows and q columns with the following properties:

- The positions in the principal diagonal are blank.
- The $\frac{q(q-1)}{2}$ positions above the principal diagonal are filled by the numbers 1, 2, …, $\frac{q(q-1)}{2}$.
- The array is symmetric about the principal diagonal.
- The ones that lie in the same row and same column are treated as first associate, the others are treated as the second associate.

Thus, these association matrices of a triangular association scheme are indexed by pairs (i, j), $1 \le j < l \le q$ and defined as follows:

$$\mathbf{B_0}=\frac{\mathbf{I_{q(q-1)}}}{\mathbf{2}},$$
$$\mathbf{B_1}=b_{(jl,j'l')},$$

where $b_{(jl,j'l')}=\begin{cases} 1 & \text{if } (j=j' \text{ or } j=l' \text{ or } l=j' \text{ or } l=l') \text{ but } (j=j' \text{ and } l=l') \\ 0 & \text{otherwise} \end{cases}$

$$\mathbf{B_2}=\frac{\mathbf{J_{q(q-1)}}}{\mathbf{2}}-\mathbf{B_0}-\mathbf{B_1}.$$

Note that

$$\mathbf{A_{21}A_{12}}=\frac{1}{32}\mathbf{B_0}+\frac{1}{64}\mathbf{B_1}.$$

The following results from Raghavarao (1971),

$$\mathbf{B_1B_2}=(q-3)\mathbf{B_1}+(2q-8)\mathbf{B_2}, \quad (28)$$

$$\mathbf{B_1^2}=2(q-2)\mathbf{B_0}+(q-2)\mathbf{B_1}+4\mathbf{B_2}, \quad (29)$$

$$\mathbf{B_2^2}=\frac{(q-2)(q-3)}{2}\mathbf{B_0}+\frac{(q-3)(q-4)}{2}\mathbf{B_1}+\frac{(q-4)(q-5)}{2}\mathbf{B_2}, \quad (30)$$

are used to obtain

$$\begin{aligned}\mathbf{F}&=\mathbf{A_{22}}-\mathbf{A_{21}A_{11}}^{-1}\mathbf{A_{12}}\\ &=\tfrac{1}{16}\mathbf{B_0}-\tfrac{4}{q+2}\left(\tfrac{1}{32}\mathbf{B_0}+\tfrac{1}{64}\mathbf{B_1}\right)+\tfrac{1}{8(q+1)(q+2)}(\mathbf{B_0}+\mathbf{B_1}+\mathbf{B_2}).\end{aligned} \quad (31)$$

Hence $\mathbf{D} = \mathbf{F}^{-1} = 24\mathbf{B_0} + 4\mathbf{B_1}$. And

$$\mathbf{B}=(24\mathbf{B_0}+4\mathbf{B_1})\mathbf{A_{21}}\frac{-4}{q+2}\left[\mathbf{B_0}-\frac{1}{2(q+1)}(\mathbf{B_0}+\mathbf{B_1}+\mathbf{B_2})\right]=-16\mathbf{A_{21}},$$

$\mathbf{B}'$ = $-16\mathbf{A_{12}}$, and

$$\mathbf{A}=\mathbf{A_{11}}^{-1}(\mathbf{I_q}+\mathbf{A_{12}F}^{-1}\mathbf{A_{21}A_{11}}^{-1})=\mathbf{I_q}.$$

Thus, we have

$$(\mathbf{X}'\mathbf{X})^{-1}=\begin{bmatrix}\mathbf{A} & \mathbf{B}'\\ \mathbf{B} & \mathbf{D}\end{bmatrix}=\begin{bmatrix}\mathbf{I_q} & -16\mathbf{UV}'\\ -16\mathbf{U}'\mathbf{V} & 24\mathbf{B_0}+4\mathbf{B_1}\end{bmatrix}. \quad (32)$$

3. Matrix (X′X)−1 for Additive Quadratic Mixture Model

The blocks of $(\mathbf{X}'\mathbf{X})^{-1}$ in (5) are given by $\mathbf{A} = a_1(q, \delta)\mathbf{I}_q + a_2(q, \delta)\mathbf{J}_q$, $\mathbf{B} = b_1(q, \delta)\mathbf{I}_q + b_2(q, \delta)\mathbf{J}_q$ and $\mathbf{D} = d_1(q, \delta)\mathbf{I}_q + d_2(q, \delta)\mathbf{J}_q$.

$$a_1(q,\delta)=\frac{2-4(-1+q)\delta+2(2-6q+3q^2)\delta^2-4q(2-3q+q^2)\delta^3+(-2+q)^2q^2\delta^4}{(-2+q)^2\delta^2(-1+q\delta)^2},$$

$$a_2(q,\delta)=2q^6\delta^5-q^5\delta^4(11+8\delta)+8(1+\delta+\delta^2)+2q^4\delta^3(12+20\delta+5\delta^2)-q^3\delta^2(26+76\delta+45\delta^2+4\delta^3)+2q^2\delta(8+33\delta+36\delta^2+8\delta^3)-2q(3$$

$$b_1(q,\delta)=\frac{(1+(1-q\delta)(-\delta^2+(1-(-1+q)\delta)^2))}{(2-2q\delta+q^2\delta^2)},$$

$$b_2(q,\delta)=-q^6\delta^5-2q^5\delta^4(3+2\delta)-2q(1+\delta)^2(3+5\delta)+4(2+\delta+\delta^2)+q^4\delta^3(15+21\delta+5\delta^2)-q^3\delta^2(19+44\delta+23\delta^2+2\delta^3)+q^2\delta(14+$$

$$d_1(q,\delta)=\frac{2-2q\delta+q^2\delta^2}{(-2+q)^2\delta^2(-1+q\delta)^2},$$

$$d_2(q,\delta)=\frac{(8-q^5\delta^4+2q^4\delta^3(3+\delta)-q^3\delta^2(12+12\delta+\delta^2)-2q(3+8\delta+3\delta^2)+2q^2\delta(6+10\delta+3\delta}{(-2+q)^2(-1+q)^2\delta^2(-2+q\delta)^2(-1+q\delta)^2}$$

4. Matrix (X′X)−1 for Special Cubic Model

The blocks of $(\mathbf{X}'\mathbf{X})^{-1}$ are given by $\mathbf{A} = \mathbf{I}_q$, $\mathbf{B}=\begin{bmatrix} -16\mathbf{U}'\mathbf{V} \\ \mathbf{E}_1' \end{bmatrix}$ and

$\mathbf{D}=\begin{bmatrix} 24\mathbf{B_0}+4\mathbf{B_1} & \mathbf{E_2} \\ \mathbf{E}_2' & \mathbf{D_{22}} \end{bmatrix}$, where $\mathbf{U}'\mathbf{V}$, $\mathbf{B_0}$ and $\mathbf{B_1}$ are from quadratic mixture model (12). Here $\mathbf{D_{22}}$ is the matrix of order $C(q, 3)$,

$$\mathbf{D_{22}}=(x_{ijk,i'j'k'})=\begin{cases} 1188 & \text{when } i=i' \text{ and } j=j' \text{ and } k=k' \\ 162 & \text{when } ijk \text{ and } i'j'k' \text{ have two factors in common,} \\ 9 & \text{when } ijk \text{ and } i'j'k' \text{ have one factor in common,} \\ 0 & \text{when } i \neq i' \text{ and } j \neq j' \text{ and } k \neq k'. \end{cases}$$

with ijk, $i'j'k'$ representing all three factor interaction terms i, j, k and i', j', k'. Also $(C(q, 1)) \times C(q, 3)$ matrix $\mathbf{E_1}$,

$$\mathbf{E_1}=(x_{i,i'j'k'})=\begin{cases} 3 & \text{when } i=i' \text{ or } i=j' \text{ or } j=k', \\ 0 & \text{otherwise.} \end{cases}$$

and $(C(q, 2)) \times C(q, 3)$ matrix $\mathbf{E_2}$,

$$\mathbf{E_2}=(x_{ij,i'j'k'})=\begin{cases} -60 & \text{when } ij \text{ and } i'j'k' \text{ have two factors in common,} \\ -6 & \text{when } ij \text{ and } i'j'k' \text{ have one factor in common,} \\ 0 & \text{otherwise.} \end{cases}$$

with i, j, k representing the rows, ij and ijk representing two factor and three factor interactions respectively.

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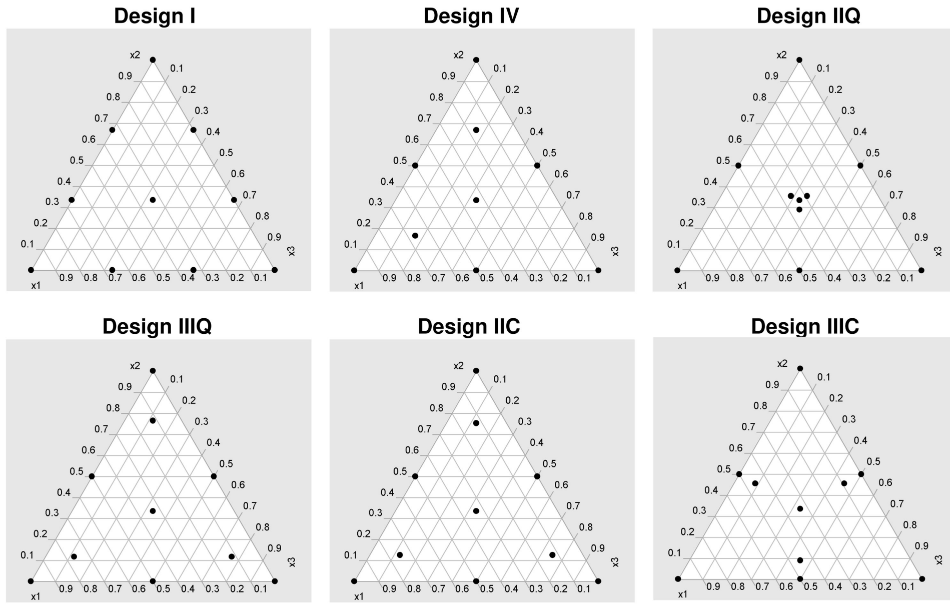

Figure 1. The Ten-point Designs

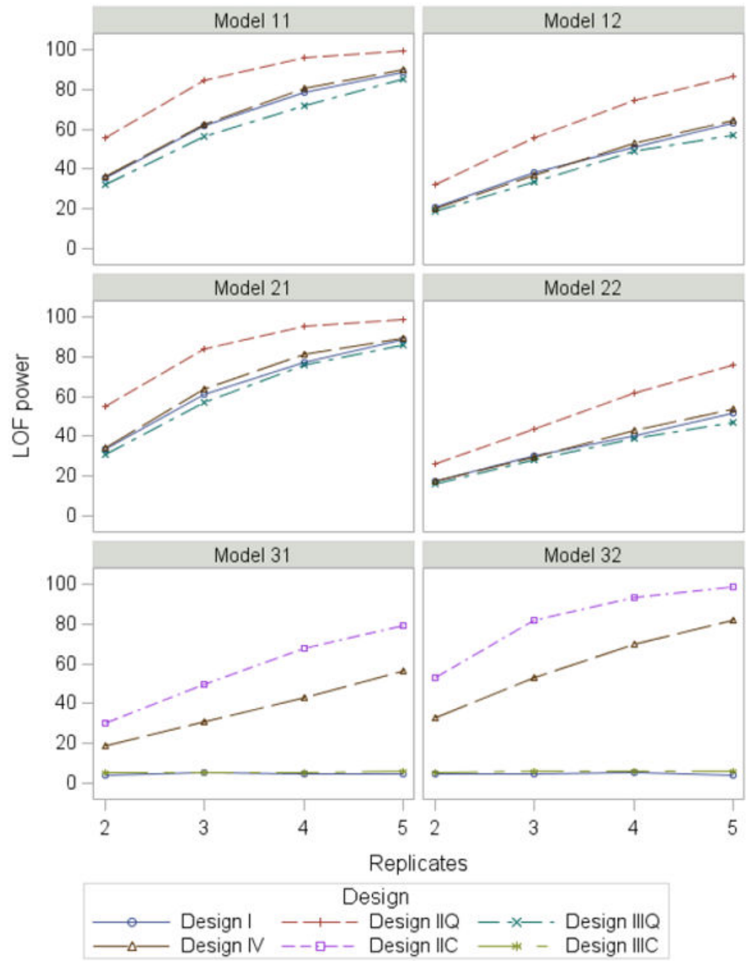

Figure 2. The LOF Power for Three Mixture Models in Table 5

Table 1

Minimal Plus (q + 1) Points Designs for Quadratic Mixture Model

Factors	Designs	Additional Points to the D-optimal Minimal Design	D_{q+1}
3	IIQ	$x \leftrightarrow$ (0.290, 0.355, 0.355) and $(1/31_3^{\prime})$	3.089
	IIIQ	$x \leftrightarrow$ (0.765,0.117,0.117) and $(1/31_3^{\prime})$	3.184
	IV	$x \leftrightarrow$ (2/3,1/6,1/6) and $(1/31_3^{\prime})$	3.148
	V	$x \leftrightarrow$ (1/2,1/4,1/4) and $(1/31_3^{\prime})$	3.121
	VI	$x \leftrightarrow$ (1/6, 5/12,1/12) and $(1/31_3^{\prime})$	3.212 *
4	IIQ	$x \leftrightarrow$ (0.322,0.226,0.226,0.226) and $(1/41_4^{\prime})$	1.423
	IIIQ	$x \leftrightarrow$ (0,707,0.098,0.098,0.098) and $(1/41_4^{\prime})$	1.454 *
	IIV	$x \leftrightarrow$ (5/8,1/8,1/8,1/8) and $(1/41_4^{\prime})$	1.447
	V	$x \leftrightarrow$ (1/2,1/6,1/6,1/6) and $(1/41_4^{\prime})$	1.442
	VI	$x \leftrightarrow$ (1/8, 7/24, 7/24, 7/24) and $(1/41_4^{\prime})$	1.444
5	IIQ	$x \leftrightarrow (1/3, /61_4^{\prime})$ and $(1/51_5^{\prime})$	0.812
	IIIQ	$x \leftrightarrow (2/3, /121_4^{\prime})$ and $(1/51_5^{\prime})$	0.822 *
	IV	$x \leftrightarrow (3/5, /101_4^{\prime})$ and $(1/51_5^{\prime})$	0.820
	V	$x \leftrightarrow (1/2, /81_4^{\prime})$ and $(1/51_5^{\prime})$	0.819
	VI	$x \leftrightarrow (1/10, 9/401_4^{\prime})$ and $(1/51_5^{\prime})$	0.814
6	IIQ	$x \leftrightarrow (0.337, 0.1331_5^{\prime})$ and $(1/61_6^{\prime})$	0.522
	IIIQ	$x \leftrightarrow (0.638, 0.0731_5^{\prime})$ and $(1/61_6^{\prime})$	0.526 *
	IV	$x \leftrightarrow (7/12, 1/121_5^{\prime})$ and $(1/61_6^{\prime})$	0.525
	V	$x \leftrightarrow (1/2, 1/101_5^{\prime})$ and $(1/61_6^{\prime})$	0.525
	VI	$x \leftrightarrow (1/12, 11/601_5^{\prime})$ and $(1/61_6^{\prime})$	0.520

Factors	Designs	Additional Points to the D-optimal Minimal Design	D_{q+1}
7	IIQ	$x \leftrightarrow (0.337, 0.1101_{6}^{\prime})$ and $(1/71_{7}^{\prime})$	0.363
	IIIQ	$x \leftrightarrow (0.616, 0.0641_{6}^{\prime})$ and $(1/71_{7}^{\prime})$	0.364*
	IV	$x \leftrightarrow (4/7, 1/141_{6}^{\prime})$ and $(1/71_{7}^{\prime})$	0.364
	V	$x \leftrightarrow (1/2, 1/121_{6}^{\prime})$ and $(1/71_{7}^{\prime})$	0.364
	VI	$x \leftrightarrow (1/14, 13/841_{6}^{\prime})$ and $(1/71_{7}^{\prime})$	0.361
8	IIQ	$x \leftrightarrow (0.336, 0.0951_{7}^{\prime})$ and $(1/81_{8}^{\prime})$	0.266
	IIIQ	$x \leftrightarrow (0.599, 0.0571_{7}^{\prime})$ and $(1/81_{8}^{\prime})$	0.267*
	IV	$x \leftrightarrow (9/16, 1/161_{7}^{\prime})$ and $(1/81_{8}^{\prime})$	0.267
	V	$x \leftrightarrow (1/2, 1/141_{7}^{\prime})$ and $(1/81_{8}^{\prime})$	0.267
	VI	$x \leftrightarrow (1/16, 15/1121_{7}^{\prime})$ and $(1/81_{8}^{\prime})$	0.265

Note:

*Maximum D-efficiency for each factor.

Table 2

Minimal Plus (q + 1) Points Designs for Additive Quadratic Mixture Model

Factors	Designs	Additional Points to the D-optimal Minimal Design	D_{q+1}
3	IIA	$x \leftrightarrow$ (0.290,0.355,0.355) and $(1/3 1_3')$	3.892
	IIIA	$x \leftrightarrow$ (0.765,0.117,0.117) and $(1/3 1_3')$	4.012
	IV	$x \leftrightarrow$ (2/3,1/6,1/6) and $(1/3 1_3')$	3.966
	V	$x \leftrightarrow$ (1/2,1/4,1/4) and $(1/3 1_3')$	3.932
	VI	$x \leftrightarrow$ (1/6, 5/12,1/12) and $(1/3 1_3')$	4.047*
4	IV	$x \leftrightarrow$ (5/8,1/8,1/8,1/8) and $(1/4 1_4')$	2.807*
	V	$x \leftrightarrow$ (1/2,1/6,1/6,1/6) and $(1/4 1_4')$	2.741
	VI	$x \leftrightarrow$ (1/8, 7/24, 7/24, 7/24) and $(1/4 1_4')$	2.698
5	IIA	$x \leftrightarrow (0.635, 0.091 1_4')$ and $(1/5 1_5')$	2.059*
	IIIA	$x \leftrightarrow (0.821, 0.045 1_4')$ and $(1/5 1_5')$	2.037
	IV	$x \leftrightarrow (3/5, 1/10 1_4')$ and $(1/5 1_5')$	2.055
	V	$x \leftrightarrow (1/2, 1/8 1_4')$ and $(1/5 1_5')$	2.007
	VI	$x \leftrightarrow (1/10, 9/40 1_4')$ and $(1/5 1_5')$	1.812
6	IIA	$x \leftrightarrow (0.605, 0.079 1_5')$ and $(1/6 1_6')$	1.602*
	IIIA	$x \leftrightarrow (0.893, 0.021 1_5')$ and $(1/6 1_6')$	1.493
	IV	$x \leftrightarrow (7/12, 1/12 1_5')$ and $(1/6 1_6')$	1.601
	V	$x \leftrightarrow (1/2, 1/10 1_5')$ and $(1/6 1_6')$	1.568
	VI	$x \leftrightarrow (1/12, 11/60 1_5')$ and $(1/6 1_6')$	1.275
7	IIA	$x \leftrightarrow (0.550, 0.075 1_6')$ and $(1/7 1_7')$	1.394*
	IIIA	$x \leftrightarrow (0.866, 0.022 1_6')$ and $(1/7 1_7')$	1.262

Factors	Designs	Additional Points to the D-optimal Minimal Design	D_{q+1}
	IV	$x \leftrightarrow (4/7, 1/141_6')$ and $(1/71_7')$	1.393
	V	$x \leftrightarrow (1/2, 1/121_6')$ and $(1/71_7')$	1.385
	VI	$x \leftrightarrow (1/14, 13/841_6')$ and $(1/71_7')$	1.117
8	IIA	$x \leftrightarrow (0.543, 0.0651_7')$ and $(1/81_8')$	1.231 *
	IIIA	$x \leftrightarrow (0.864, 0.02011_7')$ and $(1/81_8')$	1.067
	IV	$x \leftrightarrow (9/16, 1/161_7')$ and $(1/81_8')$	1.228
	V	$x \leftrightarrow (1/2, 1/141_7')$ and $(1/81_8')$	1.229
	VI	$x \leftrightarrow (1/16, 15/1121_7')$ and $(1/81_8')$	0.958

Note:

*Maximum D-efficiency for each factor.

Table 3

Minimal Plus (q + 1) Points Designs for Special Cubic Model

Factors	Designs	Additional Points to the D-optimal Minimal Design	D_{q+1}
3	IIC	$x \leftrightarrow$ (0.090,0.455,0.455) and $(1/3\,1_3')$	1.418 *
	IIIC	$x \leftrightarrow$ (0.751,0.124,0.124) and $(1/3\,1_3')$	1.353
	IV	$x \leftrightarrow$ (2/3,1/6,1/6) and $(1/3\,1_3')$	1.340
	V	$x \leftrightarrow$ (1/2,1/4,1/4) and $(1/3\,1_3')$	1.354
	VI	$x \leftrightarrow$ (1/6, 5/12,1/12) and $(1/3\,1_3')$	1.375
4	IIC	$x \leftrightarrow$ (0.108,0.297,0.297,0.297) and $(1/4\,1_4')$	0.281 *
	IIIC	$x \leftrightarrow$ (0.070,0.070,0.430,0.430) and $(1/4\,1_4')$	0.280
	IVC	$x \leftrightarrow$ (0.699,0.100,0.100,0.100) and $(1/4\,1_4')$	0.271
	IV	$x \leftrightarrow$ (5/8,1/8,1/8,1/8) and $(1/4\,1_4')$	0.270
	V	$x \leftrightarrow$ (1/2,1/6,1/6,1/6) and $(1/4\,1_4')$	0.273
	VI	$x \leftrightarrow$ (1/8, 7/24, 7/24, 7/24) and $(1/4\,1_4')$	0.279
5	IIC	$x \leftrightarrow (0.126, 0.218\,1_4')$ and $(1/5\,1_5')$	0.082
	IIIC	$x \leftrightarrow (0.099\,1_2', 0.267\,1_3')$ and $(1/5\,1_5')$	0.083 *
	IVC	$x \leftrightarrow (0.413\,1_2', 0.058\,1_3')$ and $(1/5\,1_5')$	0.082
	VC	$x \leftrightarrow (0.665, 0.084\,1_4')$ and $(1/5\,1_5')$	0.081
	IV	$x \leftrightarrow (3/5, 1/10\,1_4')$ and $(1/5\,1_5')$	0.080
	V	$x \leftrightarrow (1/2, 1/8\,1_4')$ and $(1/5\,1_5')$	0.081
	VI	$x \leftrightarrow (1/10, 9/40\,1_4')$ and $(1/5\,1_5')$	0.082
6	IIC	$x \leftrightarrow (0.142, 0.172\,1_5')$ and $(1/6\,1_6')$	0.031
	IIIC	$x \leftrightarrow (0.131\,1_2', 0.185\,1_4')$ and $(1/6\,1_6')$	0.032

Factors	Designs	Additional Points to the D-optimal Minimal Design	D_{q+1}
	IVC.	$x \leftrightarrow (0.0971_3', 0.2371_3')$ and $(1/61_6')$	0.032 *
	VC.	$x \leftrightarrow (0.4011_2', 0.0491_4')$ and $(1/61_6')$	0.032
	VIC	$x \leftrightarrow (0.640, 0.0721_5')$ and $(1/61_6')$	0.031
	IV	$x \leftrightarrow (7/12, 1/121_5')$ and $(1/61_6')$	0.031
	V	$x \leftrightarrow (1/2, 1/101_5')$ and $(1/61_6')$	0.031
	VI	$x \leftrightarrow (1/12, 11/601_5')$ and $(1/61_6')$	0.032

Note:

* Maximum D-efficiency for each factor.

Table 4

D-Efficiency for Quadratic, Additive Quadratic and Special Cubic Mixture Models

Quadratic	D-Eff	Additive Quadratic	D-Eff	Special Cubic	D-Eff
Design I	3.523	Design I	4.439	Design I	1.511
Design IV	3.148	Design IV	3.966	Design IV	1.378
Design IIQ	3.089	Design IIQ	3.892	Design IIC	1.456
Design IIIQ	3.184	Design IIIQ	4.012	Design IIIC	1.367

Table 5

Fitted and True Models for Three Mixture Models

1) Fitted Model:	**Quadratic Mixture Model**
True Model 11:	$y = 2x_1 + 1.9x_2 + 1.8x_3 + 0.5x_1x_2 + 0.5x_1x_3 + 0.5x_2x_3 + 6x_1x_2x_3 + \epsilon$
True Model 12:	$y=2x_1+1.9x_2+1.8x_3+0.5x_1x_2+0.5x_1x_3+0.5x_2x_3+5x_1^2x_2x_3+4.5x_1x_2^2x_3+4x_1x_2x_3^2+\varepsilon$
2) Fitted Model:	Additive Quadratic Mixture Model
True Model 21:	$y=2x_1+1.9x_2+1.8x_3+x_1^2+x_2^2+x_3^2+2x_1^3+2x_2^3+2x_3^3+\varepsilon$
True Model 22:	$y=2x_1+1.9x_2+1.8x_3+x_1^2+x_2^2+x_3^2+4x_1x_2x_3+\varepsilon$
3) Fitted Model:	Special Cubic Mixture Model
True Model 31:	$y=2x_1+1.9x_2+1.8x_3+2x_1x_2+2x_1x_3+2x_2x_3+3x_1x_2x_3+6x_1^2x_2^2+6x_1^2x_3^2+6x_2^2x_3^2+\varepsilon$
True Model 32:	$y = 2x_1 + 1.9x_2 + 1.8x_3 + 1x_1x_2 + 1x_1x_3 + 1x_2x_3 + 2x_1x_2x_3 +4(x1^4 + x2^4 + x3^4) + \epsilon$