Robust A-optimal designs for mixture experiments in Scheffé models

by

Chao-Jin Chou

Advisor

Mong-Na Lo Huang

Department of Applied Mathematics
National Sun Yat-sen University
Kaohsiung, Taiwan, 804, R.O.C.

June, 2003

Abstract

A mixture experiment is an experiments in which the q-ingredients are nonnegative and subject to the simplex restriction $\sum_{i=1}^{q} x_i = 1$ on the $(q-1)$-dimentional probability simplex S_{q-1}. In this work , we investigate the robust A-optimal designs for mixture experiments with uncertainty on the linear, quadratic models considered by Scheffé (1958). In Chan (2000), a review on the optimal designs including A-optimal designs are presented for each of the Scheffé's linear and quadratic models. We will use these results to find the robust A-optimal design for the linear and quadratic models under some robust A-criteria. It is shown with the two types of robust A-criteria defined here, there exists a convex combination of the individual A-optimal designs for linear and quadratic models respectively to be robust A-optimal. In the end, we compare efficiencies of these optimal designs with respect to different A-criteria.

Keywords : Convex combination, equivalence theorem, invariant symmetric block matrices, robust design.

Contents

1 Introduction

Experiments are considered in which the response to a mixture depends on the proportions of components, but not on the total amount of the mixture. Let q be the number of components and x_i be the proportion of the ith component in the mixture, so that

$$x_1 + x_2 + ... + x_q = 1, x_i \geq 0, (i = 1, 2, ..., q).$$

The design space is the (q-1)-dimensional probability simplex S^{q-1}, where

$$S^{q-1} = \{\mathbf{x} = (x_1, ..., x_q)' \in [0, 1]^q : \sum_{i=1}^{q} x_i = 1\}.$$

For the mixture models, we assume the response can be adequately graduated by a polynomial in the x_i. It is usually assumed that the observed response at $\mathbf{x}$=$(x_1, x_2, ..., x_q)'$ may be expressed as y($\mathbf{x}$)=$E(\mathbf{x}) + \varepsilon(\mathbf{x})$, where the $E(\mathbf{x})$ is the mixture model and $\varepsilon(\mathbf{x})$ is the error term, which are uncorrelated and have common unknown variance for all observations.

In this work, we take $f(\mathbf{x})$ as a multivariable polynomial regression model and a design ξ as a probability measure on S^{q-1} with finite supports. Denote a probability measure for a mixture experiment as follows

$$\xi = \begin{pmatrix} \begin{pmatrix} x_{1,1} \\ x_{1,2} \\ \vdots \\ x_{1,q} \end{pmatrix} & \begin{pmatrix} x_{2,1} \\ x_{2,2} \\ \vdots \\ x_{2,q} \end{pmatrix} & \cdots & \begin{pmatrix} x_{n,1} \\ x_{n,2} \\ \vdots \\ x_{n,q} \end{pmatrix} \\ p_1 & p_2 & \cdots & p_n \end{pmatrix},$$

where $\mathbf{x}_i = (x_{i,1}, x_{i,2}, ..., x_{i,q})'$ for $i = 1, 2, ..., q$ and $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n$ represent the finite supports and the corresponding weights are $p_1, p_2, ..., p_n$. The information matrix for the model $f(\mathbf{x})$ is therefore defined by

$$M_f(\xi) = \int_{S^{q-1}} f(\mathbf{x}) f'(\mathbf{x}) d\xi(\mathbf{x}),$$

and the dispersion matrix is equal to $M_f^{-1}(\xi)$. Thus we call a design ξ^* A-optimal if a design ξ^* minimizes $\mathrm{tr} M_f^{-1}(\xi)$ among all feasible designs defined on S^{q-1}. Minimization of $\mathrm{tr} M_f^{-1}(\xi)$ is equivalent to minimization of the mean dispersion of the estimates of the parameters.

On the other hand, while considering A-optimality as above, there is an equivalence theorem for characterizing the A-optimal designs, that is, ξ^* is A-optimal for a model $f(\mathbf{x})$. If and only if

$$f'(\mathbf{x}) M_f^{-2}(\xi^*) f(\mathbf{x}) \leq \mathrm{tr} M_f^{-1}(\xi^*),$$

for any point $\mathbf{x} \in S^{q-1}$, or

$$\mathrm{tr}(M_f(\xi) M_f^{-2}(\xi^*)) \leq \mathrm{tr} M_f^{-1}(\xi^*),$$

for ξ is an arbitrary design on S^{q-1}, with equality if and only if $\mathbf{x}$ or ξ is assigned to the design points (Pukelsheim (1993, p.221)).

Usually, the model is a single regression function. But in practice, the experimenters are often uncertain which model is suitable. That is, if there are several possible regression models in consideration, experimenters are not certain which one is more proper before accomplishing the experiments. In order to resolve such problems, model robust optimal designs are considered.

The aim of this work is to discuss robust designs between the Scheffé's linear and quadratic models. The criterion of selecting an optimal design is to minimize a convex combination of respective trace function of the dispersion matrices for these two models. This is called the robust A-optimal criterion. In this work, a real number $r \in [0, 1]$ is chosen to be the model convex combination coefficient.

In Chan (2000), an extensive review on some known results is given about analytic solutions and numerical solutions of optimal designs for various regression models for experiments with mixture. Guan and Chao (1987), Yu and Guan (1993) have determine the A-optimal design for the simplex weighted centroid designs considered where Scheffé's models are considered. At the moment, we can denote ξ_1^* and ξ_2^* as A-optimal designs for Scheffé's linear and quadratic models respectively for later use.

As the robust A-optimal criterion is a convex combination of the individual A-optimal criterion, it is speculated that there is a convex combination of the individual A-optimal designs to be robust A-optimal. In what follows, we will first find an optimal α^* to be the best one among all convex designs, and later verify that it is indeed A-optimal.

To do this, first note that equivalence theorem in Dette (1990) has been provided for D- and D_1- optimal designs, which are generalized to the problem of determining optimal product designs in the case of multivariable polynomial regression. Analogous to the robust criterion there, a robust A-optimal criterion is also defined and an equivalence theorem is provided for two or more models in this work.

In the past, the way to verify the A-optimal designs for different mixture models is usually quite complicated. In this work, it is even more difficult while adding an unknown convex design coefficient α in the robust criterion. However, due to a complete class result of Draper, et al. (2000) on weighted centroid designs, the problem can be substantially reduced. That is, we merely need to discuss designs on centroid points but not all other ones, then we will use the result to deal with our robust optimal problem.In Klein (2002), there is a quite nice method to verify a candidate optimal design obtained to satisfy the equivalence theorem in the complete class of weighted centroid designs. He analyzes a quadratic subspace of block matrices which are invariant under the action of a group $\mathcal{H}$ arising from the design of mixture experiments, and the matrices have been used to find the D-, A- and E-optimal designs respectively.

In general, the investigators assume that the fitted model is focused on a single regression function. But in practice, experimenters are often uncertain about which model is suitable. It dates back to Box and Draper (1959), if we use a simple linear function to estimate the expected value of the response when the true model is quadratic, it would result in a large bias for estimation. Thus, while designing an experiment for regression models, robustness has always been an important issue.

In the first part of next section, we provide an A-optimal equivalence theorem on multivariable regression. The problem of finding an optimal design is reduced to one in the class of weighted centroid designs in the second part. In the third part, results about a multiplication table for the blocks of $\mathcal{H}$-invariant symmetric matrices introduced in Klein (2002) are stated. In Section

3, the robust A-optimal design is obtained by verifying that in the corresponding equivalence theorem, which is considered on weighted centroid designs. Section 4 presents some plots of the relation between α and r, defined under different criteria. Finally, in Section 5, we conclude our work here and discuss some possible further works.

2 Preliminary for robust A-optimal design

In the first part of the section, the model robust A-optimality criteria analogous to Dette (1990) will be provided. In the second part, we state the weighted centroid designs in the experiments for mixture models. Finally, invariant symmetric block matrices by Klein (2002) will be introduced.

2.1 Generalized A-optimal equivalence theorem

The following result due to Dette (1990) characterizes the generalized D-optimal designs. Analogous to the results, we will provide a generalized A-optimality criterion to deal with our robust A-optimal designs for mixture experiments later as well.

In Dette (1990), the generalized D-optimal design criterion is defined and a class of polynomial regression models is as follows. Let

$$\mathcal{F}_n = \{f_l | f_l(x) = \sum_{i=0}^{l} \theta_{l,i} x^i, l = 0, 1, ..., n, x \in [-1, 1]\}$$

A vector $\gamma = (\gamma_0, \gamma_1, ..., \gamma_n)$ of real numbers is called a prior for $\mathcal{F}_n$ where γ is a probability measure on $\{0, 1, ..., n\}$ or is, for $s \in \{1, ..., n-1\}$, of the form

$$\gamma_0 = ... = \gamma_{n-s-1} = 0, \gamma_{n-s} = -\frac{n-s+1}{s},$$
$$\gamma_{n-s+1} = ... = \gamma_{n-1} = 0, \gamma_n = \frac{n+1}{s}.$$

For a given prior γ on $\{0, ..., n\}$, we call a design ξ_γ optimal for $\mathcal{F}_n$ with respect to the prior γ, if ξ_γ maximizes the function

$$\Psi_\gamma(\xi) = \sum_{l=0}^{n} \frac{\gamma_l}{l+1} \log(\det M_l(\xi)).$$

The D-optimality criterion is a special case with prior $\gamma_D = (0, ..., 0, 1)$ and D_s-optimality criterion with γ_{D_s}, $s \in (1, ..., n-1)$. Furthermore, the equivalence theorem of the generalized D-optimality criterion is also given in Dette (1990).

Analogous to the result as the above, the generalized A-optimality criteria is considered as follows. Let a vector $\mathbf{r} = (r_0, r_1, ..., r_n)$ of real numbers be a prior for $\mathcal{F}_n$. For a given prior function $\beta = \beta(\mathbf{r}) = (\beta_0, \beta_1, ..., \beta_n)$, a canonical function of a prior vector $\mathbf{r}$, we call a design ξ_β optimal $\mathcal{F}_n$ with respect to the prior β, if ξ_β minimizes the following two functions:

$$(i) \quad \Psi_\beta(\xi) = \sum_{l=0}^{n} \beta_l \mathrm{tr}(M_l^{-1}(\xi)) \tag{2.1}$$

$$(ii) \quad \Psi_\beta(\xi) = \sum_{l=0}^{n} \beta_l \log(\ \mathrm{tr}(M_l^{-1}(\xi))). \tag{2.2}$$

From the above, the aims of the two criteria are the same, that is to minimize a kind of convex combinations of some functions of the traces of dispersion matrices for two or more models to obtain a robust optimal design.

Now we also need an equivalence theorem to prove our assertion for a given criterion as the above. Analogous to Fedorov (1972, p125), we provide an equivalence theorem for the generalized L-optimal designs under the $n+1$ linear regression models $f_0, f_1, ..., f_n$, here we let the class $\mathcal{F}_n$ defined on a compact set $\aleph$ as follows.

Lemma 2.1. *For a given prior $\beta = (\beta_0, \beta_1, ..., \beta_n)$, we say the design ξ_β is optimal for the class $\mathcal{F}_n$ with $n+1$ linear regression functions $f_0, f_1, ..., f_n$ with respect to the prior β, then the following three statements are equivalent:*

(i)The design ξ_β minimizes $\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi)\}$.

(ii)For an arbitrary design ξ,

$$\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta) M_l(\xi) M_l^{-1}(\xi_\beta)\} \leq \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\}.$$

(iii)For an arbitrary single point $\mathbf{x} \in \aleph$,

$$max_{\mathbf{x}\in\aleph} \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta) f_l(\mathbf{x}) f_l(\mathbf{x})' M_l^{-1}(\xi_\beta)\} = \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\}.$$

Proof. 1° We will show that (ii) follows from (i). To do this, let ξ be an arbitrary design, the design $\xi_s = (1-s)\xi_\beta + s\xi$ is considered and also $M(\xi_s) = (1-s)M(\xi_\beta) + sM(\xi)$. In view of the linearity of the functional L

$$\frac{\partial}{\partial s} L\{M^{-1}(\xi_s)\} = L\{\frac{\partial}{\partial s} M^{-1}(\xi_s)\}.$$

From this, we obtain

$$\begin{aligned} \frac{\partial}{\partial s}\Psi_\beta(\xi_s) &= \frac{\partial}{\partial s}\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_s)\} = \sum_{l=0}^{n} \beta_l L\{\frac{\partial}{\partial s} M_l^{-1}(\xi_s)\} \\ &= \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_s)(M_l(\xi_\beta) - M_l(\xi)) M_l^{-1}(\xi_s)\}. \end{aligned}$$

Now set $s = 0$, due to the convexity of $L(M^{-1}(\xi))$ and if ξ_β is optimal, the following inequality must be satisfied, i.e.

$$\frac{\partial}{\partial s}\Psi_\beta(\xi_s)|_{s=0} = \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)(M_l(\xi_\beta) - M_l(\xi)) M_l^{-1}(\xi_\beta)\} \geq 0,$$

which implies

$$\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta) M_l(\xi) M_l^{-1}(\xi_\beta)\} \leq \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\},$$

for an arbitrary design ξ and the equality holds if and only if $\xi = \xi_\beta$.

2° We will show that (*iii*) follows from (*ii*). To do this, consider the design ξ concentrated at a single point $\mathbf{x}$ and $M_l(\xi) = f_l(\mathbf{x}) f_l(\mathbf{x})'$ such that

$$\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta) f_l(\mathbf{x}) f_l(\mathbf{x})' M_l^{-1}(\xi_\beta)\} \leq \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\}. \tag{2.3}$$

On the other hand, for any design ξ with finite support points $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_p$,

$$\begin{aligned}
\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi)\} &= \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi) M_l(\xi) M_l^{-1}(\xi)\} \\
&= \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi)(\sum_{\mathbf{x}_i \in \xi} p_i f_l(\mathbf{x}_i) f_l(\mathbf{x}_i)') M_l^{-1}(\xi)\} \\
&= \sum_{l=0}^{n} \beta_l \sum_{\mathbf{x}_i \in \xi} p_i L\{M_l^{-1}(\xi) f_l(\mathbf{x}_i) f_l(\mathbf{x}_i)' M_l^{-1}(\xi)\}.
\end{aligned}$$

Meanwhile, since ξ_β is optimal, then

$$\begin{aligned}
&\max_{\mathbf{x}} \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi) f_l(\mathbf{x}) f_l(\mathbf{x})' M_l^{-1}(\xi)\} \\
\geq\ & \max_{i} \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi) f_l(\mathbf{x}_i) f_l(\mathbf{x}_i)' M_l^{-1}(\xi)\} \\
\geq\ & \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi)\} \\
\geq\ & \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\}.
\end{aligned}$$

$$(2.4)$$

Therefore, comparing (2.3) and (2.4), it is not difficult to see that for a robust linear-optimal design, $\max_{\mathbf{x}} \Phi(\mathbf{x}, \xi_\beta) = max_{\mathbf{x}} \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta) f_l(\mathbf{x}) f_l(\mathbf{x})' M_l^{-1}(\xi_\beta)\}$ attains the smallest possible value. For brevity, we call the design ξ_β minimizing $\max_{\mathbf{x}} \Phi(\mathbf{x}, \xi)$ the minimax design. Furthermore, for the design ξ is arbitrary given, the robust linear-optimal design ξ_β will also satisfy the following equation:

$$\begin{aligned}
\max_{\mathbf{x} \in \aleph} \Phi(\mathbf{x}, \xi_\beta) &= \max_{\mathbf{x} \in \aleph} \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta) f_l(\mathbf{x}) f_l(\mathbf{x})' M_l^{-1}(\xi_\beta)\} \\
&= \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\}.
\end{aligned}$$

3° We will show that (i) follows from (iii). If the design ξ_β satisfies the equation,

$$\max_{\mathbf{x} \in \aleph} \Phi(\mathbf{x}, \xi_\beta) = \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\},$$

but not linear-optimal. We can assume that the minimax design ξ_β does not satisfy (i), that is, $\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\} > min_\xi \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi)\}$. Then a design ξ can be found such that $\frac{\partial}{\partial s} \Psi_\beta(\xi_s) < 0$, where $\xi_s = (1-s)\xi_\beta + s\xi$. For example, we could choose a design $\xi_\circ$ minimizing $\sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi)\}$ as the design it is possible. Besides,

$$\begin{aligned}
\frac{\partial}{\partial s} \Psi_\beta(\xi_s)|_{s=0} &= \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta)\} - \sum_{l=0}^{n} \beta_l L\{M_l^{-1}(\xi_\beta) M_l(\xi) M_l^{-1}(\xi_\beta)\} \\
&= \Psi_\beta(\xi_\beta) - \sum_{l=0}^{n} \beta_l \sum_{\mathbf{x}_i \in \xi} p_i L\{M_l^{-1}(\xi_\beta) f_l(\mathbf{x}_i) f_l(\mathbf{x}_i)' M_l^{-1}(\xi_\beta)\} \\
&\geq \Psi_\beta(\xi_\beta) - \max_{\mathbf{x} \in \aleph} \Phi(\mathbf{x}, \xi_\beta) = 0.
\end{aligned}$$

The obtained contradiction proves our assertion.

Lemma 2.2. *For a given prior $\beta = (\beta_0, \beta_1, ..., \beta_n)$, the following three conditions are equivalent:*

(i)The design ξ_β is optimal for the class $\mathcal{F}_n$ with respect to the prior β

(ii)The design ξ_β minimizes

$$\Phi_\beta(\xi) = max_{\mathbf{x}\in\aleph} \sum_{l=0}^{n} \beta_l \frac{L\{M_l^{-1}(\xi) f_l(\mathbf{x}) f_l(\mathbf{x})' M_l^{-1}(\xi)\}}{L\{M_l^{-1}(\xi)\}}$$

(iii)

$$\Phi_\beta(\xi_\beta) = max_{\mathbf{x}\in\aleph} \sum_{l=0}^{n} \beta_l \frac{L\{M_l^{-1}(\xi_\beta) f_l(\mathbf{x}) f_l(\mathbf{x})' M_l^{-1}(\xi_\beta)\}}{L\{M_l^{-1}(\xi_\beta)\}} = 1$$

Proof. For the generalized L-optimal equivalence theorem according to criteria(ii), the proof can be obtained similarly in Lemma 2.1.

Although the above criterion and equivalence theorem is originally defined and established for polynomial regression models on compact intervals, it can be used for mixture experiments without any problem. Therefore, we may find the robust designs with the corresponding criterion and the equivalence theorem for mixture experiments as well.

2.2 Optimal weighted centroid designs

Based on a result of Draper, et al. (2000) on weighted centroid designs, which will be introduced in the following, the problem can be substantially reduced.

Definition 2.1. *For $q \geq 2$ and $j \in 1, 2, ..., q$, the j-th elementary centroid design η_j is the uniform distribution on the centroids of depth j, that is, on all points taking the form $\frac{1}{j}\sum_{i=1}^{j} e_{k_i} \in S^{q-1}$ with $1 \leq k_1 < k_2 < ... < k_{j-1} < k_j \leq q$.*

That is, a design η_j assigns equal weights $\frac{1}{\binom{q}{j}}$ to each of points of $\mathbf{x} \leftrightarrow (\frac{1}{j}, ..., \frac{1}{j}, 0, ..., 0)$, where $j = 1, 2, ..., q$. A convex combination $\eta_\alpha = \sum_{j=1}^{q} \alpha_j \eta_j$ with $\alpha = (\alpha_1, ..., \alpha_q)' \in S^{q-1}$ is called a weighted centroid design with weight vector α. We denote the set of weighted centroid designs by $\eta(S^{q-1})$.

By Draper and Pukelsheim (1999) and Draper, et al. (2000), it is shown that the set $\eta(S^{q-1})$ of weighted centroid designs is an essentially complete class in the second-degree Kronecker models $f_k(\mathbf{x})$ for mixture experiments with $q \geq 2$ ingredients. That is, for every design ξ on S^{q-1}, there exists a weighted centroid design η with $\mathrm{tr}\{M_k^{-1}(\eta)\} \leq \mathrm{tr}\{M_k^{-1}(\xi)\}$. The same completeness property holds within the second degree Scheffé models $f_s(\mathbf{x})$, which will be shown in next section.

As a consequence of the above, the search for an A-optimal design can be restricted to the set of competing designs on $\eta(S^{q-1})$. Thus, a simpler design problem to solve is finding an optimal design $\xi^* \in \eta(S^{q-1})$ with equivalence theorem.

2.3 Invariant symmetric block matrices for the design of mixture experiments

In dealing with the problems about the calculations of the matrices, especially in the general cases as $q \geq 2$, we need to obtain a general form of the information matrices in the quadratic models. Klein (2002) presents that the information matrices for a mixture experiment can be decomposed into blocks of $\mathcal{H}$-invariant symmetric matrices and a multiplication table is provided there. It is also shown that the matrices have seven distinct entries at most. The $\mathcal{H}$-invariant symmetric matrices representation in Klein (2002) are given as follows. Let $\mathcal{G}_q$ be the symmetric group of order q. Given a permutation $\pi \in \mathcal{G}_q$ of the ingredients $1, ..., q$, we denote the corresponding permutation matrix by R_π,

$$R_\pi = \sum_{i=1}^{q} e_{\pi(i)} e_i',$$

where e_i denotes the ith Euclidean unit vector of $\Re^q$, with ith entry one and zeros elsewhere. Let $Perm(q)$ be the group of all $q \times q$ permutation matrices. Define the group,

$$\begin{aligned} \mathcal{H} &:= \{H_\pi = \begin{pmatrix} R_\pi & 0 \\ 0 & S_\pi \end{pmatrix} : \pi \in \mathcal{G}_q\}, \\ S_\pi &:= \sum_{i,j=1, i<j}^{q} E_{(\pi(i),\pi(j))_\uparrow} E_{ij}' \in Perm(\binom{q}{2}), \end{aligned}$$

where $(\pi(i), \pi(j))_\uparrow$ for all $\pi \in \mathcal{G}_q$ denotes the pair of indices $\pi(i), \pi(j)$ in ascending order.

We can see that the group $\mathcal{H}$ is a subgroup of the orthogonal group, the space

$$Sym(\binom{q+1}{2}, \mathcal{H}) := \{C \in Sym(\binom{q+1}{2}) : HCH' = C, \forall H \in \mathcal{H}\}$$

of $\mathcal{H}$-invariant symmetric matrices is a quadratic subspace of $Sym(\binom{q+1}{2})$, that is, a subspace closed under formation of powers C^n with $n \in \mathbf{N}$. We briefly introduce the results of this analysis by Klein (2002). First we define the identity matrices $U_1 = I_q$ and $W_1 = I_{\binom{q}{2}}$, and write $1_q = (1, ..., 1)' \in \Re^q$. Furthermore, we define

$$
\begin{aligned}
U_2 &= 1_q 1_q' - I_q \in Sym(q), \\
V_1 &= \sum_{i,j=1,i<j}^{q} E_{ij}(e_i + e_j)' \in \Re^{\binom{q}{2}\times q}, \\
V_2 &= \sum_{i,j=1,i<j}^{q} \sum_{k=1,k\notin\{i,j\}}^{q} E_{ij} e_k' \in \Re^{\binom{q}{2}\times q}, \\
W_2 &= \sum_{i,j=1,i<j}^{q} \sum_{k,l=1,k<l,|\{i,j\}\cap\{k,l\}|=1}^{q} E_{ij} E_{kl}' \in Sym(\binom{q}{2}), \\
W_3 &= \sum_{i,j=1,i<j}^{q} \sum_{k,l=1,k<l,|\{i,j\}\cap\{k,l\}|=0}^{q} E_{ij} E_{kl}' \in Sym(\binom{q}{2}),
\end{aligned}
$$

as the invariant symmetric block matrices.

Lemma 2.3. *Any matrix $C \in Sym(\binom{q+1}{2}, \mathcal{H})$ can be uniquely represented in the form*

$$
C = \begin{pmatrix} aI_q + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eW_1 + fW_2 + gW_3 \end{pmatrix}
$$

with coefficients $a,...,g \in \Re$. The term V_2, W_2 and W_3 only occur for $q \geq 3$ or $q \geq 4$, respectively. In particular,

$$
dimSym(\binom{q+1}{2}, \mathcal{H}) = \begin{cases} 4 & , \ \textit{for } q = 2 \\ 6 & , \ \textit{for } q = 3 \\ 7 & , \ \textit{for } q \geq 4. \end{cases}
$$

Lemma 2.4. *For any $q \geq 2$, the matrices $U_1, U_2 \in Sym(q), V_1, V_2 \in \Re^{\binom{q}{2}\times q}$, and $W_1, W_2, W_3 \in Sym(\binom{q}{2})$ from Lemma 2.3 satisfy the following equations:*

(i)(Products in span$\{U_1, U_2\}$)

$$
\begin{aligned}
V_1'V_1 &= (q-1)U_1 + U_2, & V_2'V_2 &= \tbinom{q-1}{2}U_1 + \tbinom{q-2}{2}U_2, \\
V_1'V_2 &= V_2'V_1 = (q-2)U_2, & V_2'V_2 &= (q-1)U_1 + (q-2)U_2.
\end{aligned}
$$

(ii)(Products in span$\{V_1, V_2\}$*)*

$$
\begin{aligned}
V_1U_2 &= V_1 + 2V_2, & V_2U_2 &= (q-2)V_1 + (q-3)V_2,\\
W_2V_1 &= (q-2)V_1 + 2V_2, & W_2V_2 &= (q-2)V_1 + 2(q-3)V_2,\\
W_3V_1 &= (q-3)V_2, & W_3V_2 &= \binom{q-2}{2}V_1 + \binom{q-3}{2}V_2.
\end{aligned}
$$

(iii)(Products in span$\{W_1, W_2, W_3\}$*)*

$$
\begin{aligned}
V_1V_1' &= 2W_1 + W_2, & V_1V_2' &= V_2V_1' = W_2 + 2W_3,\\
V_2V_2' &= (q-2)W_1 + (q-3)W_2 + (q-4)W_3,\\
W_2^2 &= 2(q-2)W_1 + (q-2)W_2 + 4W_3,\\
W_3^2 &= \binom{q-2}{2}W_1 + \binom{q-3}{2}W_2 + \binom{q-4}{2}W_3,\\
W_2W_3 &= W_3W_2 = (q-3)W_2 + 2(q-4)W_3.
\end{aligned}
$$

3 The robust A-optimal designs for Scheffé's linear and quadratic models

In this section, we concentrate on the robust A-optimal designs for the Scheffé's linear and quadratic models. First we introduce the two mixture models and the A-optimal designs respectively, which will be used later. To the end, our candidate robust optimal design will be verified with the equivalence theorem to confirm that it is indeed A-optimal.

3.1 Scheffé's linear and quadratic models and the corresponding A-optimal designs

The first type of mixture model was the polynomial suggested by Scheffé (1958). Let $E_{q,1}(\mathbf{x})$ and $E_{q,2}(\mathbf{x})$ denote Scheffé linear and quadratic polynomials on the simplex S^{q-1} , which are defined as follows.

(i) Scheffé's linear model:

$$E_{q,1}(\mathbf{x}) = \sum_{1\leq i\leq q} \theta_i x_i = \theta_1' f_1(\mathbf{x}),$$

(ii) Scheffé's quadratic model:

$$E_{q,2}(\mathbf{x}) = \sum_{1\leq i\leq q} \theta_i x_i + \sum_{1\leq i\leq j\leq q} \theta_{ij} x_i x_j = \theta_2' f_2(\mathbf{x}).$$

Using the equivalence theorem, it is easy to prove that the design ξ_1^* which assigns a weight $1/q$ to each $\mathbf{x} \leftrightarrow (1, 0, ..., 0)$ is A-optimal for the linear polynomial $E_{q,1}(\mathbf{x})$, and these points are the only possible support points. Guan and Chao (1987), Yu and Guan (1993) have given that the $\{q, 2\}$ simplex weighted centroid design with $w_1 : w_2 = \sqrt{4q-3} : 4$ is A-optimal for Scheffé's quadratic models with $q \geq 4$. That is, the design ξ_2^* assigns equal weights w_1 to $\mathbf{x} \leftrightarrow (1, 0, ..., 0)$ and w_2 to $\mathbf{x} \leftrightarrow (\frac{1}{2}, \frac{1}{2}, 0, ..., 0)$, i.e.

$$w_1 = \frac{\sqrt{4q-3}}{q\sqrt{4q-3} + 2q(q-1)}, w_2 = \frac{4}{q\sqrt{4q-3} + 2q(q-1)},$$

for $q \geq 4$, where $C_1^q w_1 + C_2^q w_2 = 1$.

To be more precise, it is understood that the Scheffé's linear A-optimal design ξ_1^* can be expressed as follows,

$$\xi_1^* = \left(\begin{array}{cccc} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \\ \frac{1}{q} & \frac{1}{q} & \cdots & \frac{1}{q} \end{array} \right), \tag{3.1}$$

and the Scheffé's quadratic A-optimal design ξ_2^* as follows,

$$\xi_2^* = \left(\begin{array}{cccccccc} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} & \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1/2 \\ 1/2 \end{pmatrix} \\ w_1 & w_1 & \cdots & w_1 & w_2 & w_2 & \cdots & w_2 \end{array} \right). \tag{3.2}$$

Meanwhile, we denote $f_1(\mathbf{x}) = (x_1, x_2, ..., x_q)'$ and $f_2(\mathbf{x}) = (x_1, x_2, ..., x_q, x_1x_2, x_1x_3, ..., x_{q-1}x_q)'$ as Scheffé's linear models and quadratic models respectively, and the corresponding information matrices are $M_1(\xi)$ and $M_2(\xi)$ with a design ξ on S^{q-1}.

3.2 Robust A-optimality criteria for Scheffé models

In Section 2, the generalized A-optimality criteria defined in (2.1) and (2.2) have been defined, and now problems with uncertainties on linear and quadratic models, i.e. $l = 2$ will be considered. Therefore, the robust A-optimal criteria can be written as

$$(i) \quad \Psi_\beta(\xi) = \beta_1 \mathrm{tr} M_1^{-1}(\xi) + \beta_2 \mathrm{tr} M_2^{-1}(\xi) \tag{3.3}$$

$$(ii) \quad \Psi_\beta(\xi) = \beta_1 \log(\mathrm{tr} M_1^{-1}(\xi)) + \beta_2 \log(\mathrm{tr} M_2^{-1}(\xi)). \tag{3.4}$$

Then the equivalence theorem for the two criteria given in Section 2 can be used here. Thus, a design ξ_β is robust A-optimal for Scheffé's linear and quadratic models if ξ_β minimizes the functions $\Psi_\beta(\xi)$, and it can be verified through the equivalence theorems, such that for all $\mathbf{x} \in S^{q-1}$,

$$\begin{aligned}\Phi(\mathbf{x}, \xi_\beta) &= \beta_1 f_1(\mathbf{x})' M_1^{-2}(\xi_\beta) f_1(\mathbf{x}) + \beta_2 f_2(\mathbf{x})' M_2^{-2}(\xi_\beta) f_2(\mathbf{x}) \\ &= \beta_1 \phi_1(\mathbf{x}, \xi_\beta) + \beta_2 \phi_2(\mathbf{x}, \xi_\beta) \leq \beta_1 \mathrm{tr} M_1^{-1}(\xi_\beta) + \beta_2 \mathrm{tr} M_2^{-1}(\xi_\beta),\end{aligned}$$

or

$$\begin{aligned}\Upsilon(\mathbf{x}, \xi_\beta) &= \beta_1 \frac{f_1(\mathbf{x})' M_1^{-2}(\xi_\beta) f_1(\mathbf{x})}{\mathrm{tr} M_1^{-1}(\xi_\beta)} + \beta_2 \frac{f_2(\mathbf{x})' M_2^{-2}(\xi_\beta) f_2(\mathbf{x})}{\mathrm{tr} M_2^{-1}(\xi_\beta)} \\ &= \beta_1 \upsilon_1(\mathbf{x}, \xi_\beta) + \beta_2 \upsilon_2(\mathbf{x}, \xi_\beta) \leq 1.\end{aligned}$$

In what follows, we will show that the function $\phi_l(\mathbf{x}, \xi_\beta)$ can be considered as a trace of the products of certain matrices, where $l = 1$ or 2, which has some good properties and can be used later.

3.3 Exchangeability and Kiefer ordering

By Draper and Pukelsheim (1999), we call a design $\tau = \tau(\mathbf{x})$ as a single-point permutation design, which assigns weights on each of points of the subset$\{\mathbf{x} :$ a single point $\mathbf{x} \leftrightarrow (x_1, x_2, ..., x_q)\}$, where $\mathbf{x}$ is an arbitrary point defined on S^{q-1}. A design τ is said to be permutationally invariant when $\tau^R = \tau$ for all $R \in Perm(q)$, where τ^R is the image of τ under R. We call a design with this invariance property an exchangeable design. Moreover, we may obtain an exchangeable design $\bar{\tau}$ by averaging over the permutation group,

$$\bar{\tau} = \frac{1}{q!} \sum_{R \in Perm(q)} \tau^R.$$

To illustrate the notation, we give an example for $q = 3$ and an arbitrary point $\mathbf{x} = (\frac{1}{3}, \frac{2}{3}, 0)'$, then the set of

$$\{\mathbf{x} \leftrightarrow (x_1, x_2, x_3)\} = \{(\frac{1}{3}, \frac{2}{3}, 0), (\frac{1}{3}, 0, \frac{2}{3}), (\frac{2}{3}, \frac{1}{3}, 0), (\frac{2}{3}, 0, \frac{1}{3}), (0, \frac{1}{3}, \frac{2}{3}), (0, \frac{2}{3}, \frac{1}{3})\}.$$

Suppose a design τ is chosen as

$$\tau = \left(\begin{array}{cccc} \begin{pmatrix} 1/3 \\ 2/3 \\ 0 \end{pmatrix} & \begin{pmatrix} 2/3 \\ 0 \\ 1/3 \end{pmatrix} & \begin{pmatrix} 0 \\ 1/3 \\ 2/3 \end{pmatrix} & \begin{pmatrix} 0 \\ 2/3 \\ 1/3 \end{pmatrix} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{6} \end{array} \right),$$

which assigns weights on the subset of $\{\mathbf{x} \leftrightarrow (x_1, x_2, x_3)\}$. Now, if a permutation matrix R is considered by

$$R = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

which will imply

$$R\tau = \left(\begin{array}{cccc} \begin{pmatrix} 0 \\ 1/3 \\ 2/3 \end{pmatrix} & \begin{pmatrix} 1/3 \\ 2/3 \\ 0 \end{pmatrix} & \begin{pmatrix} 2/3 \\ 0 \\ 1/3 \end{pmatrix} & \begin{pmatrix} 1/3 \\ 0 \\ 2/3 \end{pmatrix} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{6} \end{array} \right).$$

Therefore, while considering all the permutation matrices $R \in Perm(3)$, then

$$\bar{\tau} = \left(\begin{array}{cccccc} \begin{pmatrix} 1/3 \\ 2/3 \\ 0 \end{pmatrix} & \begin{pmatrix} 1/3 \\ 0 \\ 2/3 \end{pmatrix} & \begin{pmatrix} 2/3 \\ 1/3 \\ 0 \end{pmatrix} & \begin{pmatrix} 2/3 \\ 0 \\ 1/3 \end{pmatrix} & \begin{pmatrix} 0 \\ 1/3 \\ 2/3 \end{pmatrix} & \begin{pmatrix} 0 \\ 2/3 \\ 1/3 \end{pmatrix} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \end{array} \right).$$

If the original design τ itself is exchangeable, then no modification is necessary, $\bar{\tau} = \tau$. Otherwise, the average $\bar{\tau}$ is an improvement over τ, in that it exhibits more symmetry, or balance. In terms of matrix majorization, the moment matrix of the averaged design $\bar{\tau}$ is majorized by the moment of τ, $M(\bar{\tau}) \prec M(\tau)$. As a consequence, the design $\bar{\tau}$ yields better than τ, under a large class of optimality criteria. For more details, see Pukelsheim (1993, p.343). Furthermore, for the calculation of the equivalence theorem, we need some useful properties of $\bar{\tau}$ as follows.

Corollary 3.1. *For an arbitrary point* $\mathbf{x}$ *and a single-point permutation design* $\tau = \tau(\mathbf{x})$*, we have*

$$\phi_l(\mathbf{x}, \xi) = f_l(\mathbf{x})' M_l^{-2}(\xi) f_l(\mathbf{x}) = \operatorname{tr}\{M_l(\bar{\tau}) M_l^{-2}(\xi)\}$$

for any exchangeable design ξ*, where* $l = 1$ *or* 2 *and* $\bar{\tau}$ *is an averaged design over design* τ*.*

Proof. For $\bar{\tau} = \frac{1}{q!} \sum \tau^R$, $R \in Perm(q)$,

$$M(\bar{\tau}) \;=\; \frac{1}{q!} \sum_R M(\tau^R) = \sum_{\mathbf{x}_i \in \bar{\tau}} \frac{1}{q!} f(\mathbf{x}_i) f(\mathbf{x}_i)'.$$

All the points $\mathbf{x}_i \in \bar{\tau}$ can be produced by one point $\mathbf{x}_1 \in \tau$ under the permutation matrix R_i, that is, $\mathbf{x}_i = R_i \mathbf{x}_1$, $R_i \in Perm(q)$. For convenience, we denote that

$$\begin{aligned}(\mathbf{x}_{(1)})' &= (x_1, x_2, ..., x_q)' \\ (\mathbf{x}_{(2)})' &= (x_1x_2, x_1x_3, ..., x_{q-1}x_q)'.\end{aligned}$$

By Draper et al. (1993), for every orthogonal $q \times q$ matrix R_i, there exists a unique nonsingular $q \times q$ matrix R_{1i} such that

$$f_1(R_i\mathbf{x}) = R_i^{(1)}(\mathbf{x}_{(1)})' = R_{1i}f_1(\mathbf{x})',$$

and a $\binom{q+1}{2} \times \binom{q+1}{2}$ matrix R_{2i} such that

$$f_2(R_i\mathbf{x}) = \begin{pmatrix} R_i^{(1)} & . \\ . & R_i^{(2)} \end{pmatrix} \begin{pmatrix} \mathbf{x}_{(1)} \\ \mathbf{x}_{(2)} \end{pmatrix} = R_{2i}f_2(\mathbf{x})',$$

where $R^{(2)}$ is a matrix, changed with $R^{(1)}$. Moreover, $R_{li}R'_{li} = R'_{li}R_{li} = I_{q_l}$ for $l = 1$ or 2. Hence, from the right hand side of the equation, we have

$$\begin{aligned}\mathrm{tr}\{M_l(\bar{\tau})M_l^{-2}(\xi)\} &= \mathrm{tr}\{\sum_{\mathbf{x}_i \in \bar{\tau}} \frac{1}{q!} f_l(\mathbf{x}_i)f_l(\mathbf{x}_i)'M_l^{-2}(\xi)\} \\ &= \mathrm{tr}\{\sum_{\mathbf{x}_1 \in \bar{\tau}} \frac{1}{q!} f_l(R_i\mathbf{x}_1)f_l(R_i\mathbf{x}_1)'M_l^{-2}(\xi)\} \\ &= \sum_{\mathbf{x}_1 \in \bar{\tau}} \frac{1}{q!} \mathrm{tr}\{R_{li}f_l(\mathbf{x}_1)f_l(\mathbf{x}_1)'R'_{li}M_l^{-2}(\xi)\} \\ &= \mathrm{tr}\{f_l(\mathbf{x}_1)f_l(\mathbf{x}_1)'R'_{li}M_l^{-2}(\xi)R_{li}\}.\end{aligned}$$

Since the design ξ assigns one weight p_1 to each of points $\mathbf{x} \leftrightarrow (1, 0, ..., 0)$ and another weight

p_2 to $\mathbf{x} \leftrightarrow (\frac{1}{2}, \frac{1}{2}, 0, ..., 0)$, it is clear that ξ is an exchangeable design, i.e.

$$\begin{aligned} M_l(\xi) &= \int f_l(\mathbf{x}) f_l(\mathbf{x})' d\xi = \int f_l(\mathbf{x}) f_l(\mathbf{x})' d\xi^R = \int f_l(R\mathbf{x}) f_l(R\mathbf{x})' d\xi \\ &= R_l \int f_l(\mathbf{x}) f_l(\mathbf{x})' d\xi R_l' = R_l M_l(\xi) R_l', \end{aligned}$$

where $R \in Perm(q)$ and $R_l R_l' = R_l' R_l = I_{q_l}$ for $l = 1$ or 2. Then we have

$$\begin{aligned} M_l^{-1}(\xi) &= (R_l M_l(\xi) R_l')^{-1} = (R_l')^{-1} M_l^{-1}(\xi)(R_l)^{-1} = R_l M_l^{-1}(\xi) R_l' \\ M_l^{-2}(\xi) &= (R_l M_l^{-1}(\xi) R_l')^{-1} = R_l M_l^{-2}(\xi) R_l' \end{aligned}$$

Thus, as ξ is an exchangeable design,

$$\begin{aligned} \mathrm{tr}\{M_l(\bar{\tau}) M_l^{-2}(\xi)\} &= \mathrm{tr}\{f_l(\mathbf{x}_1) f_l(\mathbf{x}_1)' R_{li}' M_l^{-2}(\xi) R_{li}\} \\ &= \mathrm{tr}\{f_l(\mathbf{x}_1) f_l(\mathbf{x}_1)' R_{li}' R_{li} M_l^{-2}(\xi) R_{li}' R_{li}\} \\ &= \mathrm{tr}\{f_l(\mathbf{x}_1) f_l(\mathbf{x}_1)' M_l^{-2}(\xi)\} = f_l(\mathbf{x}_1)' M_l^{-2}(\xi) f_l(\mathbf{x}_1). \end{aligned}$$

Since $\mathbf{x}_1$ must be one point belonging to supports of the design τ, the equality certainly holds true. Then the proof is completed.

Note that the convex complete class results obtained by Draper and Pukelsheim (1999) and Draper et al. (2000) are for Kronecker regression models. But it is mentioned that the Scheffé models contains some properties as Kronecker models by a linear transformation. For convenience, let f_k and f_s represent the Kronecker and Scheffé models respectively, and M_k and M_s represent the information matrices of the two models respectively. Moreover, we denote that a symmetric matrix $M \geq 0$ if the matrix is nonegative definite. Now a weighted centroid design $\eta \in \eta(S^{q-1})$ and a feasible design τ on S^{q-1} are considered for Scheffé models, then we have a property as follows.

Corollary 3.2. *In the second-degree Scheffé models for mixture experiments with $q \geq 2$ ingredients, consider a weighted centroid design $\eta \in \eta(S^{q-1})$, we have*

$$M_s(\eta) \geq M_s(\bar{\tau}),$$

where τ is any feasible design on S^{q-1}.

Proof. By Draper et al. (2000), it is known that $M_k(\eta) \geq M_k(\bar{\tau})$. Now choose a $\binom{q+1}{2} \times q^2$ transform matrix L, defined as

$$L = \begin{pmatrix} I_q & \frac{1}{2}V_1' & \frac{1}{2}V_1' \\ 0 & \frac{1}{2}W_1 & \frac{1}{2}W_1 \end{pmatrix}.$$

Then there is a correspondence between the Scheffé model $f_s(\mathbf{x})$ and the Kronecker model $f_k(\mathbf{x})$ through the linear transformation by the matrix L, where

$$\begin{aligned} f_s(\mathbf{x}) &= (x_1, x_2, ..., x_m, x_1x_2, x_1x_3, ..., x_{q-1}x_q)', \\ f_k(\mathbf{x}) &= (x_1^2, x_2^2, ..., x_m^2, x_1x_2, x_1x_3, ..., x_{q-1}x_q, x_2x_1, x_3x_1, ..., x_qx_{q-1})', \end{aligned}$$

such that

$$f_s(\mathbf{x}) = Lf_k(\mathbf{x}),$$

which implies that the information matrices of any design ξ for the Scheffé model and those for the Kronecker model have a relationship as

$$M_s(\bar{\tau}) = \int f_s(\mathbf{x})f_s(\mathbf{x})'d\bar{\tau} = L\int f_k(\mathbf{x})f_k(\mathbf{x})'d\bar{\tau}L' = LM_k(\bar{\tau})L'.$$

Therefore,

$$M_k(\eta) - M_k(\bar{\tau}) \geq 0 \Rightarrow M_s(\eta) - M_s(\bar{\tau}) = L(M_k(\eta) - M_k(\bar{\tau}))L' \geq 0,$$

which implies that

$$M_s(\eta) \geq M_s(\bar{\tau}). \tag{3.5}$$

Then the proof is completed.

3.4 The equivalence theorem on weighted centroid designs

By those properties stated above, the verification of robust A-optimality through equivalence theorem for Scheffé's linear and quadratic models can be substantially reduced.

Lemma 3.1. *For an exchangeable design ξ^*, it is robust A-optimal for Scheffé's linear and quadratic models if and only if*

$$\beta_1 \mathrm{tr}\{M_1(\eta_j)M_1^{-2}(\xi^*)\} + \beta_2 \mathrm{tr}\{M_2(\eta_j)M_2^{-2}(\xi^*)\} \leq \beta_1 \mathrm{tr} M_1^{-1}(\xi^*) + \beta_2 \mathrm{tr} M_2^{-1}(\xi^*)$$

for every centroid design η_j, where j = 1,2,...,q.

Proof. By Corollary 3.2, apply (3.5) on the Scheffé's second degree models, we can replace the character s into 2. i.e.

$$M_2(\eta) \geq M_2(\bar{\tau}). \tag{3.6}$$

Moreover, we can also use a $\binom{q+1}{2} \times q$ matrix z to reduce the inequality of the information matrix for Scheffé's quadratic models to that for Scheffé's linear models. i.e.

$$M_1(\eta) = z' M_2(\eta) z \geq z' M_2(\bar{\tau}) z = M_1(\bar{\tau}). \tag{3.7}$$

Taking inverse on (3.6) and (3.7), we have

$$M_1^{-1}(\eta) \leq M_1^{-1}(\bar{\tau}) \Rightarrow M_1^{-2}(\eta) \leq M_1^{-2}(\bar{\tau}) \tag{3.8}$$

Referring to the equivalence theorem stated in Section 3.2,

$$\begin{aligned} \phi_1(\mathbf{x}, \xi) &= f_1(\mathbf{x})' M_1^{-2}(\xi) f_1(\mathbf{x}) = f_2(\mathbf{x})' z M_1^{-2}(\xi) z' f_2(\mathbf{x}) \\ \phi_2(\mathbf{x}, \xi) &= f_2(\mathbf{x})' M_2^{-2}(\xi) f_2(\mathbf{x}), \end{aligned}$$

where ξ is a feasible design on S^{q-1}. By (3.7) and (3.8), we have the corresponding function for a design $\eta \in S^{q-1}$ such that

$$\begin{aligned} \Phi(\mathbf{x}, \eta) &= \beta_1 \phi_1(\mathbf{x}, \eta) + \beta_2 \phi_2(\mathbf{x}, \eta) \\ &= \beta_1 f_2(\mathbf{x})' z M_1^{-2}(\eta) z' f_2(\mathbf{x}) + \beta_2 f_2(\mathbf{x})' M_2^{-2}(\eta) f_2(\mathbf{x}) \\ &= f_2(\mathbf{x})' (\beta_1 z M_1^{-2}(\eta) z' + \beta_2 M_2^{-2}(\eta)) f_2(\mathbf{x}) \\ &\leq f_2(\mathbf{x})' (\beta_1 z M_1^{-2}(\bar{\tau}) z' + \beta_2 M_2^{-2}(\bar{\tau})) f_2(\mathbf{x}) \\ &= \Phi(\mathbf{x}, \bar{\tau}). \end{aligned}$$

Besides, in view of corollary 3.1, for every point $\mathbf{x} \in S^{q-1}$, we can choose a single-point permutation design τ such that

$$\begin{aligned}\Phi(\mathbf{x},\xi^*) &= \beta_1 f_1(\mathbf{x})' M_1^{-2}(\xi^*) f_1(\mathbf{x}) + \beta_2 f_2(\mathbf{x})' M_2^{-2}(\xi^*) f_2(\mathbf{x}) \\ &= \beta_1 \mathrm{tr}\{M_1(\bar{\tau}) M_1^{-2}(\xi^*)\} + \beta_2 \mathrm{tr}\{M_2(\bar{\tau}) M_2^{-2}(\xi^*)\} \\ &\leq \beta_1 \mathrm{tr}\{M_l(\eta) M_l^{-2}(\xi^*)\} + \beta_2 \mathrm{tr}\{M_2(\eta) M_2^{-2}(\xi^*)\}.\end{aligned}$$

Thus, the inequality in the robust A-optimal equivalence theorem,

$$\beta_1 f_1(\mathbf{x})' M_1^{-2}(\xi^*) f_1(\mathbf{x}) + \beta_2 f_2(\mathbf{x})' M_2^{-2}(\xi^*) f_2(\mathbf{x}) \leq \beta_1 \mathrm{tr} M_1^{-1}(\xi^*) + \beta_2 \mathrm{tr} M_2^{-1}(\xi^*)$$

for every point $\mathbf{x} \in S^{q-1}$, can be reduced to that for any $\eta \in \eta(S^{q-1})$, i.e.

$$\beta_1 \mathrm{tr}\{M_1(\eta) M_1^{-2}(\xi^*)\} + \beta_2 \mathrm{tr}\{M_2(\eta) M_2^{-2}(\xi^*)\} \leq \beta_1 \mathrm{tr} M_1^{-1}(\xi^*) + \beta_2 \mathrm{tr} M_2^{-1}(\xi^*),$$

which is equivalent to the inequality as

$$\beta_1 \mathrm{tr}\{M_1(\eta_j) M_1^{-2}(\xi^*)\} + \beta_2 \mathrm{tr}\{M_2(\eta_j) M_2^{-2}(\xi^*)\} \leq \beta_1 \mathrm{tr} M_1^{-1}(\xi^*) + \beta_2 \mathrm{tr} M_2^{-1}(\xi^*),$$

for all $\eta_j, j = 1, 2, ..., q$.

As a result of the above lemma, we merely need to check all the centroid designs η_j under the equivalence theorem while trying to verify that a design ξ^* is A-optimal, and need not to check all the points $\mathbf{x} \in S^{q-1}$ as before.

In Draper et al. (2000), the moment matrices $M(\eta_j)$ for second degree Kronecker models have been given for $j = 1, 2, ..., q$. In this work, we provide the moment matrices of the design $\eta_j \in \eta(S^{q-1})$ for second degree Scheffé models in the following lemma.

Lemma 3.2. *For second degree Scheffé model, we have*

$$
\begin{aligned}
M_1(\eta_j) &= \mu_{2,j} I_q + \mu_{11,j} U_2 \\
M_2(\eta_j) &= \begin{pmatrix} C_{11,j} & C'_{21,j} \\ C_{21,j} & C_{22,j} \end{pmatrix} = \begin{pmatrix} \mu_{2,j} I_q + \mu_{11,j} U_2 & \mu_{21,j} V'_1 + \mu_{111,j} V'_2 \\ \mu_{21,j} V_1 + \mu_{111,j} V_2 & \mu_{22,j} W_1 + \mu_{211,j} W_2 + \mu_{1111,j} W_3 \end{pmatrix},
\end{aligned}
$$

where

$\mu_{2,j} = \frac{1}{jq}$, $\mu_{11,j} = \frac{1}{jq}\frac{j-1}{q-1}$;

$\mu_{21,j} = \frac{1}{j^2 q}\frac{1}{jq}$, $\mu_{111,j} = \frac{1}{j^2 q}\frac{j-1}{q-1}\frac{j-2}{q-2}$;

$\mu_{22,j} = \frac{1}{j^3 q}\frac{1}{jq}$, $\mu_{211,j} = \frac{1}{j^3 q}\frac{j-1}{q-1}\frac{j-2}{q-2}$, $\mu_{1111,j} = \frac{1}{j^3 q}\frac{j-1}{q-1}\frac{j-2}{q-2}\frac{j-3}{q-3}$.

Proof. By Draper and Pukelsheim (1999), it is evident that η_j is exchangeable and assigns an equal weight $\frac{1}{j}$ to each of $\mathbf{x} \leftrightarrow (\frac{1}{j}, ..., \frac{1}{j}, 0, ..., 0)$ for $j = 1, 2, ..., q$. Therefore,

$$
\begin{aligned}
\mu_{2,j} &= \int x_r^2 d\eta_j &&= \frac{1}{j^2}\binom{q-1}{j-1}\frac{1}{\binom{q}{j}} &&= \frac{1}{jq} \\
\mu_{11,j} &= \int x_r x_s d\eta_j &&= \frac{1}{j^2}\binom{q-2}{j-2}\frac{1}{\binom{q}{j}} &&= \frac{1}{jq}\frac{j-1}{q-1} \\
\mu_{21,j} &= \int x_r^2 x_s d\eta_j &&= \frac{1}{j^3}\binom{q-2}{j-2}\frac{1}{\binom{q}{j}} &&= \frac{1}{j^2 q}\frac{j-1}{q-1} \\
\mu_{111,j} &= \int x_r x_s x_t d\eta_j &&= \frac{1}{j^3}\binom{q-3}{j-3}\frac{1}{\binom{q}{j}} &&= \frac{1}{j^2 q}\frac{j-1}{q-1}\frac{j-2}{q-2} \\
\mu_{22,j} &= \int x_r^2 x_s^2 d\eta_j &&= \frac{1}{j^4}\binom{q-2}{j-2}\frac{1}{\binom{q}{j}} &&= \frac{1}{j^3 q}\frac{j-1}{q-1} \\
\mu_{211,j} &= \int x_r^2 x_s x_t d\eta_j &&= \frac{1}{j^4}\binom{q-3}{j-3}\frac{1}{\binom{q}{j}} &&= \frac{1}{j^3 q}\frac{j-1}{q-1}\frac{j-2}{q-2} \\
\mu_{1111,j} &= \int x_r x_s x_t x_u d\eta_j &&= \frac{1}{j^4}\binom{q-4}{j-4}\frac{1}{\binom{q}{j}} &&= \frac{1}{j^3 q}\frac{j-1}{q-1}\frac{j-2}{q-2}\frac{j-3}{q-3}
\end{aligned} ,
$$

where $1 \leq r < s < t < u \leq q$.

In next subsection, we will find the robust A-optimal among the class Ξ_c defined below. Let ξ_1^*,..., ξ_m^* be the A-optimal designs respectively for the m candidate models.

3.5 Robust A-optimal designs for Scheffé's models

Let the class Ξ_c be the class of the convex combinations of ξ_1^*,..., ξ_m^* with a weight vector $\alpha = (\alpha_1, \alpha_2, ..., \alpha_m)' \in S^{m-1}$ for $m \in \mathbf{N}$ such as

$$\Xi_c = \{\xi_\alpha = \alpha_1\xi_1^* + \alpha_2\xi_2^* + ... + \alpha_m\xi_m^*, \quad \alpha = (\alpha_1, \alpha_2, ..., \alpha_m)' \in S^{m-1}\}.$$

In this work, as we would like to find a robust design with uncertainties on Scheffé's linear and quadratic models, we consider a design $\xi_\alpha \in \Xi_c$ and it is conjectured that a convex combination of ξ_1^* and ξ_2^* would be robust A-optimal with a weight vector $\alpha = (\alpha, 1-\alpha, 0, ..., 0)'$ such as

$$\xi_\alpha = \alpha\xi_1^* + (1-\alpha)\xi_2^*. \tag{3.9}$$

Note that the convex design ξ_α also belongs to the class $\eta(S^{q-1})$, so that it is clearly an exchangeable design. By robust A-optimality function in (3.3), the prior (β_1, β_2) can be chosen as $(r, 1-r)$,$(\frac{r}{q_1}, \frac{1-r}{q_2})$ or $(\frac{r}{\mathrm{tr}M_1^{-1}(\xi_1^*)}, \frac{1-r}{\mathrm{tr}M_2^{-1}(\xi_2^*)})$, where $q_1 = q$ and $q_2 = \binom{q+1}{2}$. For given $r \in [0,1]$ in the case with $\beta = (\beta_1, \beta_2) = (r, 1-r)$, we will find a corresponding $\alpha_r^* \in [0,1]$ such that $\xi_{\alpha_r^*}$ minimizes the function $\Psi_r(\xi_\alpha)$, and later verify that $\xi_{\alpha_r^*}$ is indeed robust A-optimal.

On the other hand, we can also show that for $(\beta_1, \beta_2) = (\frac{r}{q_1}, \frac{1-r}{q_2})$ and $(\frac{r}{\mathrm{tr}M_1^{-1}(\xi_1^*)}, \frac{1-r}{\mathrm{tr}M_2^{-1}(\xi_2^*)})$, robust A-optimal designs can be obtained through that for $(\beta_1, \beta_2) = (r, 1-r)$. Thus, we merely need to consider the criterion with $(\beta_1, \beta_2) = (r, 1-r)$ and others can be obtained accordingly.

Theorem 3.1. *For a given prior $r \in [0,1]$, consider a design $\xi_\alpha \in \Xi_c$ for mixture experiments with $q \geq 4$ ingredients, there exists an optimal α_r^* with $\alpha_r^* = g(r) \in [0,1]$ such that the corresponding function g(*) is one-one and onto.*

Proof. As the robust A-criterion is

$$\Psi_r(\xi_\alpha) = r\mathrm{tr}M_1^{-1}(\xi_\alpha) + (1-r)\mathrm{tr}M_2^{-1}(\xi_\alpha),$$

In order to find an optimal α_r^* to minimize $\Psi_r(\xi_\alpha)$, we take the derivative on $\Psi_r(\xi_\alpha)$ with respect to α and set it equal to zero. Then we have

$$\begin{aligned}
\frac{\partial}{\partial\alpha}\Psi_r(\xi_\alpha) &= r\frac{\partial}{\partial\alpha}\mathrm{tr}(M_1^{-1}(\xi_\alpha)) + (1-r)\frac{\partial}{\partial\alpha}\mathrm{tr}(M_2^{-1}(\xi_\alpha)) \\
&= -r\mathrm{tr}\{M_1^{-1}(\xi_\alpha)(\frac{\partial}{\partial\alpha}M_1(\xi_\alpha))M_1^{-1}(\xi_\alpha)\} - (1-r)\mathrm{tr}\{M_2^{-1}(\xi_\alpha)(\frac{\partial}{\partial\alpha}M_2(\xi_\alpha))M_2^{-1}(\xi_\alpha)\} \\
&= r\mathrm{tr}\{M_1^{-1}(\xi_\alpha)(M_1(\xi_2^*) - M_1(\xi_1^*))M_1^{-1}(\xi_\alpha)\} \\
&\quad +(1-r)\mathrm{tr}\{M_2^{-1}(\xi_\alpha)((M_2(\xi_2^*) - M_2(\xi_1^*)))M_2^{-1}(\xi_\alpha)\} \\
&= r\mathrm{tr}\{M_1^{-2}(\xi_\alpha)(M_1(\xi_2^*) - M_1(\xi_1^*))\} + (1-r)\mathrm{tr}\{M_2^{-2}(\xi_\alpha)(M_2(\xi_2^*) - M_2(\xi_1^*))\}.
\end{aligned}$$

Thus, the optimal α_r^* holds the following equality.

$$r\mathrm{tr}\{M_1^{-2}(\xi_{\alpha_r^*})(M_1(\xi_2^*) - M_1(\xi_1^*))\} + (1-r)\mathrm{tr}\{M_2^{-2}(\xi_{\alpha_r^*})(M_2(\xi_2^*) - M_2(\xi_1^*))\} = 0. \quad (3.10)$$

Moreover, observe that $\xi_1^* = \eta_1$ and $\xi_2^* = C_1^q w_1\eta_1 + C_2^q w_2\eta_2$ such that

$$\begin{aligned}
M(\xi_2^*) - M(\xi_1^*) &= M(C_1^q w_1\eta_1 + C_2^q w_2\eta_2) - M(\eta_1) \\
&= M((C_1^q w_1 - 1)\eta_1 + C_2^q w_2\eta_2) \\
&= C_2^q w_2(M(\eta_2) - M(\eta_1)),
\end{aligned}$$

where $C_1^q w_1 + C_2^q w_2 = 1$. Hence, (3.10) yields that

$$r\mathrm{tr}\{M_1^{-2}(\xi_\alpha)(M_1(\eta_2) - M_1(\eta_1))\} + (1-r)\mathrm{tr}\{M_2^{-2}(\xi_\alpha)((M_2(\eta_2) - M_2(\eta_1))\} = 0. \quad (3.11)$$

While solving the equation, as those matrices have some special forms as shown in Lemma 2.3, we can compute $M_l(\eta_2) - M_l(\eta_1)$ by using Lemma 3.2 for $l = 1, 2$. Therefore, we can express those matrices with q ingredients as

$$M_1(\eta_2) - M_1(\eta_1) = \begin{pmatrix} \frac{-1}{2q} I_q + \frac{1}{2q(q-1)} U_2 \end{pmatrix} \quad (3.12)$$

$$M_2(\eta_2) - M_2(\eta_1) = \begin{pmatrix} \frac{-1}{2q} I_q + \frac{1}{2q(q-1)} U_2 & \frac{1}{4q(q-1)} V_1' \\ \frac{1}{4q(q-1)} V_1 & \frac{1}{8q(q-1)} W_1 \end{pmatrix}. \quad (3.13)$$

For the convex design $\xi_\alpha \in \Xi_c$, the corresponding information matrices for Scheffé models can be written as

$$M_l(\xi_\alpha) = \alpha M_l(\xi_1^*) + (1-\alpha) M_l(\xi_2^*), \quad (3.14)$$

where $l = 1, 2$. Hence, in order to calculate $M_1^{-2}(\xi_\alpha)$ and $M_2^{-2}(\xi_\alpha)$, we first need to find the moment matrices $M_1(\xi_1^*)$, $M_1(\xi_2^*)$, $M_2(\xi_1^*)$ and $M_2(\xi_2^*)$. After some computations, we obtain

$M_1(\xi_1^*) = \frac{1}{q} I_q$,

$M_1(\xi_2^*) = \begin{pmatrix} w_1 I_q + w_2(\frac{1}{4}(q-1) I_q + \frac{1}{4} U_2) \end{pmatrix}$,

$M_2(\xi_1^*) = \begin{pmatrix} \frac{1}{q} I_q & 0 \\ 0 & 0 \end{pmatrix}$,

$M_2(\xi_2^*) = \begin{pmatrix} M_1(\xi_2^*) & \frac{1}{8} w_2 V_1' \\ \frac{1}{8} w_2 V_1 & \frac{1}{16} w_2 W_1 \end{pmatrix}$, then substitute the above moments matrices into (3.14), we have

$$M_1(\xi_\alpha) = \left(\frac{\alpha}{q} + (1-\alpha)w_1 + \frac{1}{4}(1-\alpha)(q-1)w_2)I_q + \frac{1}{4}(1-\alpha)w_2U_2 \right), \qquad (3.15)$$

$$M_2(\xi_\alpha) = \begin{pmatrix} M_1(\xi_\alpha) & \frac{1}{8}(1-\alpha)w_2V_1' \\ & \\ \frac{1}{8}(1-\alpha)w_2V_1 & \frac{1}{16}(1-\alpha)w_2W_1 \end{pmatrix}. \qquad (3.16)$$

For simplicity, take $p_1 = \frac{\alpha}{q} + (1-\alpha)w_1$ and $p_2 = (1-\alpha)w_2$ to express the convex design ξ_α as

$$\xi_\alpha = \left(\begin{array}{ccccccc} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} & \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1/2 \\ 1/2 \end{pmatrix} \\ p_1 & p_1 & \cdots & p_1 & p_2 & p_2 & \cdots & p_2 \end{array} \right),$$

which assigns p_1 to each of $\mathbf{x} \leftrightarrow (1,0,...,0)$ and p_2 to each of $\mathbf{x} \leftrightarrow (1/2,1/2,0,...,0)$ such that the moment matrices (3.15) and (3.16) can be rewrote as

$$M_1(\xi_\alpha) = \left((p_1 + \frac{1}{4}(q-1)p_2)I_q + \frac{1}{4}p_2U_2 \right),$$

$$M_2(\xi_\alpha) = \begin{pmatrix} M_1(\xi_\alpha) & \frac{1}{8}p_2V_1' \\ & \\ \frac{1}{8}p_2V_1 & \frac{1}{16}p_2W_1 \end{pmatrix}.$$

Thus, we can use these matrices to calculate the inverse matrices respectively in the next step. For a block matrix $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$, the inverse of M can be computed as

$$M^{-1} = \begin{pmatrix} K^{-1} & -K^{-1}BD^{-1} \\ -D^{-1}CK^{-1} & D^{-1} + D^{-1}CK^{-1}BD^{-1} \end{pmatrix},$$

where $K^{-1} = A - BD^{-1}C$, see Fedorov (1972, p.16,17). Moreover, due to quadratic subspace property of $Sym(\binom{q+1}{2}, \mathcal{H})$ by Klein (2002), we can assume that the inverse matrices $M_l^{-1}(\xi_{\alpha_r^*})$ have a form the same as $M_l(\xi_{\alpha_r^*})$ for $l = 1, 2$. Using the inverse formula above and Lemma 2.3

and Lemma 2.4, we obtain the following results,

$$\begin{aligned} M_1^{-1}(\xi_\alpha) &= \left(\; a_1 I_q + b_1 U_2 \; \right), \\ M_2^{-1}(\xi_\alpha) &= \begin{pmatrix} a_2 I_q + b_2 U_2 & c_2 V_1' + d_2 V_2' \\ & \\ c_2 V_1 + d_2 V_2 & e_2 W_1 + f_2 W_2 + g_2 W_3 \end{pmatrix}, \end{aligned}$$

where

$$a_1 = \frac{8p_1 + (4q-6)p_2}{(4p_1 + (q-2)p_2)(2p_1 + (q-1)p_2)}, \quad b_1 = \frac{-2p_2}{(4p_1 + (q-2)p_2)(2p_1 + (q-1)p_2)},$$

$$a_2 = \frac{1}{p_1}, \quad b_2 = 0, \quad c_2 = \frac{-2}{p_1}, \quad d_2 = 0, \quad e_2 = \frac{8}{p_1} + \frac{16}{p_2}, \quad f_2 = \frac{4}{p_1}, \quad g_2 = 0.$$

Similarly, we compute $M_l^{-2}(\xi_\alpha)$ by $M_l^{-1}(\xi_\alpha) * M_l^{-1}(\xi_\alpha)$ for $l = 1, 2$ and the forms of the matrices are still invariant, i.e.

$$\begin{aligned} M_1^{-2}(\xi_\alpha) &= \left(\; a_1' I_q + b_1' U_2 \; \right), \\ M_2^{-2}(\xi_\alpha) &= \begin{pmatrix} a_2' I_q + b_2' U_2 & c_2' V_1' + d_2' V_2' \\ & \\ c_2' V_1 + d_2' V_2 & e_2' W_1 + f_2' W_2 + g_2' W_3 \end{pmatrix}, \end{aligned}$$

where

$$a_1' = \frac{4(16p_1^2 + 8(2q-3)p_1p_2 + (4q^2 - 11q + 8)p_2^2)}{(4p_1 + (q-2)p_2)^2(2p_1 + (q-1)p_2)^2}, \quad b_1' = \frac{-4(8p_1p_2 + (3q-4)p_2^2)}{(4p_1 + (q-2)p_2)^2(2p_1 + (q-1)p_2)^2},$$

$$a_2' = \frac{4q-3}{p_1^2}, \quad b_2' = \frac{4}{p_1^2}, \quad c_2' = -\frac{2(16p_1 + (4q+1)p_2)}{p_1^2 p_2}, \quad d_2' = -\frac{16}{p_1^2},$$

$$e_2' = \frac{8(32p_1^2 + 32p_1p_2 + (4q+1)p_2^2)}{p_1^2 p_2^2}, \quad f_2' = \frac{4(32p_1 + (4q+9)p_2)}{p_1^2 p_2}, \quad g_2' = \frac{64}{p_1^2}.$$

In what follows, we substitute the above results into equation (3.11), then we have

$$\operatorname{tr}\{M_1^{-2}(\xi_\alpha)(M_1(\eta_2) - M_1(\eta_1))\} = t_1(q,\alpha) = -\frac{8}{(4p_1 + (q-2)p_2)}, \tag{3.17}$$

$$\operatorname{tr}\{M_2^{-2}(\xi_\alpha)(M_2(\eta_2) - M_2(\eta_1))\} = t_2(q,\alpha) = \frac{16}{p_2^2} - \frac{4q-3}{p_1^2}, \tag{3.18}$$

and solving equation (3.11) and obtain that there exists a real number $\alpha_r^* \in [0,1]$ such that

$$r = \frac{t_2(q,\alpha_r^*)}{t_2(q,\alpha_r^*) - t_1(q,\alpha_r^*)}. \tag{3.19}$$

On the other hand, for the function $r = g^{-1}(\alpha_r^*)$ is considered, taking the derivation on r with respect to α_r^*, then we have

$$\frac{\partial}{\partial \alpha_r^*} g^{-1}(\alpha_r^*) = \frac{t_2(q,\alpha_r^*)t_1'(q,\alpha_r^*) - t_2'(q,\alpha_r^*)t_1(q,\alpha_r^*)}{(t_2(q,\alpha_r^*) - t_1(q,\alpha_r^*))^2}, \tag{3.20}$$

where all functions of the numerator of (3.20) as follows.

$$t_1(q,\alpha_r^*) = \frac{-2q(2(q-1)+\sqrt{4q-3})}{(q\alpha_r^* + (q-2) + \sqrt{4q-3})} < 0, \tag{3.21}$$

$$t_2(q,\alpha_r^*) = q^2(2(q-1)+\sqrt{4q-3})^2\left(\frac{1}{(1-\alpha_r^*)^2} - \frac{1}{(1+\frac{2(q-1)}{\sqrt{4q-3}}\alpha_r^*)^2}\right) > 0, \tag{3.22}$$

and the derivations on $t_1(q,\alpha_r^*)$ and $t_2(q,\alpha_r^*)$ with respect to α_r^* as follows,

$$t_1'(q,\alpha_r^*) = \frac{2q^2(2(q-1)+\sqrt{4q-3})}{(q\alpha_r^* + (q-2) + \sqrt{4q-3})^2} > 0, \tag{3.23}$$

$$t_2'(q,\alpha_r^*) = q^2(2(q-1)+\sqrt{4q-3})^2\left(\frac{2}{(1-\alpha_r^*)^3} + \frac{4(q-1)(4q-3)}{(2(q-1)\alpha_r^* + \sqrt{4q-3})^3}\right) > 0. \tag{3.24}$$

Thus, for $\alpha_r^* \in [0,1)$, the four inequalities (3.21), (3.22), (3.23) and (3.24) above make the derivative function (3.20) greater than zero. Moreover, by (3.21) and (3.22), we also find that $g^{-1}(0) = 0$ and $\lim_{\alpha_r^* \to 1} g^{-1}(\alpha_r^*) = 1$. Therefore, the relation function $g^{-1}(\alpha_r^*)$ is strictly-increasing on $[0,1]$ and this function from α_r^* to r is one-one and onto. That is, for a given $r \in [0,1]$, there exists an optimal $\alpha_r^* \in [0,1]$ and thus the relation function $\alpha_r^* = g(r)$ is one-one and onto. The proof is completed.

Usually, we use $r = g^{-1}(\alpha_r^*)$ as the relation function because it is easier to get α_r^* this way. Moreover, as (β_1, β_2) is of different form, the relation function between r and α_r^* can be still obtained easily by applying the results for $(r, 1-r)$.

Theorem 3.2. *For a given $r \in [0,1]$, the design $\xi_{\alpha_r^*} \in \Xi_c$ with optimal $\alpha_r^* \in [0,1]$ is robust A-optimal.*

Proof. To prove that the convex design $\xi_{\alpha_r^*}$ is robust A-optimal, the equivalence theorem in Lemma 3.1,

$$r\mathrm{tr}\{M_1(\eta_j)M_1^{-2}(\xi_{\alpha_r^*})\} + (1-r)\mathrm{tr}\{M_2(\eta_j)M_2^{-2}(\xi_{\alpha_r^*})\} \leq r\mathrm{tr}M_1^{-1}(\xi_{\alpha_r^*}) + (1-r)\mathrm{tr}M_2^{-1}(\xi_{\alpha_r^*})$$

for every $j = 1, 2, ..., q$, must be satisfied.

After some computations, we find that the equality holds on the support points of the design $\xi_{\alpha_r^*}$ at each of the points $\mathbf{x} \leftrightarrow (1, 0, ..., 0)$ and $\mathbf{x} \leftrightarrow (\frac{1}{2}, \frac{1}{2}, 0, ..., 0)$. By Corollary 3.1, it is shown the equality also holds on $j = 1, 2$ because the centroid designs η_1 and η_2 are the permutation designs of each $\mathbf{x} \leftrightarrow (1, 0, ..., 0)$ and $\mathbf{x} \leftrightarrow (\frac{1}{2}, \frac{1}{2}, 0, ..., 0)$ respectively. Now we take $C_j := r\mathrm{tr}\{M_1(\eta_j)M_1^{-2}(\xi_{\alpha_r^*})\} + (1-r)\mathrm{tr}\{M_2(\eta_j)M_2^{-2}(\xi_{\alpha_r^*})\}$, then if we can show that

$$C_2 > C_3 > C_4 > ... > C_q, \tag{3.25}$$

the proof is completed.

The inequality above is equivalent to $C_j - C_{j+1} > 0$, for $j = 2, ..., q-1$. According to the properties of weighted centroid designs, the moment matrices $M_1(\eta_j)$ and $M_2(\eta_j)$ have been given in Lemma 3.2. After some simplifications, we have

$C_j - C_{j+1} = (8(j-1)(64p_1^* p_2^*(j^3 - 3j^2 - 5j - 2) + 32p_1^{*2}(j^3 + 11j_2 + 12j + 4) - p_2^{*2}((17j^3 - 37j_2 - 68j - 28) + 4q(j^3 + 11j^2 + 12j + 4))))/(j^3(j+1)^3(256p_1^{*4} + 128(q-2)p_1^{*3}p_2^* + 8(2q^2 - 16q + 15)p_1^{*2}p_2^{*2} - 8(4q^2 - 11q + 6)p_1^* p_2^{*3} - (q-2)^2(4q-3)p_2^{*4}))$.

Since we merely need to discuss the function above on $j \geq 2$, $C_j - C_{j+1}$ can be rewrite as follows, i.e.

$$C_j - C_{j+1} = \frac{8(j-1)(a(j-2)^3 + b(j-2)^2 + c(j-2) + d)}{j^3(j+1)^3 p_1^{*2} p_2^{*2}(4p_1^* + (q-2)p_2^*)^2(t_2(q,\alpha_r^*) - t_1(q,\alpha_r^*))}, \tag{3.26}$$

where

$$\begin{aligned}
a &= 64p_1^* p_2^* + 32p_1^{*2} - (4q+17)p_2^{*2} \\
&\propto \sqrt{4q-3}(16 + (8q-24)\alpha_r^*) + (8\alpha_r^{*2}(q-4)^2 + (12\alpha_r^{*2} + 40\alpha_r^* + 4)(q-4) - 57\alpha_r^{*2} + 162\alpha_r^* - 7, \\
b &= -128p_1^* p_2^* + 448p_1^{*2} - (56q+14)p_2^{*2} \\
&\propto \sqrt{4q-3}(48 + (136q-184)\alpha_r^*) + (\alpha_r^{*2}(136q^2 - 436q + 167) + \alpha_r^*(232q+34) + 68q - 167, \\
c &= -512p_1^* p_2^* + 1184p_1^{*2} - (148q-91)p_2^{*2} \\
&\propto \sqrt{4q-3}(-20 + (136q-116)\alpha_r^*) + \alpha_r^{*2}(136q^2 - 300q + 99) + \alpha_r^*(96q+34) + 68q - 99, \\
d &= -576p_1^* p_2^* + 896p_1^{*2} - (112q-16)p_2^{*2} \\
&\propto \sqrt{4q-3}(-16 + (40q-24)\alpha_r^*) + \alpha_r^{*2}(40q^2 - 68q + 19) + \alpha_r^*(8q+10) + 20q - 19.
\end{aligned}$$

Through some more computations, we can find the four coefficients a, b, c, d are greater then zero for $q \geq 4$, which implies the numerator of (3.26) is greater than zero as $j \geq 2$. On the other hand, by (3.21) and (3.22), the inequality $t_2(q,\alpha_r^*) - t_1(q,\alpha_r^*) > 0$ is easy to be obtained. As the results above, the function (3.26) is greater than zero.

Therefore, for $q \geq 4$, the inequalities $C_j - C_{j+1} > 0$ for all $j = 2, 3, ..., q-1$ have been proved. That is, for a given $r \in [0, 1]$, the optimal $\alpha_r^* \in [0, 1]$ implies that the convex design $\xi_{\alpha_r^*} \in \Xi_c$ is indeed robust A-optimal for Scheffé's linear and quadratic models.

4 Relationship between r and α_r^*

In Section 2, the criteria (2.1) and (2.2) for $n = 2$ can be considered with some different prior (β_1, β_2), such as

$$(\beta_1, \beta_2) = (r, 1-r), \quad (\frac{r}{q_1}, \frac{1-r}{q_2}), \quad \text{or} \quad (\frac{r}{\mathrm{tr}M_1^{-1}(\xi_1^*)}, \frac{1-r}{\mathrm{tr}M_2^{-1}(\xi_2^*)}).$$

Given a criterion as the above, we could get the relationship between r and α_r^* with $q \geq 4$ ingredient. In Section 3, we have shown that the convex design $\xi_{\alpha_r^*}$ is robust A-optimal and there exists an one-one correspondence between r and α while choosing the prior $(\beta_1, \beta_2) = (r, 1-r)$. Therefore, if we want to find robust A-optimal designs under the other two types of prior, we can select the value $(r, 1-r)$ as

$$(r, 1-r) = (\frac{\frac{r'}{m_1}}{\frac{r'}{m_1} + \frac{1-r}{m_2}}, \frac{\frac{1-r'}{m_2}}{\frac{r'}{m_1} + \frac{1-r}{m_2}}), \tag{4.1}$$

where $(m_1, m_2) = (q_1, q_2)$ or $(\mathrm{tr}M_1^{-1}(\xi_1^*), \mathrm{tr}M_2^{-1}(\xi_2^*))$. By (4.1), we have

$$r' = h(r) = \frac{\frac{r}{m_2}}{\frac{1-r}{m_1} + \frac{r}{m_2}}. \tag{4.2}$$

Thus, for a given $r \in [0, 1]$, the value r' also belongs to $[0, 1]$ and is one-one corresponding to r. Now consider the convex combination coefficient α. If the one-one correspondence between r and the optimal α_r^* holds true, it is obvious that r' and α_r^* have the same result. Therefore, for a given r, we say the design $\xi_{\alpha_r^*}$ is robust A-optimal, then for a given $r' = h(r)$, we can also find a robust A-optimal design $\xi_{\alpha_{r'}^*} = \xi_{\alpha_{h(r)}^*}$.

Although the prior $(\beta_1, \beta_2) = (1-r)$ can be extended to other ones, the relationship between

r and α_r^* on different type of (β_1, β_2) are different. In what follows, we will show these different types of relationship and present with plots.

For the three types of prior (β_1, β_2), we denote (β_1, β_2) as $(\frac{r}{m_1}, \frac{1-r}{m_2})$, where $(m_1, m_2) = (1,1), (q_1, q_2)$, or $(\mathrm{tr}M_1^{-1}(\xi_1^*), \mathrm{tr}M_2^{-1}(\xi_2^*))$. For a given $r \in [0,1]$, a function $g(*)$ from r to the corresponding optimal $\alpha_r^* \in [0,1]$ is one-one and onto. Hence, for criteria (2.1) with $n = 2$, the relation functions between r and α_r^* are as follows and the corresponding plots are shown in Figure 1.

$$r = \frac{t_2(q, \alpha_r^*)}{t_2(q, \alpha_r^*) - \dfrac{m_2}{m_1} t_1(q, \alpha_r^*)}, \tag{4.3}$$

where $t_1(q, \alpha_r^*)$ and $t_2(q, \alpha_r^*)$ defined as (3.17) and (3.18).

On the other hand, for criteria (2.2) with $n = 2$, the relation functions between r and α_r^* are as follows and the corresponding plots are shown in Figure 2.

$$r = \frac{t_2(q, \alpha_r^*)}{t_2(q, \alpha_r^*) - \dfrac{m_2 \mathrm{tr}M_2^{-1}(\xi_{\alpha_r^*})}{m_1 \mathrm{tr}M_1^{-1}(\xi_{\alpha_r^*})} t_1(q, \alpha_r^*)}. \tag{4.4}$$

Note that the results of criteria(ii) are equivalent to those in minimize the function

$$\beta_1 \log\{\frac{1}{m_1}\mathrm{tr}M_1^{-1}(\xi_\alpha)\} + \beta_2 \log\{\frac{1}{m_2}\mathrm{tr}M_2^{-1}(\xi_\alpha)\},$$

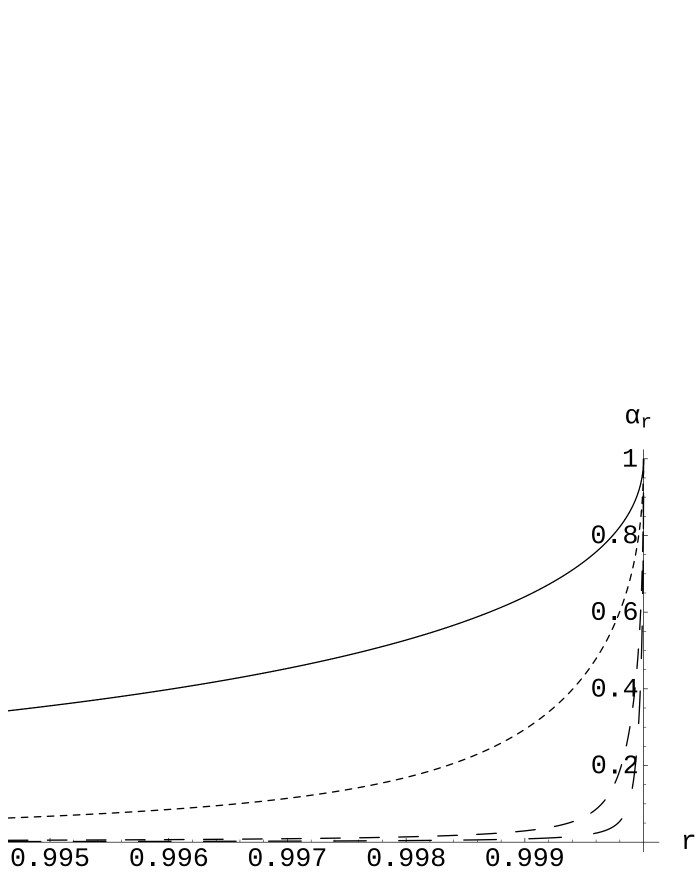
where $(m_1, m_2) = (1,1), (q_1, q_2)$, or $(\mathrm{tr}M_1^{-1}(\xi_1^*), \mathrm{tr}M_2^{-1}(\xi_2^*))$. Thus, we merely need to discuss in $m_1 = m_2 = 1$.

(a)

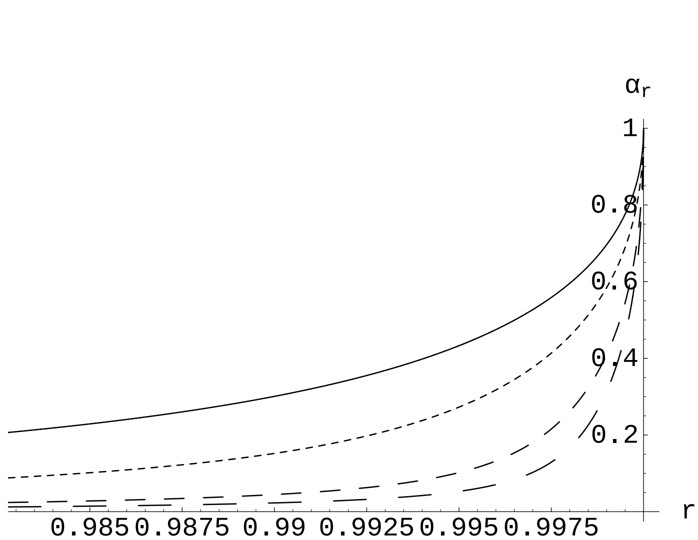
(b)

(c)

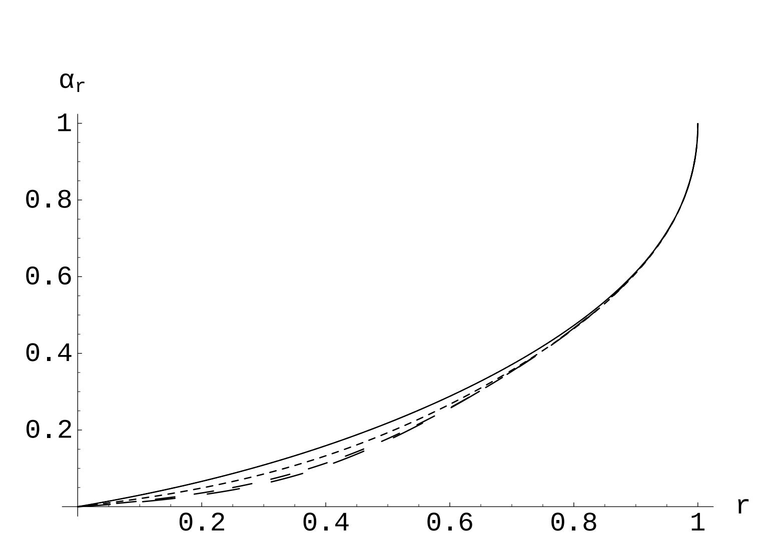
Figure 1. The relation functions between r and α_r^* for criterion (2.1) under different prior (β_1, β_2) with $q = 4, 10, 30$ and 50. (a)$(\beta_1, \beta_2) = (r, 1-r)$, (b) $(\beta_1, \beta_2) = (\frac{r}{q_1}, \frac{1-r}{q_2})$ and (c) $(\beta_1, \beta_2) = (\frac{r}{\mathrm{tr}M_1^{-1}(\xi_1^*)}, \frac{1-r}{\mathrm{tr}M_2^{-1}(\xi_2^*)})$.



α_r
1
0.8
0.6
0.4
0.2
0.995
0.996
0.997
0.998
0.999
r



α_r
1
0.8
0.6
0.4
0.2
r
0.985
0.9875
0.99
0.9925
0.995
0.9975



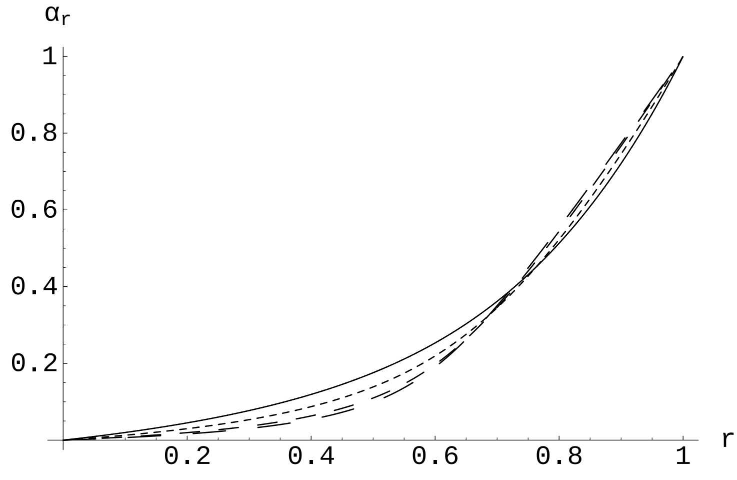
α_r
1
0.8
0.6
0.4
0.2
r
0.2
0.4
0.6
0.8
1

(a)

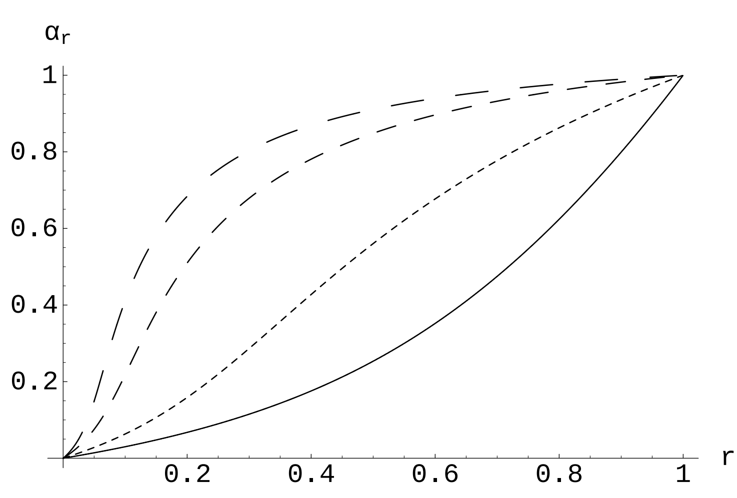
(b)

(c)

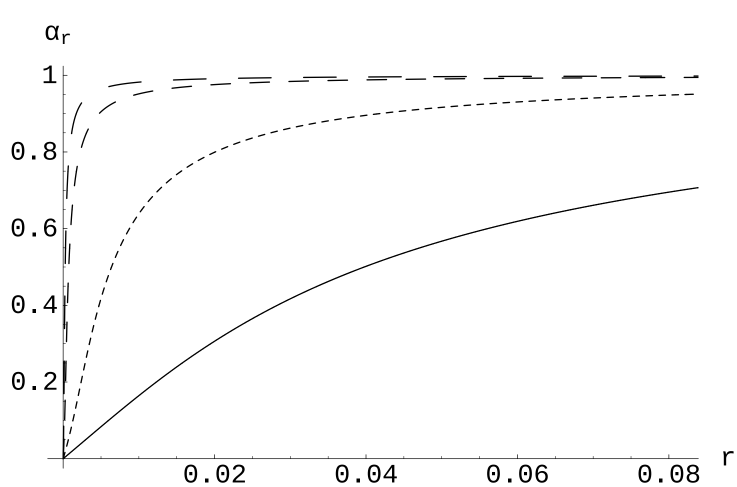
Figure 2. The relation functions between r and α_r^* for criterion (2.2) under different prior (β_1, β_2) with $q = 4, 10, 30$ and 50. (a)$(\beta_1, \beta_2) = (r, 1-r)$, (b) $(\beta_1, \beta_2) = (\frac{r}{q_1}, \frac{1-r}{q_2})$ and (c) $(\beta_1, \beta_2) = (\frac{r}{\mathrm{tr} M_1^{-1}(\xi_1^*)}, \frac{1-r}{\mathrm{tr} M_2^{-1}(\xi_2^*)})$.



α_r
1
0.8
0.6
0.4
0.2
0.2
0.4
0.6
0.8
1
r



α_r
1
0.8
0.6
0.4
0.2
r
0.2
0.4
0.6
0.8
1



α_r
1
0.8
0.6
0.4
0.2
r
0.02
0.04
0.06
0.08

5 Summary and some further works

The main results in this work are finding the robust A-optimal designs under different robust A-optimal criteria, where each criterion is a convex combination of a function of the traces of dispersion matrices respectively with a convex coefficient $r \in [0,1]$. We have therefore, for one of the robust A-optimal criteria, found for each given $r \in [0,1]$, there does exist a convex combination coefficient $\alpha_r^* \in [0,1]$ such that the convex combination of individual A-optimal design $\xi_{\alpha_r^*} = \alpha_r^* \xi_1^* + (1-\alpha_r^*)\xi_2^*$ is robust A-optimal under uncertainties between Scheffé's linear and quadratic models. Furthermore, it is proved that there exists an one-one and onto function between a given value r and the corresponding optimal coefficient α_r^*.

In order to verify whether a candidate design is robust A-optimal, a generalized A-optimal equivalence theorem is considered on Scheffé models. Moreover, the complete class results of weighted centroid designs (Draper, et al. (2000)) and the property of $\mathcal{H}$-invariant symmetric matrices (Klein (2002)) have been very useful in finding the optimal designs in the robust settings and making the computation tractable.

Furthermore, in this work, the value of r is predetermined, it is also of interest to discuss whether the performances of $\xi_{\alpha_r^*}$ is still acceptable under other values of r. In other words, under which criterion, i.e. choice of r value, such that the performances are not too bad even for other criterion, we will discuss along this direction in the future.

References

[1] Box, G. E. P., and Draper, N. R. (1959). A Basis for the Selection of a Response Surface Design, *Journal of the American Statistical Association*, 54, 622-654.

[2] Chan, L. Y. (2000). Optimal Design for Experiments with Mixtures: A Survey. *Communications in Statistions Instatistics-Theory and Methods*, **29** (9 & 10), 2281-2312.

[3] Guan, Y., Chao, X. (1987). On the A-optimal Allocation of Observations for the Generalized Simplex-Centroid Design (in Chinese). *Journal of Engineering Mathematics, 4(3)*, 33-39.

[4] Dette, H. (1990). A Generalization of D- and D_s- Optimal Design in Polynomial Regression. *The Annals of Statistics.* Vol. 18, No. 4, 1784-1804.

[5] Draper, N. R., Gaffke, N. and Pukelsheim, F. (1993) Rotatability of Cariance Surfaces and Moment Matrices. *Journal of Statistical Planning and Inference.* 36, 347-356.

[6] Draper, N. R., Heiligers, B. and Pukelsheim, F. (2000). Kiffer Ordering of Simplex Designs for Second-Degree Mixture Models with four or more Ingredients. *The Annals of Statistics*, Vol. 28. No. 2, 578-590.

[7] Draper, N. R., Pukelsheim, F. (1999). Kiffer Ordering of Simplex Designs for first- and second-degree Mixture Models. *Journal of Statistical Planning and Inference* **79**, 325-348.

[8] Draper, N. R., Pukelsheim, F. (1998). Mixture Models based on Homogeneous Polynomials. *Journal of Statistical Planning and Inference* 71, 303-311.

[9] Fedorov V. V. (1972). Theory of Optimal Experiments. Translated and edited by W. J. Studden and E. M. Klimko. Academic press, New York.

[10] Kiefer, J. (1961). Optimal Designs in Regression Problems, II. *Annals of Mathematical Statistics*, Vol. 32, Issue 1, 298-325.

[11] Klein, T. (2002). Invariant Sysmmetric Block Matrices for the Design of Mixture Experiments. *Institutfür Mathematik, Universität Augsburg, Report No. 443.*

[12] Klein, T. (2002). Optimal Designs for Second-degree Kronecker Model Mixture Experiments. *Institutfür Mathematik, Universität Augsburg, Report No. 444.*

[13] Pukelshiem, F. (1993). Optimal Design of Experiments. Wiley, New York.

[14] Scheffé, H. (1958). Experiments with Mixtures. *Journal of the Royal Statistical Society Series B* 20, 344-360.