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混合實驗在 Scheffè 模型之穩健 D-最適設計

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摘要

在本論文中，我們探討在混合實驗上的取點問題。一混合實驗，是在一包含q 個非負的成分$\{x_i, i = 1, \cdots, q\}$的$(q-1)$ 維之單純型機率空間S^{q-1}上所設計的實驗，並且以單純的限制式$\sum_{i=1}^{q} x_i = 1$ 為實驗的條件。在此，我們研究當混合實驗的模型屬於Scheffé（1958）所定義模型集合中，但並不確定其模型究竟屬於線性、二次或沒有交互作用之三次的情況下，如何尋找一穩健D型最適設計的問題。在不確知Scheffé 模型的型態時，我們希望利用個別模型下之D型最適設計，來尋找出相關的穩健D型最適設計。若不確定實驗的模型是Scheffé的線性或二次之下，我們得證其穩健D型最適設計為個別D型最適設計的最佳凸組合。針對在考慮Scheffé線性和沒有交互作用之三次模型的情況，相關的穩健D型最適設計有一些數值上的驗證和推測結果，對線性、二次和沒有交互作用的三次模型，我們也有類似的結果。最後，我們討論在給定Scheffé線性和二次模型下之穩健D型最適設計，探討其在小中取大準則下的效率D_r問題。

關鍵字: 完備集合，凸組合，等價定理，不變的對稱區塊矩陣，D_r-效率。

Robust D-optimal designs for mixture experiments in Scheffé models

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Abstract

A mixture experiment is an experiment in which the q-ingredients $\{x_i, i = 1, \cdots, q\}$ are nonnegative and subject to the simplex restriction $\sum_{i=1}^{q} x_i = 1$ on the $(q-1)$-dimensional probability simplex S^{q-1}. In this work, we investigate the robust D-optimal designs for mixture experiments with consideration on uncertainties in the Scheffé's linear, quadratic and cubic model without 3-way effects. The D-optimal designs for each of the Scheffé's models are used to find the robust D-optimal designs. With uncertianties on the Scheffé's linear and quadratic models, the optimal convex combination of the two model's D-optimal designs can be proved to be a robust D-optimal design. For the case of the Scheffé's linear and cubic model without 3-way effects, we have some numerical results about the robust D-optimal designs, as well as that for Scheffé's linear, quadratic and cubic model without 3-way effects. Ultimately, we discuss the efficiency of a maxmin type criterion D_r under given the robust D-optimal designs for the Scheffé's linear and quadratic models.

Keywords : Complete classes, convex combination, equivalence theorem, invariant symmetric block matrices, D_r-efficiency.

Contents

1 Introduction

Optimal design problems for general polynomial regression models have been investigated extensively. In this work, we focus our attention on mixture experiments. In mixture experiments, early important work was done by Scheffé (1958) where the simplex-lattice designs were introduced. The design problems for models considered by Scheffé for the mixture experiments will be investigated here. Suppose that in a mixture experiment with q nonnegative components, the proportions are subject to the simplex restriction $\sum_{i=1}^{q} x_i = 1, x_i \geq 0$ for all i. The q proportions can be expressed as a column vector $\mathbf{x} = (x_1, \cdots, x_q)'$ in the $(q-1)$-dimensional probability simplex

$$S^{q-1} = \{(x_1, \cdots, x_q)' \in [0,1]^q : x_1 + \cdots + x_q = 1, \quad x_i \geq 0 \quad i = 1, \cdots, q\}.$$

Let $\eta(\mathbf{x}) = E(y(\mathbf{x})) = \theta' f(\mathbf{x})$ be a corresponding regression function on S^{q-1} under the given Scheffé models, where $f(\mathbf{x})$ is a known function and θ is the unknown parameter vector. It is assumed the response variable $y(\mathbf{x})$ has mean $\theta' f(\mathbf{x})$ and variance σ^2 independence of $\mathbf{x}$.

An exact design is a probability measure on design space which puts weight p_i at distinct $\mathbf{x}_i$ and np_i , $i = 1, \cdots, n$ are integers. An approximate optimal design removes the integer restrictions on np_i , $i = 1, \cdots, n$. We will study the approximate design here. Now a design is a probability measure ξ on S^{q-1} with finite supports. Denote a probability measure ξ for a mixture experiment as follows

$$\xi = \begin{pmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_n \\ p_1 & \cdots & p_n \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} x_{1,1} \\ \vdots \\ x_{1,q} \end{pmatrix} & \cdots & \begin{pmatrix} x_{n,1} \\ \vdots \\ x_{n,q} \end{pmatrix} \\ \\ p_1 & \cdots & p_n \end{pmatrix},$$

where $\mathbf{x}_1, \cdots, \mathbf{x}_n$ represent the finite supports and the corresponding weights are $p_1, \ldots, p_n$. The information matrix is therefore defined by

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

and the corresponding dispersion function is given by

$$d(\mathbf{x}, \xi) = f'(\mathbf{x}) M^{-1}(\xi) f(\mathbf{x}).$$

A design ξ^* is called D-optimal if it maximizes the determinate of $M(\xi)$. For models with a continue regression models and compact design space, by the well known equivalence theorem, ξ^* minimizes the maximum of $d(\mathbf{x}, \xi)$ among all feasible designs ξ, in other words the D-optimal design and the minimax design are equivalent, and $\max_{\mathbf{x}} d(\mathbf{x}, \xi^*) \leq q$ for any point $\mathbf{x} \in S^{q-1}$ and equality hold at the design points.

For different types of mixture polynomial models as Scheffé's linear, quadratic, cubic models, log contrast models, the D-optimal designs for the models just mentioned have been obtained. For example, Kiefer (1961) has determined the D-optimal designs for the quadratic models. Mikaeili (1989, 1993) have found the D-optimal designs for cubic without 3-way effect and full cubic on the q-simplex, and Lim (1990) has given the D-optimal design for cubic polynomial regression on the q-simplex. Cornell (1990) has numerous examples and applications of mixture experiments. An extensive review has been given by Chan (2000) on known results about analytic and numerical solutions of optimal designs on various regression models for experiments with mixture. In the past, the way to find the D-optimal designs for different mixture models has almost always used the orthogonal polynomials approach provided by Kiefer (1961) to compute the dispersion function. Such method does not utilize the inverse of information matrix to prove that the optimal designs satisfy the equivalence theorem. Although using orthogonal polynomials does not require computation of the inverse of the information matrix, it is usually proved through a complex computation that a design is D-optimal. Draper and Pukelsheim (1999), Draper et al. (2000) have provided a useful complete class result which makes the research of an optimal design under very general criteria much more easier. Draper and Pukelsheim (1999) shows that the vertex points design is the unique optimal design under the Kiefer ordering in the first-degree mixture model. For the second-degree mixture model with two or three ingredients, complete class results under the Kiefer ordering are also derived there. Draper et al. (2000) shows that the set of weighted centroid designs constitutes a convex complete class under Kiefer ordering for the second-degree mixture models. For four ingredients, the class is minimal complete. With the complete class result, we are able to focus on finding an optimal design in that class. Klein (2002) has that in the complete class of weighted centroid designs, a method to prove equivalence theorem. It has analyzed a quadratic subspace of block matrices which are invariant under the action of a group $\mathcal{H}$ arising from the design of mixture experiments. Later these results are 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, the experimenters are often uncertain about which model is suitable i.e. if there are several possible regression models in consideration, experimenters do not know which model is proper before accomplishing the experiments. Actually concerns about uncertainty of the models for the experiments dates back to Box and Draper (1959), where it is observed that if we use simple linear function to estimate the expected value of the response when the true model is quadratic, it would result in a large bias term for estimation. Since then while designing an experiment for regression models, robustness has always been an important issue. Many papers thereafter have addressed this issue and provided different design strategies, for some examples see Stigler (1971), Atkinson and Cox (1974), Huber (1975), Studden (1982), Sacks and Ylvisaker (1984), Huang and Studden (1988), Dette (1990, 1991, 1993, 1994a, 1994b, 1995), Pukelsheim and Rosenberger (1993), Dette and Studden (1995) and Dette and Wong (1996). For more details about different types of optimal design criteria see Pukelsheim (1993).

The paper is organized as follows. In Section 2, some lemmas and theorems useful for finding and verifying the robust optimal designs are provided. In Section 3, the robust D-optimal design for Scheffé's linear and quadratic models are obtained and the efficiencies of the D-optimal designs with different weighting on the models are computed and compared using the maxmin criterion as originated from Pukelsheim and Rosenberger (1993) and Zen and Tsai (2003) are discussed. In Section 4, we list some robust D-optimal designs obtained numerically. In the Appendix A, the Scheffé's models and the corresponding D-optimal designs reviewed in Chan (2000) are provided for completeness.

2 Preliminary for the robust D-optimal design

Now we introduce the model robust D-optimal design criterion. A model robust D-optimal design criterion for mixture experiments is defined to be that for given constants $r_j \in [0,1], \sum_{j=1}^{\ell} r_j = 1$, the following function is maximized

$$\psi_r(\xi) = \prod_{j=1}^{\ell} |M_j(\xi)|^{\frac{r_j}{m_j}}, \tag{2.1}$$

where $M_j(\xi), j = 1, \ldots, \ell$, are the corresponding information matrix for the ℓ candidate models for the experiment, where m_j is the dimension of the unknown parameter vector in model j,$j = 1, \cdots, \ell$.

To find the model robust D-optimal designs for classes with Sheffé's polynomial models, complete class results under Kiefer ordering derived by Draper and Pukelsheim (1999), Draper et al. (2000), the invariant symmetric block matrices representation by Klein (2002) as well as the equivalent theorem in Dette (1990) will be utilized.

2.1 Complete classes for second degree mixture models

In this subsection, we present results by Draper and Pukelsheim (1999), Draper et al. (2000), where it is stated that the implication of the complete class theorems is that any design not of a mixture of the elementary centroid designs can be improved upon by using an appropriate combination of the elementary centroid designs. Such consequence is very instrumental in finding the optimal designs so that we may restrict our attentions on the classes of weighted centroid designs introduced below.

Definition 2.1.1. *For $q \geq 2$ and $j \in \{1, \cdots, q\}$, the j-th elementary centroid design η_j takes uniform weight on the centroid points of depth j, i.e. taking the form $\frac{1}{j}\sum_{i=1}^{j} e_{k_i} \in S^{q-1}$ with $1 \leq k_1 < k_2 < \cdots < k_{j-1} < k_j \leq q$. A convex combination $\eta(\lambda) = \sum_{j=1}^{q} \lambda_j \eta_j$ with $\lambda = (\lambda_1, \cdots, \lambda_q)' \in S^{q-1}$ is called a weighted centroid design with weight vector λ.*

The following theorem about complete class of optimal designs under Kiefer ordering is due to Draper and Pukelsheim (1999), Draper et al. (2000) for the first and second-degree mixture models on Kronecker regression functions. Now we give the second-degree Kronecker model for illustration.

$$E(Y(\mathbf{x})) = f'(\mathbf{x})\boldsymbol{\theta} = (\mathbf{x} \otimes \mathbf{x})'\boldsymbol{\theta} = \sum_{i=1}^{q} \theta_i x_i + \sum_{\substack{i,j=1 \\ i<j}}^{q} (\theta_{ij} + \theta_{ji}) x_i x_j \tag{2.2}$$

Since the convex complete class results are under Kiefer ordering, we give the introduce of the Kiefer ordering, see Pukelsheim (1993,p12,p352,p354) for detail.

Definition 2.1.2. *Give two matrices $C, D \in Sym(q)$,*

(i) *We say that C is majorized by D, denoted by $C \prec D$, when C lies in the convex hull of the orbit of D under congruence action of the group $\mathcal{H}$, i.e.*

$$C \prec D \iff C \in \{HDH' : H \in \mathcal{H}\}.$$

(ii) *The Loewner ordering of symmetric matrices is defined as*

$$C \geq D \iff C - D \geq 0 \iff C - D \in CCD(q).$$

We call C is more informative than D and write $C \gg D$ when C is better in the Loewner ordering than some intermediate matrix E which is majorized by D,

$$C \gg D \iff C \geq E \in conv\{HDH' \in \mathcal{H}\} \quad \text{for some } E \in Sym(q).$$

Therefore, we call the relation of $\gg$ *the Kiefer ordering on Sym(q) relative to the group* $\mathcal{H}$. *The notation* $\gg$ *is represented as* $C \geq E \prec D$.

The convex complete class of weighted centroid designs on Kronecker models are presented by the following theorem.

Theorem 2.1.3. *In the second-degree mixture model (2.2) for* $q \geq 2$ *ingredients, the set of weighted centroid designs*

$$\mathcal{W} = \{\lambda_1\eta_1 + \cdots + \lambda_q\eta_q : (\lambda_1, \cdots, \lambda_q)' \in S^{q-1}\}$$

is convex and constitutes a complete class of designs under Kiefer ordering. For $q = 2, 3, 4$, *the class is minimal complete.*

Note that any of the weighted centroid design η is an exchangeable design, an important property that will be utilized throughout this work. The definition of an exchangeable design is stated below for clarity. Let $Perm(q)$ be the group of all $q \times q$ permutation matrices.

Definition 2.1.4. *A design* τ *is said to be permutation invariant when*

$$\tau^R = \tau \qquad \text{for all } R \in Perm(q),$$

where $\tau^R(t) = \tau(R^{-1}t)$ *is the image of* τ *under* R. *A design with this invariant property is called an exchangeable design.*

Note that for an arbitrary design τ, a corresponding exchangeable design $\bar{\tau}$ can be obtained by averaging over the permutation group,

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

If $\bar{\tau} = \tau$, then τ itself is exchangeable. Moreover, the information matrix of $\bar{\tau}$ is majorized by the information matrix τ denoted as $M(\bar{\tau}) \prec M(\tau)$.

Besides, a information matrix is said to be permutationally invariant when

$$M = RMR' \quad \text{for all} \quad R \in Perm(m), \text{ where } m \text{ is the dimension of } M$$

which is also called an exchangeable information matrix.

2.2 Invariant symmetric block matrices

Next we introduce the invariant symmetric matrices results by Klein (2002). In Klein (2002), 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 the matrices have seven distinct entries at most. With these block matrices representation, the D- ,A- and E-optimal designs for quadratic models have been obtained there. The results and methods there is very help in finding optimal designs here. The $\mathcal{H}$-invariant symmetric matrices representation in Klein (2002) are given as follows. Suppose $\mathcal{Q}_q$ designate the symmetric group of degree q. Let

$$\begin{aligned} \mathcal{H} &= \left\{ H_\pi = \begin{pmatrix} R_\pi & 0 \\ 0 & S_\pi \end{pmatrix} : \pi \in \mathcal{Q}_q \right\}, \qquad \text{with} \\ R_\pi &= \sum_{i=1}^{q} e_{\pi(i)} e_i' \qquad \text{and} \\ S_\pi &= \sum_{\substack{i,j=1 \\ i<j}}^{q} E_{(\pi(i),\pi(j))_\uparrow} E_{ij}' \in Perm\left(\binom{q}{2}\right) \qquad \text{for all } \pi \in \mathcal{Q}_q, \end{aligned}$$

where $(\pi(i), \pi(j))_\uparrow$ denotes the pair of indices $\pi(i)$,$\pi(j)$ in ascending order. The set $\mathcal{H}$ acts on the space $\mathrm{Sym}\left(\binom{q+1}{2}\right)$ through the congruence transformation $H, C \mapsto HCH'$ and induces the subspace

$$\text{Sym}\left(\binom{q+1}{2}, \mathcal{H}\right) = \left\{C \in \text{Sym}\left(\binom{q}{2}\right) : HCH' = C \quad \text{for all } H \in \mathcal{H}\right\}$$

of $\mathcal{H}$-invariant symmetric matrices. For completeness, we will present the block matrices on the quadratic subspace $\text{Sym}\left(\binom{q+1}{2}, \mathcal{H}\right)$ as follows.

Let $U_1 = I_q$, $W_1 = I_{\binom{q}{2}}$, and $1_q = (1, \cdots, 1)' \in \mathbb{R}^q$,

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

Now, an important result and a multiplication table given in Klein (2002) are stated in the next two lemmas.

Lemma 2.2.1. *Any matrix* $C \in Sym\left(\binom{q}{2}, \mathcal{H}\right)$ *can be uniquely represented in the form*

$$C = \begin{pmatrix} C_{11} & C_{21}' \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} aI_q + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{q}{2}} + fW_2 + gW_3 \end{pmatrix} \tag{2.3}$$

with coefficients $a, \cdots, g \in \mathbb{R}$. *The term* V_2, W_2 *and* W_3 *only occur for* $q \geq 3$ *or* $q \geq 4$, *respectively. In particular,*

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

The next lemma represents a multiplication table for these matrices.

Lemma 2.2.2. *For any* $q \geq 2$, *the matrices* $U_1, U_2 \in Sym(q), V_1, V_2 \in \mathbb{R}^{\binom{q}{2}\times q}$, *and* $W_1, W_2, W_3 \in Sym\left(\binom{q}{2}\right)$ *satisfy the following equations:*

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

$$V_1'V_1 = (q-1)U_1 + U_2, \qquad V_2'V_2 = \binom{q-1}{2}U_1 + \binom{q-2}{2}U_2,$$

$$V_1'V_2 = V_2'V_1 = (q-2)U_2, \qquad U_2^2 = (q-1)U_1 + (q-2)U_2.$$

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

$$V_1U_2 = V_1 + 2V_2, \qquad V_2U_2 = (q-2)V_1 + (q-3)V_2,$$

$$W_2V_1 = (q-2)V_1 + 2V_2, \qquad W_2V_2 = (q-2)V_1 + 2(q-3)V_2,$$

$$W_3V_1 = (q-3)V_2, \qquad W_3V_2 = \binom{q-2}{2}V_1 + \binom{q-3}{2}V_2.$$

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

$$V_1V_1' = 2W_2 + W_2, \qquad V_2V_2' = (q-2)W_2 + (q-3)W_2 + (q-4)W_3,$$

$$V_1V'2 = V_2V_1' = W_2 + 2W_3,$$

$$W_2^2 = 2(q-2)W_1 + (q-2)W_2 + 4W_3,$$

$$W_3^2 = \binom{q-2}{2}W_1 + \binom{q-3}{2}W_2 + \binom{q-4}{2}W_3,$$

$$W_2W_3 = W_3W_2 = (q-3)W_2 + 2(q-4)W_3.$$

2.3 Generalized D-optimal equivalence theorem

The following result due to Dette (1990) characterizes the generalized D-optimal designs ξ^* and will be employed to verify the robust D-optimal designs for mixture experiments as well.

Now we state the generalized D-optimal design criterion defined in Dette (1990). Consider a class of polynomial regression models

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

The variance of the $f_\ell(x)$ at the point $x \in [-1, 1]$ is proportional to

$$d_\ell(x, \xi) = (1, x, \cdots, x^\ell) M_\ell^{-1}(\xi)(1, x, \cdots, x^\ell)'$$

where

$$M_\ell(\xi) = \int (1, x, \cdots, x^\ell)'(1, x, \cdots, x^\ell)\lambda(x) d\xi(x)$$

denotes the information matrix of the design ξ and $\lambda(x)$ is called the efficiency function. A vector $\beta = (\beta_0, \beta_1, \cdots, \beta_n)$ of real numbers is called a prior for $\mathcal{F}_n$ where β is a probability measure on $\{0, \cdots, n\}$ or is, for $s \in \{1, \cdots, n-1\}$, of the form

$$\beta_0 = \cdots = \beta_{n-s-1} = 0, \quad \beta_{n-s} = -\frac{n-s+1}{s},$$

$$\beta_{n-s+1} = \cdots = \beta_{n-1} = 0, \quad \beta_n = \frac{n+1}{s}.$$

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

$$\Psi_\beta(\xi) = \sum_{\ell=0}^{n} \frac{\beta_\ell}{\ell+1} \log(det M_\ell(\xi)). \tag{2.4}$$

The D-optimality criterion is a special case with prior $\beta_D = (0, \cdots, 0, 1)$ and D_s-optimality criterion with the prior $\beta_{D_s}, s \in (1, \cdots, n-1)$.

The following is the equivalence theorem of the generalized D- optimality criterion given in Dette (1990).

Theorem 2.3.1. *For a given prior $\beta = (\beta_0, \cdots, \beta_n)$ on $\{0, 1, \cdots, n\}$ 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*

$$\Phi_\beta(\xi) = \max_{x \in [-1,1]} \lambda(x) \sum_{\ell=0}^{n} \frac{\beta_\ell}{\ell+1} d_\ell(x, \xi).$$

(iii)

$$\Phi_\beta(\xi_\beta) = \max_{x \in [-1,1]} \lambda(x) \sum_{\ell=0}^{n} \frac{\beta_\ell}{\ell+1} d_\ell(x, \xi_\beta) = 1.$$

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

3 Robust D-optimal designs for the Scheffé's linear and quadratic model

In this section, we will concentrate on robust D-optimal designs for the Scheffé's linear and quadratic models. We first state the mixture models and D-optimal designs for the Scheffé's linear and quadratic models that will be used later. For the Scheffé's linear model, the corresponding regression function is

$$E_1(y(\mathbf{x})) = \boldsymbol{\theta}'_1 f_1(\mathbf{x}) = \sum_{1\le i\le q} \theta_i x_i,$$

where $f_1(\mathbf{x}) = (x_1, \cdots, x_q)', 0 \le x_i \le 1$, $\boldsymbol{\theta}_1 = (\theta_1, \cdots, \theta_q)'$ and the D-optmal design ξ_1^* assigns a equal weight $\frac{1}{q}$ to each of the points $\mathbf{x} \leftrightarrow (1, 0, \cdots, 0)$ which means

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

Therefore, the corresponding information matrix and dispersion function are

$$M_1(\xi_1^*) = \sum_{\mathbf{x}_i \in \xi_1^*} \frac{1}{q} f_1(\mathbf{x}_i) f'_1(\mathbf{x}_i),$$

$$d_1(\mathbf{x}, \xi_1^*) = f'(\mathbf{x}) M_1^{-1}(\xi_1^*) f(\mathbf{x}).$$

For the Scheffé's quadratic model, the corresponding regression function is

$$E_2(y(\mathbf{x})) = \boldsymbol{\theta}'_2 f_2(\mathbf{x}) = \sum_{1\le i\le q} \theta_i x_i + \sum_{1\le i<j\le q} \theta_{ij} x_i x_j,$$

where $f_2(\mathbf{x}) = (x_1, \cdots, x_q, x_1x_2, \cdots, x_{q-1}x_q)', 0 \le x_i \le 1$, $\boldsymbol{\theta}_2 = (\theta_1, \cdots, \theta_q, \theta_{12}, \cdots, \theta_{q-1q})'$ and the D-optimal design ξ_2^* assigns a weight $\frac{1}{\binom{q+1}{2}}$ to each of the points $\mathbf{x} \leftrightarrow (1, 0, \cdots, 0)$

and $\mathbf{x} \leftrightarrow (\frac{1}{2}, \frac{1}{2}, 0, \cdots, 0)$ which means that

$$\xi_2^*(\mathbf{x}) = \left(\begin{array}{ccccccccc} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} & \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \\ \vdots \\ \frac{1}{2} \end{pmatrix} & \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \\ \frac{1}{\binom{q+1}{2}} & \cdots & \frac{1}{\binom{q+1}{2}} & \frac{1}{\binom{q+1}{2}} & \cdots & \frac{1}{\binom{q+1}{2}} & \frac{1}{\binom{q+1}{2}} & \cdots & \frac{1}{\binom{q+1}{2}} \end{array} \right).$$

Then the corresponding information matrix and dispersion function are

$$M_2(\xi_2^*) = \sum_{\mathbf{x}_i \in \xi_2^*} \frac{1}{\binom{q+1}{2}} f_2(\mathbf{x}_i) f_2'(\mathbf{x}_i),$$
$$d_2(\mathbf{x}, \xi_2^*) = f'(\mathbf{x}) M_2^{-1}(\xi_2^*) f(\mathbf{x}).$$

In the following, these results will be used to find the robust D-optimal designs.

3.1 Robust D-optimal designs

In this subsection, model robust D-optimal designs for mixture experiments under criterion defined in (2.1) are discussed, where problems with uncertainties on linear and quadratic models, i.e. $\ell = 2$, will be considered. Then

$$\psi_r(\xi) = |M_1(\xi)|^{\frac{r_1}{m_1}} |M_2(\xi)|^{\frac{r_2}{m_2}}, \quad \text{where } r = r_1 = 1 - r_2. \tag{3.1}$$

Taking log on (3.1), we have

$$\Psi_r(\xi) = \log \psi_r(\xi) = \frac{r_1}{m_1} \log(|M_1(\xi)|) + \frac{r_2}{m_2} \log(|M_2(\xi)|). \tag{3.2}$$

The form is equivalent to (2.4) as provided by Dette(1990). Therefore, by Dette(1990) a design ξ_r^* is robust D-optimal for a given prior r if ξ_r^* maximizes the function $\Psi_r(\xi)$, and it can be verified through the equivalence theorem, such that for all $\mathbf{x} \in S^{q-1}$,

$$\begin{aligned} d(\mathbf{x}, \xi_r^*) &= \frac{r_1}{m_1} f_1'(\mathbf{x}) M_1^{-1}(\xi_r^*) f(\mathbf{x}) + \frac{r_2}{m_2} f_2'(\mathbf{x}) M_2^{-1}(\xi_r^*) f(\mathbf{x}) \\ &= \frac{r_1}{m_1} d_1(\mathbf{x}, \xi_r^*) + \frac{r_2}{m_2} d_2(\mathbf{x}, \xi_r^*) \le 1. \end{aligned}$$

Note that the convex complete class results obtained by Draper and Pukelsheim (1999), Draper et al. (2000) are for the Kronecker regression models. Although as the Kiefer ordering does not depend on the basis that is chosen for the regression function, we can get the same class $\mathcal{W}$ of weighted centroid designs for the Scheffé models by a linear transformation. For convenience, let K and S represent the Kronecker and Scheffé models respectively, and M_K,M_S represent the information matrices of Kronecker and Scheffé models.

Let L be the linear transformation matrix between Kronercker and Scheffé models and be defined as

$$L' = \begin{pmatrix} I_q & \frac{1}{2}V_1' & \frac{1}{2}V_1' \\ 0_{\binom{q}{2}} & \frac{1}{2}I_{\binom{q}{2}} & \frac{1}{2}I_{\binom{q}{2}} \end{pmatrix}_{\binom{q+1}{2}\times q^2} \tag{3.3}$$

where V_1 is the matrix in Lemma 2.2.1. Let $\bar{\tau}$ be an exchangeable design on S^{q-1}, we have the relationship that

$$M_S(\bar{\tau}) = L' M_K(\bar{\tau}) L. \tag{3.4}$$

The next corollary can be obtained through the equality (3.4) and nonnegative definite matrix, see Pukelsheim (1993, p.9) for the definition. A symmetric matrix A is a nonnegative definite matrix is defined through

$$A \in NND(q) \Longleftrightarrow A \in \mathrm{Sym}(q) \text{ and } x'Ax \geq 0 \text{ for all } x \in \mathbb{R}^q \ .$$

Corollary 3.1.1. *The class $\mathcal{W}$ of weighted centroid design also forms a complete class for Scheffé model.*

Proof. According to Draper and Pukelsheim (1999), Draper et al. (2000), for $\eta \in \mathcal{W}$, $\bar{\tau}$ is an exchangeable design on S^{q-1} , then we have

$$M_K(\eta) \geq M_K(\bar{\tau}).$$

Hence,

$$M_K(\eta) - M_K(\bar{\tau}) \geq 0 \quad \text{i.e. } M_K(\eta) - M_K(\bar{\tau}) \text{ is nonnegative define.}$$

Suppose y' is a nonnegative $1 \times q^2$ vector and $y' = x'L'$ where x' is also a nonnegative $1 \times \binom{q+1}{2}$ vector. Then

$$\begin{aligned} x'(M_S(\eta) - M_S(\bar{\tau}))x &= x'L'(M_K(\eta) - M_K(\bar{\tau}))Lx \\ &= y'(M_K(\eta) - M_K(\bar{\tau}))y \geq 0. \end{aligned}$$

Therefore, for all L defined in (3.3)

$$M_S(\eta) - M_S(\bar{\tau}) \geq 0 \quad \text{i.e.} \quad M_S(\eta) \geq M_S(\bar{\tau}), \tag{3.5}$$

Hence, the class $\mathcal{W}$ is also the complete class for Scheffé models under Kiefer ordering .

□

Because our theme is focus on robust D-optimal designs. Therefore, the next step is to derive the convex complete class for robust D-optimal designs.

Lemma 3.1.2. *The class $\mathcal{W}$ of weighted centroid designs forms a complete class for robust D-criterion under Kiefer ordering.*

Proof. By Corollary 3.1.1, apply (3.5) on the second-degree model, we can replace the character S into 2. Therefore, for the Scheffé's quadratic model.

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

Moreover, by the above inequality, we have

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

where z is a $\binom{q+1}{2} \times \binom{q+1}{2}$ matrix defined as $z' = \begin{pmatrix} I_q & 0_{q\times\binom{q}{2}} \end{pmatrix}_{q\times\binom{q+1}{2}}$. Taking inverse on (3.6),(3.7), then

$$M_1^{-1}(\eta) \leq M_1^{-1}(\bar{\tau}), \quad M_2^{-1}(\eta) \leq M_2^{-1}(\bar{\tau}). \tag{3.8}$$

By (3.8), we have

$$\frac{r}{q}(zM_1^{-1}(\eta)z') + \frac{1-r}{\binom{q+1}{2}}M_2^{-1}(\eta) \leq \frac{r}{q}(zM_1^{-1}(\bar{\tau})z') + \frac{1-r}{\binom{q+1}{2}}M_2^{-1}(\bar{\tau}).$$

Moreover, for $\mathbf{x} \in \mathcal{S}^{q-1}$, it can be shown that

$$\begin{aligned} d(\mathbf{x},\eta) &= f_2'(\mathbf{x})\left(\frac{r}{q}(zM_1^{-1}(\eta)z') + \frac{1-r}{\binom{q+1}{2}}M_2^{-1}(\eta)\right)f_2(\mathbf{x}) \\ &\leq f_2'(\mathbf{x})\left(\frac{r}{q}(zM_1^{-1}(\bar{\tau})z') + \frac{1-r}{\binom{q+1}{2}}M_2^{-1}(\bar{\tau})\right)f_2(\mathbf{x}) = d(\mathbf{x},\bar{\tau}). \end{aligned}$$

That is the class $\mathcal{W}$ of weighted centroid designs forms a complete class for robust D-criterion under Kiefer ordering. □

Now, let ε represent a single point design which assigns weight $p = 1$ to the point $\mathbf{x}$ i.e. $\varepsilon = \begin{pmatrix} \mathbf{x} \\ p \end{pmatrix}$. In the next lemma, a useful representation of the dispersion function at its support points are given

Lemma 3.1.3. *Let a point $\mathbf{x} \in \varepsilon$, and ξ is an exchangeable design, then we have the following results.*

$$d_1(\mathbf{x},\xi) = f_1'(\mathbf{x})M_1^{-1}(\xi)f_1(\mathbf{x}) = \mathrm{Tr}(M_1(\varepsilon)M_1^{-1}(\xi)), \tag{3.9}$$

$$d_2(\mathbf{x},\xi) = f_2'(\mathbf{x})M_2^{-1}(\xi)f_2(\mathbf{x}) = \mathrm{Tr}(M_2(\varepsilon)M_2^{-1}(\xi)). \tag{3.10}$$

Moreover,

$$d(\mathbf{x},\xi) = \frac{r}{q}\mathrm{Tr}(M_1(\varepsilon)M_1^{-1}(\xi)) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}(M_2(\varepsilon)M_2^{-1}(\xi))$$

Proof. At first, (3.9) will be proved. As ξ is an exchageable design, then

$$M_1(\xi) = RM_1(\xi)R', \qquad \forall R \in Perm\,(q)\,,$$

Therefore,

$$M_1^{-1}(\xi) = (RM_1(\xi)R')^{-1} = R'^{-1}M_1^{-1}(\xi)R^{-1} = RM_1^{-1}(\xi)R',$$

Let $\mathbf{x} = (x_1, \cdots, x_q)' \in \varepsilon$,

$$f_1(R\mathbf{x}) = R(x_1, \cdots, x_q)' = Rf_1(\mathbf{x}).$$

Furthermore,

$$\begin{aligned} M_1(\bar{\varepsilon}) &= \frac{1}{q!}\sum_{R\in Perm(q)} M_1(\varepsilon^R(\mathbf{x})) = \frac{1}{q!}\sum_{R\in Perm(q)} M_1(\varepsilon(R^{-1}\mathbf{x})) = \frac{1}{q!}\sum_{R\in Perm(q)} M_1(\varepsilon(R\mathbf{x})) \\ &= \frac{1}{q!}\sum_{R\in Perm(q)} f_1(R\mathbf{x})f_1'(R\mathbf{x}) \\ &= \frac{1}{q!}\sum_{R\in Perm(q)} Rf_1(\mathbf{x})f_1'(\mathbf{x})R'. \end{aligned}$$

Then we have

$$\begin{aligned} \mathrm{Tr}(M_1(\bar{\varepsilon})M_1^{-1}(\xi)) &= \mathrm{Tr}(\frac{1}{q!}\sum_{R\in Perm(q)} Rf_1(\mathbf{x})f_1'(\mathbf{x})R'M_1^{-1}(\xi)) \\ &= \mathrm{Tr}(\frac{1}{q!}\sum_{R\in Perm(q)} f_1(\mathbf{x})f_1'(\mathbf{x})RM_1^{-1}(\xi)R') \\ &= \mathrm{Tr}(\frac{1}{q!}\sum_{R\in Perm(q)} f_1(\mathbf{x})f_1'(\mathbf{x})M_1^{-1}(\xi)) \\ &= \mathrm{Tr}(f_1(\mathbf{x})f_1'(\mathbf{x})M_1^{-1}(\xi)) \\ &= f_1'(\mathbf{x})M_1^{-1}(\xi)f_1(\mathbf{x}) = d_1(\mathbf{x}, \xi). \end{aligned}$$

Similarly, we obtain the analogous result of (3.10) by the same steps. Moreover,

$$\begin{aligned} d(\mathbf{x},\xi) &= f_2'(\mathbf{x})\left(\frac{r}{q}(zM_1^{-1}(\xi)z') + \frac{1-r}{\binom{q+1}{2}}(\mathbf{x})M_2^{-1}(\xi)\right)f_2(\mathbf{x}) \\ &= \frac{r}{q}f_1'(\mathbf{x})z'(zM_1^{-1}(\xi)z')zf_1(\mathbf{x}) + \frac{1-r}{\binom{q+1}{2}}f_2'(\mathbf{x})M_2^{-1}(\xi)f_2(\mathbf{x}) \\ &= \frac{r}{q}f_1'(\mathbf{x})M_1^{-1}(\xi)f_1(\mathbf{x}) + \frac{1-r}{\binom{q+1}{2}}f_2'(\mathbf{x})M_2^{-1}(\xi)f_2(\mathbf{x}) \\ &= \frac{r}{q}\mathrm{Tr}(M_1(\bar{\varepsilon})M_1^{-1}(\xi)) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}(M_2(\bar{\varepsilon})M_2^{-1}(\xi)) \end{aligned}$$

This lemma is proved. □

3.2 Robust D-optimal designs for Scheffé's models

In this subsection, we will find the robust D-optimal among the class Ξ_c which is defined below. Let $\xi_1^*, \cdots, \xi_\ell^*$ be the optimal designs for the ℓ candidate models.

Definition 3.2.1. *Let the class Ξ_c be the convex combinations of $\xi_1^*, \cdots, \xi_\ell^*$.*

$$\Xi_c = \{\xi_\alpha = \alpha_1\xi_1^* + \alpha_2\xi_2^* + \cdots + \alpha_\ell\xi_\ell^*\ , \quad \alpha_i \in [0,1] \quad \textit{and} \sum_{i=1}^{\ell} \alpha_i = 1\}$$

We will first find an optimal α^* which maximizes (3.2) among Ξ_c. Later we prove the corresponding ξ_{α^*} is indeed robust D-optimal among all feasible designs. Since the design $\xi_\alpha = \alpha\xi_1^* + (1-\alpha)\xi_2^*$ for the Scheffé's linear and quadratic models also belong to W, so that ξ_α is an exchangeable design.

We will find a corresponding α_r^* such that $\xi_{\alpha_r^*}$ maximizes $\Psi_r(\xi_\alpha)$, and later prove that $\xi_{\alpha_r^*}$ is robust D-optimal with respcet to the given r.

Lemma 3.2.2. *For a given r, the optimal α_r^* can be expressed as follows*

$$\alpha_r^* = \frac{-2 - r + q\ (-1 + 2\,r) + \sqrt{-8\,r\ (-q + r) + (2 + q + r - 2\,q\,r)^2}}{2\ (q - r)}.$$

Proof. As

$$\Psi_r(\xi_\alpha) = \frac{r}{m_1}\log(|M_1(\xi_\alpha)|) + \frac{1-r}{m_2}\log(|M_2(\xi_\alpha)|).$$

In order to find the optimal α^* which minimizes $\Psi_(\xi_\alpha)$, we take the derivative of $\Psi_r(\xi_\alpha)$ with respect to α and set it equal to zero. It is known that (see Fedorov (1972, p21)) if A is a square matrix and $|A| \neq 0$, then

$$\frac{d}{dt}\ln|A| = \mathrm{Tr}A^{-1}(\frac{dA}{dt}).$$

Then we have

$$\begin{aligned} \frac{d}{d\alpha}\Psi_r(\xi_\alpha) &= \frac{r}{q}\mathrm{Tr}M_1^{-1}(\xi_\alpha)\frac{d}{d\alpha}M_1(\xi_\alpha) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}M_2^{-1}(\xi_\alpha)\frac{d}{d\alpha}M_2(\xi_\alpha) \\ &= \frac{r}{q}\mathrm{Tr}M_1^{-1}(\xi_\alpha)(M_1(\xi_1^*) - M_1(\xi_2^*)) \\ &\quad + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}M_2^{-1}(\xi_\alpha)(M_2(\xi_1^*) - M_2(\xi_2^*)). \end{aligned} \tag{3.11}$$

In order to simplify (3.11), the first and second-degree moment matrices of ξ_1^* and ξ_2^* provided by Draper and Pukelsheim (1999) and the block matrices obtained by Klein (2002) are utilized below. Note that

$$\begin{aligned} M_1(\xi_1^*) &= \frac{1}{q}I_q\ , \\ M_1(\xi_2^*) &= (A_1 I_q + B_1 U_2) = \frac{1}{\binom{q+1}{2}}\left(\frac{q+3}{4}I_q + \frac{1}{4}U_2\right)\ , \\ M_2(\xi_1^*) &= \begin{pmatrix} \frac{1}{q}I_q & 0 \\ 0 & 0 \end{pmatrix}_{\binom{q+1}{2}\times\binom{q+1}{2}}\ , \\ M_2(\xi_2^*) &= \begin{pmatrix} A_2 I_q + B_2 U_2 & C_2 V_1' + D_2 V_2' \\ C_2 V_1 + D_2 V_2 & E_2 W_1 + F_2 W_2 + G_3 W_3 \end{pmatrix} \\ &= \begin{pmatrix} M_1(\xi_2^*) & \frac{1}{8\binom{q+1}{2}}V_1' \\ \frac{1}{8\binom{q+1}{2}}V_1 & \frac{1}{16\binom{q+1}{2}}I_{\binom{q}{2}} \end{pmatrix}_{\binom{q+1}{2}\times\binom{q+1}{2}}\ , \end{aligned}$$

where

$$A_1 = \int_{S^{q-1}} x_i^2 d\xi_2^* = \frac{1}{\binom{q+1}{2}} \frac{q+3}{4}, \qquad B_1 = \int_{S^{q-1}} x_i x_j d\xi_2^* = \frac{1}{\binom{q+1}{2}} \frac{1}{4},$$

$$A_2 = A_1, \qquad B_2 = B_1,$$

$$C_2 = \int_{S^{q-1}} x_i^2 x_j d\xi_2^* = \frac{1}{8\binom{q+1}{2}}, \qquad D_2 = \int_{S^{q-1}} x_i^2 x_j^2 d\xi_2^* = 0,$$

$$E_2 = \int_{S^{q-1}} x_i x_j x_k d\xi_2^* = \frac{1}{16\binom{q+1}{2}}, \qquad F_2 = \int_{S^{q-1}} x_i^2 x_j x_k d\xi_2^* = 0,$$

$$G_2 = \int_{S^{q-1}} x_i x_j x_k x_l d\xi_2^* = 0.$$

Then we have

$$\begin{aligned} M_1(\xi_\alpha) &= \alpha M_1(\xi_1^*) + (1-\alpha) M_1(\xi_2^*) \\ &= \left(\frac{q(2q+1+\alpha)}{(q+2)+q\alpha} I_q + \frac{q(-1+\alpha)}{(q+2)+q\alpha} U_2 \right), \end{aligned}$$

and

$$\begin{aligned} M_2(\xi_\alpha) &= \alpha M_2(\xi_1^*) + (1-\alpha) M_2(\xi_2^*) \\ &= \begin{pmatrix} \frac{q\alpha-\alpha+q+3}{2q(q+1)} I_q + \frac{1-\alpha}{2q(q+1)} U_2 & \frac{1-\alpha}{4q(q+1)} V_1' \\ \frac{1-\alpha}{4q(q+1)} V_1 & \frac{1-\alpha}{8q(q+1)} W_1 \end{pmatrix}_{\binom{q+1}{2} \times \binom{q+1}{2}}. \end{aligned}$$

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, p16,17). Using the inverse formula above and Lemma 2.2.2, we obtain the following results,

$$M_1^{-1}(\xi_\alpha) = (a_1 I_q + b_1 U_2)_{q\times q} \ ,$$

$$M_2^{-1}(\xi_\alpha) = \begin{pmatrix} a_2 I_q + b_2 U_2 & c_2 V_1' + d_2 V_2' \\ c_2 V_1 + d_2 V_2 & e_2 W_1 + f_2 W_2 + g_2 W_3 \end{pmatrix}_{\binom{q+1}{2}\times\binom{q+1}{2}} \ ,$$

where

$$a_1 = \frac{q(2q+1+\alpha)}{(q+2)+q\alpha} \ , \qquad b_1 = \frac{q(-1+\alpha)}{(q+2)+q\alpha} \ ,$$

$$a_2 = \frac{q(q+1)}{2+(q-1)\alpha} \ , \qquad b_2 = 0 \ ,$$

$$c_2 = -\frac{2q(q+1)}{2+(q-1)\alpha} \ , \qquad d_2 = 0 \ ,$$

$$e_2 = \frac{8q(q+1)(3+(q-2)\alpha)}{(1-\alpha)(2+(q-1)\alpha)} \ , \qquad f_2 = \frac{4q(q+1)}{2+(q-1)\alpha} \ , \quad g_2 = 0 \ .$$

Now by Lemmas 2.2.1 and 2.2.2, it can be computed that

$$\mathrm{Tr} M_1^{-1}(\xi_\alpha) M_1(\xi_1^*) = \mathrm{Tr}(\frac{a_1}{q} I_q + \frac{b_1}{q} U_2) = a_1 \ , \tag{3.12}$$

$$\mathrm{Tr} M_1^{-1}(\xi_\alpha) M_1(\xi_2^*) = q \left(\frac{a_1}{\binom{q+1}{2}} + \frac{(a_1+b_1)(q-1)}{4\binom{q+1}{2}} \right) \ , \tag{3.13}$$

$$\mathrm{Tr} M_2^{-1}(\xi_\alpha) M_2(\xi_1^*) = a_2 \ , \tag{3.14}$$

$$\mathrm{Tr} M_2^{-1}(\xi_\alpha) M_2(\xi_2^*) = q \left(\frac{a_2(q+3)}{4\binom{q+1}{2}} + \frac{c_2(q-1)}{8\binom{q+2}{2}} \right) + \binom{q}{2} \left(\frac{c_2}{4\binom{q+1}{2}} + \frac{e_2}{16\binom{q+2}{2}} \right). \tag{3.15}$$

Now substitute these results into (3.12), (3.13), (3.14) and (3.15) into (3.11), and set it to zero. We can get the relationship between r and α_r^* as

$$r = \frac{(q+2)\alpha_r^* + q{\alpha_r^*}^2}{2+(2q-1)\alpha_r^* + {\alpha_r^*}^2} \ . \tag{3.16}$$

By solving (3.16) and find the root between 0 and 1, we have

$$\alpha_r^* = \frac{-2 - r + q\ (-1+2\,r) + \sqrt{-8\,r\ (-q+r) + (2+q+r-2\,q\,r)^2}}{2\ (q-r)}. \tag{3.17}$$

The lemma is proved. □

The next two plots is to show the relationship of r and α_r^* and their formulas are presented in (3.16), (3.17). A difficulty with the robust D-optimal design is to show that for any

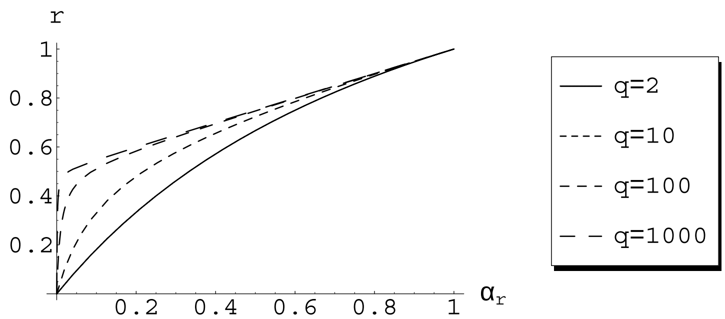

Figure 1: Plot of $r = h(\alpha_r^*)$ for $q = 2, 10, 100, 1000$.

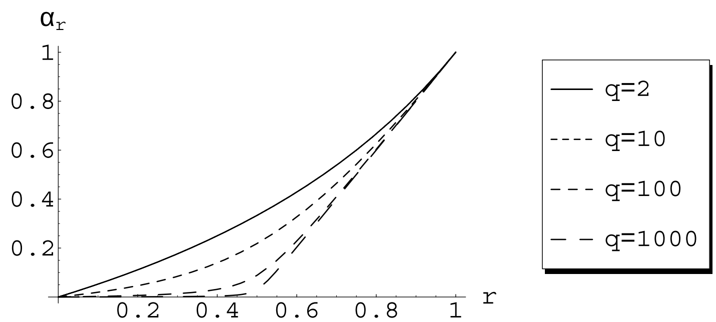

Figure 2: Plot of $\alpha_r^* = g(r)$ for $q = 2, 10, 100, 1000$.

point $\mathbf{x} \in S^{q-1}$, $d(\mathbf{x}, \xi_{\alpha_r^*})$ is less than or equal to 1 and equality holds on the support points. In the classic method by Kiefer(1951), the orthogonal polynomials is used to compute $d(\mathbf{x}, \xi)$ directly, but we will not use such an approach here. We use the approach that Klein(2002) utilizes. Now we present the method and prove that the $\xi_{\alpha_r^*} \in \Xi_c$ is indeed a robust D-optimal design in the following theorem.

Theorem 3.2.3. *The $\xi_{\alpha_r^*} \in \Xi_c$ which is convex combination of ξ_1^* and ξ_2^* by $\alpha_r^* \in [0,1]$ is the robust D-optimal design for the Scheffé's linear and quadratic models .*

Proof. Now, for an arbitrary point $\mathbf{x} \in \varepsilon$ on S^{q-1}, the equivalence theorem under robust D-optimal criterion can be verified by lemma 3.1.3 and $M(\eta) \geq M(\bar{\tau})$ where $\eta \in \mathcal{W}$, $\bar{\tau}$ is an exchangeable design. Then we have

$$
\begin{aligned}
d(\mathbf{x}, \xi_{\alpha_r^*}) &= \frac{r}{q}\mathrm{Tr}(M_1(\bar{\varepsilon})M_1^{-1}(\xi_{\alpha_r^*})) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}(M_2(\bar{\varepsilon})M_2^{-1}(\xi_{\alpha_r^*})) \\
&\leq \frac{r}{q}\mathrm{Tr}(M_1(\eta)M_1^{-1}(\xi_{\alpha_r^*})) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}(M_2(\eta)M_2^{-1}(\xi_{\alpha_r^*})) \\
&= \frac{r}{q}\mathrm{Tr}(M_1(\sum_{j=1}^{q}\lambda_j\eta_j)M_1^{-1}(\xi_{\alpha_r^*})) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}(M_2(\sum_{j=1}^{q}\lambda_j\eta_j)M_2^{-1}(\xi_{\alpha_r^*})) \\
&= \sum_{j=1}^{q}\lambda_j\left(\frac{r}{q}\mathrm{Tr}(M_1(\eta_j)M_1^{-1}(\xi_{\alpha_r^*})) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}(M_2(\eta_j)M_2^{-1}(\xi_{\alpha_r^*}))\right)
\end{aligned}
$$

Then, let

$$
N_j = \frac{r}{q}\mathrm{Tr}(M_1(\eta_j)M_1^{-1}(\xi_{\alpha_r^*})) + \frac{1-r}{\binom{q+1}{2}}\mathrm{Tr}(M_2(\eta_j)M_2^{-1}(\xi_{\alpha_r^*})).
$$

where $M_\ell(\eta_j), \ell = 1, 2$ represent the information matrix of j-th elementary centroid design for $j = 1, \cdots, q$, then we have

$$
M_1(\eta_j) = \left(\ \mu_{2,j}I_q + \mu_{11,j}U_2\ \right),
$$

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

and U_2, V_1, V_2, W_1, W_2, W_3 is the form by Lemma 2.2.1. For detail

$$\mu_{2,j} = \int_{S^{q-1}} x_i^2 d\eta_j = \frac{1}{jq}, \quad \mu_{11,j} = \int_{S^{q-1}} x_i x_j d\eta_j = \frac{j-1}{jq(q-1)},$$

$$\mu_{21,j} = \int_{S^{q-1}} x_i^2 x_j d\eta_j = \frac{j-1}{j^2 q(q-1)},$$

$$\mu_{111,j} = \int_{S^{q-1}} x_i x_j x_k d\eta_j = \frac{(j-1)(j-2)}{j^2 q(q-1)(q-2)},$$

$$\mu_{22,j} = \int_{S^{q-1}} x_i^2 x_j^2 d\eta_j = \frac{j-1}{j^3 q(q-1)},$$

$$\mu_{211,j} = \int_{S^{q-1}} x_i^2 x_j x_k d\eta_j = \frac{(j-1)(j-2)}{j^3 q(q-1)(q-2)},$$

$$\mu_{1111,j} = \int_{S^{q-1}} x_i x_j x_k x_l d\eta_j = \frac{(j-1)(j-2)(j-3)}{j^3 q(q-1)(q-2)(q-3)}.$$

Therefore, we obtain that

$$N_j = \frac{(-1+\alpha_r^*)\,\alpha_r^* j^3 - 8\,(1+\alpha_r^*\,q) + 8j\,(1+\alpha_r^* q) + 2j^2\,(1+\alpha_r^*\,q)}{j^3\,(2+\alpha_r^{*^2} + \alpha_r^*\,(-1+2\,q))}.$$

However, for $j, q \geq 2$, $\alpha_r^* \in [0,1]$,

$$N_j - N_{j+1} = \frac{2\,(-4-8j+8j^3+j^2(1+j)^2)\,(1+\alpha_r^* q)}{j^3(1+j)^3\,(2+\alpha_r^{*^2}+\alpha_r^*\,(-1+2q))} \geq 0,$$

and equality holds if and only if $j = 1$, i.e. $N_1 = N_2$.

Therefore,

$$N_1 = N_2 > N_3 > \cdots > N_q. \tag{3.18}$$

Hence, by the above inequality

$$d(\mathbf{x}, \xi_{\alpha_r^*}) = \begin{cases} 1 & \text{when } j = 1, 2 \\ < 1 & \text{when } j \geq 3, \end{cases}$$

Therefore, by the equivalence theorem, the design $\xi_{\alpha_r^*}$ is robust D-optimal with uncertainties on Scheffé's linear and quadratic models. □

3.3 D_r-efficiency of robust D-optimal design

In the previous subsection, we find the robust D-optimal designs by given a fixed $r \in [0, 1]$, but the choice of r is also a problem. In Zen and Tsai (2003), following a robust D-optimal criterion discussions in Pukelsheim and Rosenberger (1993), a robust D-optimal designs criterion has been proposed there which actually can be reduced to be a special case in the robust D-optimal design criterion as defined in Dette (1990). Although in Zen and Tsai (2003), the problem of choosing a suitable r has also been discussed, where a maximin criterion for choosing r is proposed. In this section, we will adopt a similar maxmin criterion for the robust D-optimal design problems in mixture experiments. Now we introduce the efficiencies of robust D-optimal designs $\xi_{\alpha_{r'}^*}, 0 \leq r' \leq 1$, under robust criterion with weighting r' to see whether those robust D-optimal design $\xi_{\alpha_r^*}$ is acceptable under weighting r. To see that, first note in Section 2.2, information matrices for a mixture experiments can be decomposed into blocks as (2.3). Moreover, in order to compute the efficiencies of interest, we need know the value of the determinant for information matrices. Therefore, the next formula will be used for the computation, i.e.

$$C = \begin{vmatrix} C_{11} & C_{21}' \\ C_{21} & C_{22} \end{vmatrix} = |C_{11}| \; |C_{22} - C_{21}C_{11}^{-1}C_{21}'| = |C_{11} - C_{21}'C_{22}^{-1}C_{21}| \; |C_{22}|,$$

see Fedorov (1972, p16). Hence, we can simplify $\Psi_r(\xi_\alpha)$ as follows.

$$\begin{aligned}\Psi_r(\xi_\alpha) &= |M_1(\xi_\alpha)|^{\frac{r}{m_1}}|M_2(\xi_\alpha)|^{\frac{1-r}{m_2}} \\ &= \frac{2^{\frac{(1-q)(q\,(3-2r)+r)}{q(1+q)}}(1+q)^{\frac{r}{q}}\left((1-\alpha)^{\frac{-1+q}{2}}(2-(1-q)\,\alpha)\right)^{\frac{2(1-r)}{1+q}}(2+q+q\alpha)^{\frac{(-1+q)r}{q}}}{q+q^2},\end{aligned} \tag{3.19}$$

where r is obtained through (3.16). We consider the robust D-optimal criterion (2.1) for any fixed r' under criterion with weighting r. We are interested in their performance of those robust D-optimal designs through the relative efficiency and to see if those designs are acceptable. That is, we will focus on the behaviour of the robust D-optimal design $\xi_{\alpha^*_{r'}}$ under different Ψ_r criteria. The relative efficiency of a robust D-optimal design $\xi_{\alpha^*_{r'}}$ under Ψ_r-robust D-optimal criterion is defined as follows

$$D_r\text{-eff}(\xi_{\alpha^*_{r'}}) = \frac{\Psi_r(\xi_{\alpha^*_{r'}})}{\Psi_r(\xi_{\alpha^*_r})}, \quad r, r' \in [0,1]. \tag{3.20}$$

Substituting (3.19) into (3.20), we obtain the form of $D_r\text{-eff}(\xi_{\alpha^*_{r'}})$ with respect to r and r' in the next lemma. Let

$$g(r,r') = (1-\alpha^*_{r'})^{\frac{-1+q}{2}}\left(2+(-1+q)\,\alpha^*_{r'}\right)^{\frac{2-2r}{1+q}}\left(2+q+q\alpha^*_{r'}\right)^{\frac{(-1+q)r}{q}}.$$

Lemma 3.3.1. *For any fixed $r' \in [0,1]$ and $q \geq 2$, let $\xi_{\alpha^*_{r'}}$ be the $\Psi_{r'}$-robust D-optimal design. Then the D_r-efficiency of $\xi_{\alpha^*_{r'}}$ in (3.20) can be expressed as*

$$\begin{aligned}D_r\text{-eff}(\xi_{\alpha^*_{r'}}) &= \frac{g(r,r')}{g(r,r)} \\ &= \left(\frac{1-\alpha^*_{r'}}{1-\alpha^*_r}\right)^{\frac{(-1+q)(1-r)}{1+q}}\left(\frac{2-(1-q)\,\alpha^*_{r'}}{2-(1-q)\,\alpha^*_r}\right)^{\frac{2-2r}{1+q}}\left(\frac{2+q+q\alpha^*_{r'}}{2+q+q\alpha^*_r}\right)^{\frac{(-1+q)r}{q}}\end{aligned} \tag{3.21}$$

where α^*_r is a function of r as in (3.16).

In order to find the performance of $D_r\text{-eff}(\xi_{\alpha^*_{r'}})$, we first to see the behavior of $g(r,r')$ in the following lemma.

Lemma 3.3.2. *For any fixed $r \in [0,1]$ and $q \geq 2$,*

$g(r,r')$ is strictly increasing on $[0,r)$ and strictly decreasing on $(r,1]$. Moreover, the maximum value of $g(r,r')$ is attained at $r' = r$.

Proof. If we given r' that also means given $\alpha^*_{r'}$ and in order to simplification of the computation, we utilize $\alpha^*_{r'}$ for computation. Therefore, we take log on $g(r,r')$, then take derivative of $\log g(r,r')$ and set it equal to zero, i.e.

$$\frac{d}{d\alpha^*_{r'}} \log g(r,r') = 0 \tag{3.22}$$

Then we have

$$\begin{aligned}\frac{d}{d\alpha^*_{r'}} \log g(r,r') &= \frac{d}{d\alpha^*_{r'}} \log \left((1-\alpha^*_{r'})^{\frac{-1+q}{2}} \left(2 + (-1+q)\,\alpha^*_{r'}\right)^{\frac{2-2r}{1+q}} \left(2+q+q\alpha^*_{r'}\right)^{\frac{(-1+q)r}{q}} \right) \\ &= -\frac{(-1+q)(1-r)}{(1+q)(1-\alpha^*_{r'})} + \frac{(-1+q)(2-2r)}{(1+q)(2+(-1+q)\,\alpha^*_{r'})} + \frac{(-1+q)\,r}{2+q+q\alpha^*_{r'}}.\end{aligned} \tag{3.23}$$

Therefore, (3.22) is simplified as

$$\frac{(-1+q)\left(\alpha^*_{r'}\left(2+q+q\alpha^*_{r'}\right) - r\left(2+(-1+2\,q)\,\alpha^*_{r'} + {\alpha^*_{r'}}^2\right)\right)}{(-1+\alpha^*_{r'})\left(2+(-1+q)\,\alpha^*_{r'}\right)\left(2+q+q\alpha^*_{r'}\right)} = 0,$$

solve the above equation with the (3.16) and find the root between 0 and 1, we can obtain that $\alpha^*_{r'} = \alpha^*_r$ i.e. $r = r'$. Next, we take derivative of (3.23) in order to observe that the extreme value is maximal or minimal. If the value is less than zero, we can say that $g(r,r')$ is strictly increasing on $[0,r')$ and strictly decreasing on $(r',1]$.

$$\frac{d^{\,2}}{d^{\,2}\alpha^*_{r'}} \log g(r,r') = -\left(\frac{(-1+q)(1-r)}{(1+q)\left(1-\alpha^*_{r'}\right)^2} + \frac{(-1+q)(2-2r)}{(1+q)\left(2+(-1+q)^2\,\alpha^*_{r'}\right)^2} + \frac{(-1+q)\,qr}{(2+q+q\alpha^*_{r'})^2} \right),$$

where $q \geq 2$ and $r, \alpha^*_r \in [0,1]$. Therefore,

$$\frac{d^{\,2}}{d^{\,2}\alpha^*_{r'}} \log g(r,r') < 0.$$

This lemma is proved. □

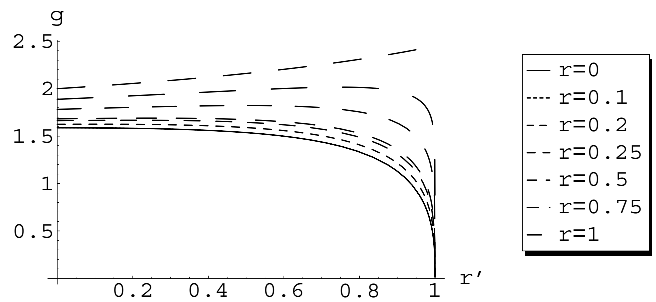

Figure 3: Plot of $g(r, r')$ for given r at $q = 2$.

Now we want to find the minimum value of D_r-eff$(\xi_{\alpha^*_{r'}})$ in the following lemma.

Lemma 3.3.3. *For given $r' \in [0, 1]$, the minimum value of D_r-eff$(\xi_{\alpha^*_{r'}})$ in [0,1] is attained at the two end points, i.e. $r = 0$ or $r = 1$.*

Proof. If we given r' that also means given $\alpha^*_{r'}$ as (3.17) and in order to simplification of the computation, we utilize α^*_r for computation. Hence, we take log on $g(r, r')$, then take derivative of $\log g(r, r')$ and set it equal to zero, i.e.

$$\frac{d}{d\alpha^*_r} \log D_r\text{-eff}(\xi_{\alpha^*_{r'}}) = 0,$$

Hence, we have the equality after simplification.

$$\frac{-2\left((q^2-q-1){\alpha^*_r}^2+2q\alpha^*_r+(2+q)\right)\left((-1+q)q\log(\frac{-1+\alpha^*_{r'}}{-1+\alpha^*_r})+2\,q\,\log(\frac{2+(-1+q)\alpha^*_{r'}}{2+(-1+q)\alpha^*_r})-\left(-1+q^2\right)\log(\frac{2+q+q\alpha^*_{r'}}{2+q+q\alpha^*_r})\right)}{q\,(1+q)\left(2+(-1+2q)\alpha^*_r+{\alpha^*_r}^2\right)^2} = 0.$$

The first expression in the fraction of the numerator is a quadratic function in α^*_r and does not have any root in [0,1] for $q \geq 2$, and the second fraction of the numerator has only root $\alpha_r^* = \alpha_{r'}^*$ which attains the maximal. Therefore, the minimum value is attained at the two end points $\alpha_r^* = 0$ or $\alpha_r^* = 1$, i.e. $r = 0$ or $r = 1$. $\square$

For clarity we give two plots, Figure 4 is represented D_r-eff$(\xi_{\alpha_{r'}^*})$ for a given $\alpha_{r'}^* \in [0, 1]$, and Figure 5 is represented D_r-eff$(\xi_{\alpha_{r'}^*})$ for a given $r' \in [0, 1]$.

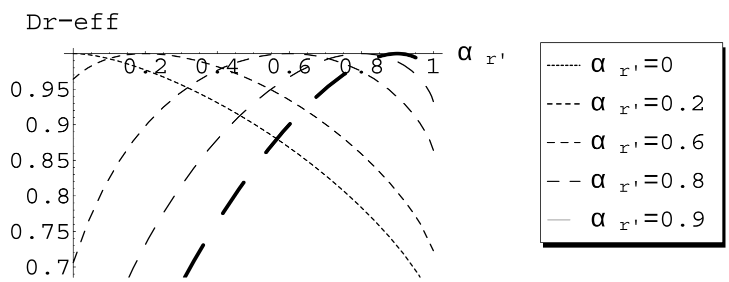

Figure 4: Plot of D_r-eff$(\xi_{\alpha_{r'}^*})$ for given $\alpha_{r'}^* = 0, 0.25, 0.75, 0.8, 0.9$ at $q = 5$.

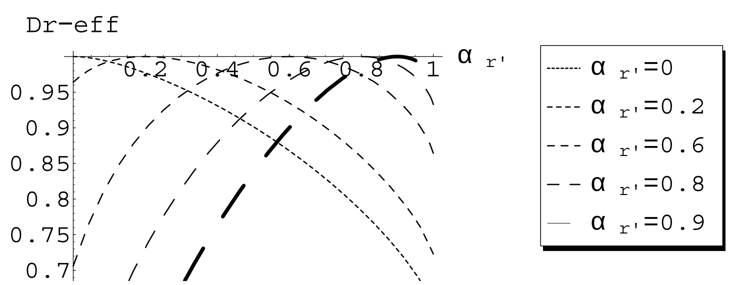

Figure 5: Plot of D_r-eff$(\xi_{\alpha_{r'}^*})$ for given $r' = 0, 0.25, 0.75, 0.8, 0.9$ at $q = 5$.

On the other hand , we can find the similar behavior of D_r-eff$(\xi_{\alpha_{r'}^*})$ in [0,1] for a given r by Figure 6.

Through Figure 5, we can observe that for a given r', the minimal of D_r-eff$(\xi_{\alpha_{r'}^*})$ will

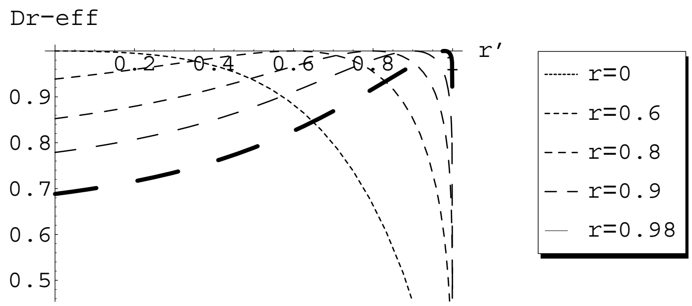

Figure 6: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ for given $r = 0, 0.6, 0.8, 0.9, 0.98$ at $q = 5$.

be obtained at either $r = 0$ or 1. Furthermore, when r' increases from 0 to 1, we can find that the minimum value changes from $r = 1$ to $r = 0$.

Let $p(r') = \frac{g(1,r')}{g(0,r')}$ which is the ratio of D_0-eff$(\xi_{\alpha^*_{r'}})$ and D_1-eff$(\xi_{\alpha^*_{r'}})$. Therefore, $p(r')$ can be simplified as

$$p(r') = \frac{D_1\text{-eff}(\xi_{\alpha^*_{r'}})}{D_0\text{-eff}(\xi_{\alpha^*_{r'}})} = \frac{g(1,r')}{g(0,r')} = \frac{(2+2q)^{\frac{-1+q}{q}} \left((1-\alpha^*_{r'})^{\frac{-1+q}{2}} \left(2 + (-1+q)\,\alpha^*_{r'}\right) \right)^{\frac{2}{1+q}}}{2^{\frac{2}{1+q}} \left(2 + q + q\alpha^*_{r'}\right)^{\frac{-1+q}{q}}},$$

and we will solve for $p(r') = 1$ to obtain the optimal r'. Furthermore, in Figure 7, it is to show that the maximum value is obtained at $p(r') = 1$ i.e. D_0-eff$(\xi_{\alpha^*_{r'}}) = D_1$-eff$(\xi_{\alpha^*_{r'}})$.

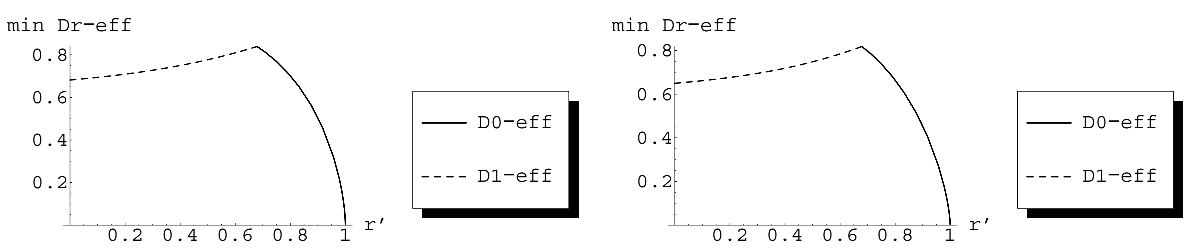

Figure 7: Plot of $\min_{0 \le r \le 1} D_r$-eff$(\xi_{\alpha^*_{r'}})$ for $q = 4, 5$.

Theorem 3.3.4. *For any fixed $r' \in [0,1]$ and $q \geq 2$, we have*

$$\min_{0\leq r\leq 1}\{D_r\text{-}eff(\xi_{\alpha^*_{r'}})\} = \begin{cases} D_0\text{-}eff(\xi_{\alpha^*_{r'}}) & , \text{ if } \quad r' \geq r^* \\ D_1\text{-}eff(\xi_{\alpha^*_{r'}}) & , \text{ if } \quad r' < r^* \end{cases},$$

where D_0-eff$(\xi_{\alpha^*_{r'}})$ and D_1-eff$(\xi_{\alpha^*_{r'}})$ are as in (3.20) with $r = 0$ and $r = 1$, respectively, and r^* is the root of $p(r') = 1$.

Theorem 3.3.5. *For any $q \geq 2$, $\min_{0\leq r\leq 1}\{D_r\text{-}eff(\xi_{\alpha^*_{r'}})\}$ is increasing first, then decreasing in r' and the maximum value of $\min_{0\leq r\leq 1}\{D_r\text{-}eff(\xi_{\alpha^*_{r'}})\}$ is attained at $r' = r^*$, i.e.*

$$r^* = arg\{\max_{0\leq r'\leq 1}\min_{0\leq r\leq 1} D_r\text{-}eff(\xi_{\alpha^*_{r'}})\},$$

where r^* is the root of $p(r') = 1$.

Next, we give the behavior of D_r-eff$(\xi_{\alpha^*_{r'}})$ for given different r' at $q = 5$

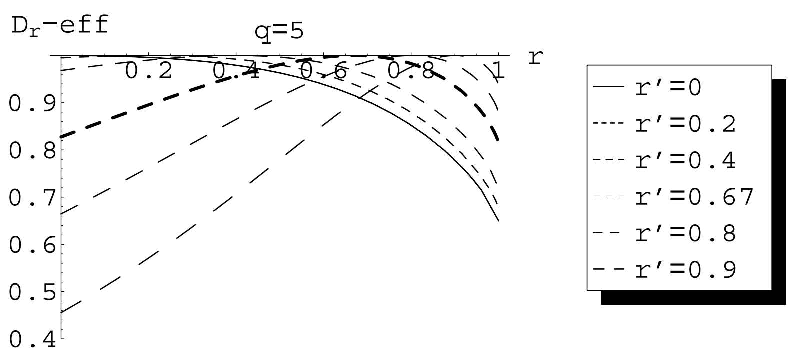

Figure 8: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ for given $r' = 0, 0.2, 0.4, 0.67, 0.8, 0.9$ at $q = 5$.

In Figure 8, the thick line indicates that at $q = 5$, $\xi_{\alpha^*_{0.67}}$ does achieve the maxmin criterion as discussed in Theorem 3.3.5. Furthermore, in Appendix C it gives some plots of D_r-eff$(\xi_{\alpha^*_{r'}})$ for $r' = 0.67$ at different q. Moreover, Table 1 gives some numerical results of r^* and the corresponding efficiencies of $\xi_{\alpha^*_{r*}}, \xi_{\alpha^*_{0.6}}, \xi_{\alpha^*_{0.67}}, \xi_{\alpha^*_{0.7}}$ and the special case of D_0-eff$(\xi_{\alpha^*_{0.67}})$ which is the efficiency of $\xi_{\alpha^*_{0.67}}$ under quadratic model.

Table 1: Table of $\min_{0\le r\le 1} D_r\text{-eff}(\xi_{\alpha^*_{r'}}) = \min_{0\le r\le 1} \frac{g(r,r')}{g(r,r)}$ for different r'

q	r^*	$\min_{0\le r\le 1} \frac{g(r,r^*)}{g(r,r)}$	$\min_{0\le r\le 1} \frac{g(r,0.6)}{g(r,r)}$	$\min_{0\le r\le 1} \frac{g(r,0.67)}{g(r,r)}$	$\min_{0\le r\le 1} \frac{g(r,0.7)}{g(r,r)}$	$\min_{0\le r\le 1} \frac{g(0,0.67)}{g(0,0)}$
2	0.679472	0.915523	0.899735	0.91357	0.905934	0.919615
3	0.679609	0.869229	0.844833	0.866132	0.854466	0.875693
4	0.679667	0.839402	0.80937	0.835551	0.821244	0.847453
5	0.679662	0.818324	0.784219	0.813938	0.797666	0.827503
6	0.679612	0.802506	0.765272	0.797728	0.779871	0.812514
7	0.679531	0.790125	0.750385	0.785055	0.765846	0.800752
10	0.679188	0.764876	0.71982	0.759294	0.736833	0.77658
100	0.672929	0.685299	0.620804	0.682612	0.6334049	0.690824

From Table 1, we can see that the values of r^* is approximating 0.67 as q becomes large and the value of $\min_{0\le r\le 1} D_r\text{-eff}(\xi_{\alpha^*_{r'}})$ is approximately 0.68. It is of interest to know the asymptotic value of $\min_{0\le r\le 1} D_r\text{-eff}(\xi_{\alpha^*_{r'}})$ when q goes to infinity. This is examined by fixing $r' = 0.67$ to compare the behavior of $D_r\text{-eff}(\xi_{\alpha^*_{r'}})$ under $r = 0$ and $r = 1$.

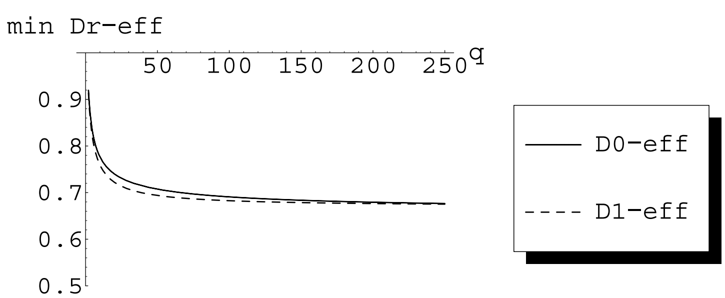

Figure 9: Plot of $D_0\text{-eff}(\xi_{\alpha^*_{r'}})$ and $D_1\text{-eff}(\xi_{\alpha^*_{r'}})$ for given $r' = 0.67$ at $q = 2, \cdots, 250$.

From Figure 9, we find that the values of $D_0\text{-eff}(\xi_{\alpha^*_{r'}})$ and $D_1\text{-eff}(\xi_{\alpha^*_{r'}})$ are stable around 0.68 as q gets large. Plots of $D_r\text{-eff}(\xi_{\alpha^*_{r'}})$ under different r for $q = 2\cdots, 250$ are presented in Appendix D and it also shows that $D_r\text{-eff}(\xi_{\alpha^*_{0.67}})$ under different r is stable and is approximately 0.68 when q becomes large. In Appendix C it is shown that when we have many ingredients i.e. q becomes large, the efficiency of D_r-eff$(\xi_{\alpha^*_{0.67}})$ is decreasing to be approximately 0.68 but when the quadratic model is more likely such as $0 \leq r \leq \frac{1}{2}$, we observe that

$$D_r\text{-eff}(\xi_{\alpha^*_{0.67}}) < D_r\text{-eff}(\xi_{\alpha^*_{r'}}) \approx 1 \qquad \text{where } 0 \leq r, r' \leq \tfrac{1}{2},$$

i.e. D_r-eff$(\xi_{\alpha^*_{r'}})$, is more efficient than D_r-eff$(\xi_{\alpha^*_{0.67}}) \approx 0.68$ when $0 \leq r, r' \leq \frac{1}{2}$.

4 Some other results and discussion

In the previous section, we have concentrated on the Scheffé's linear and quadratic models, but for mixture experiments there still are many other possible models. Therefore, the same procedures are used to find the robust D-optimal designs on the Scheffé's linear and cubic models without 3-way effect.

Firstly, we find that if ξ_α is the linear combination of the D-optimals for Scheffé's linear and cubic models without 3-way effect, then there may also be a convex combination of the individual D-optimal designs to be the robust D-optimal design for the two models. In the following, we will discuss robust D-optimal designs for the Scheffé's linear and cubic models without 3-way effect. Note that the corresponding regression function for cubic model without 3-way effect is

$$E_3(y(\mathbf{x})) = \boldsymbol{\theta}_3' f_3(\mathbf{x}) = \sum_{1\le i\le q} \theta_i x_i + \sum_{1\le i<j\le q} \theta_{ij} x_i x_j + \sum_{1\le i<j\le q} \gamma_{ij} x_i x_j (x_i - x_j),$$

where

$$f_3(\mathbf{x}) = (x_1, \cdots, x_q, x_1x_2, \cdots, x_{q-1}x_q, x_1x_2(x_1-x_2), \cdots, x_{q-1}x_q(x_{q-1}-x_q))', 0 \le x_i \le 1,$$

$$\boldsymbol{\theta}_3 = (\theta_1, \cdots, \theta_q, \theta_{12}, \cdots, \theta_{q-1q}, \gamma_{12}, \cdots, \gamma_{q-1q})'.$$

and the D-optimal design ξ_3^* assigns a weight $\frac{1}{q^2}$ to each of the $\binom{q}{1}$ points $\mathbf{x} \leftrightarrow (1, 0, \cdots, 0)$ and each of the $2\binom{q}{2}$ points $\mathbf{x} \leftrightarrow (\frac{1-\frac{1}{\sqrt{5}}}{2}, \frac{1+\frac{1}{\sqrt{5}}}{2}, 0, \cdots, 0)$ which means that

$$\xi_3^*(\mathbf{x}) = \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} & \begin{pmatrix} \frac{1-\frac{1}{\sqrt{5}}}{2} \\ \frac{1+\frac{1}{\sqrt{5}}}{2} \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots \;\; \cdots & \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \frac{1+\frac{1}{\sqrt{5}}}{2} \\ \frac{1-\frac{1}{\sqrt{5}}}{2} \end{pmatrix} \\ \frac{1}{q^2} & \cdots & \frac{1}{q^2} & \frac{1}{q^2} & \cdots \;\; \cdots & \frac{1}{q^2} \end{pmatrix}.$$

Then the corresponding information matrix and dispersion function are

$$M_3(\xi_3^*) = \sum_{\mathbf{x}_i \in \xi_3^*} \frac{1}{q^2} f_3(\mathbf{x}_i) f_3'(\mathbf{x}_i),$$

$$d_3(\mathbf{x}, \xi_3^*) = f'(\mathbf{x}) M_3^{-1}(\xi_3^*) f(\mathbf{x}).$$

Next we will use results of ξ_1^* and ξ_3^* to find the robust D-optimal designs. In the class of convex combination with $\xi_\alpha = \alpha\xi_1^* + (1-\alpha)\xi_3^*, 0 \le \alpha \le 1$, we conjecture the relationship between r and α_r^* as

$$r = \frac{q(3\alpha_r^* + 2\alpha_r^{*2})}{2 + (5q-4)\alpha_r^* + 2\alpha_r^{*2}}, \tag{4.1}$$

and corresponding plot is in Figure 9,

Then by solving Equation (4.1) and find the root between 0 and 1, we obtain

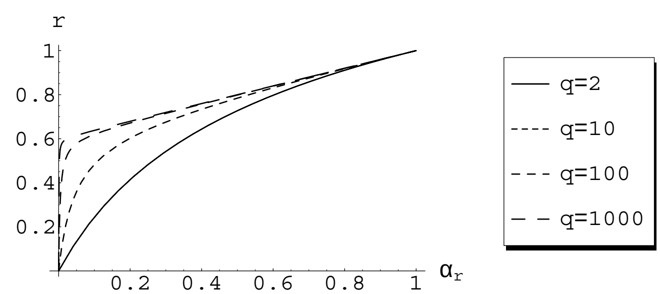

Figure 10: Plot of the relationship of r and α_r^* as (4.1) for $q = 2, 10, 100, 1000$.

$$\alpha_r^* = \frac{-4r + q\,(-3+5r) + \sqrt{q^2(3-5r)^2 - 40\,(-1+r)\,qr}}{4\,(q-r)}. \tag{4.2}$$

The next plot presents the behavior of r and α_r^* under different q.

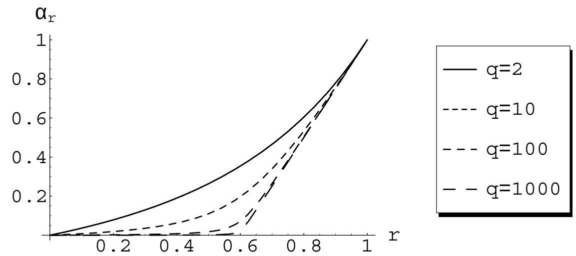

Figure 11: Plot of the relationship of α_r^* and r as (4.2) for $q = 2, 10, 100, 1000$.

Moreover, using "Mathematica",we find that $\xi_{\alpha_r^*}$ does satisfy the equivalence theorem by Dette(1990) for $q = 2, 3, 4, 5$ at the selected points tested.

Secondly, if the robust D-optimal considered by Scheffé's linear model, quadratic model and cubic model without 3-way effect for given $r, k \in [0, 1]$, $\xi_{\alpha_{r,k}^*}$ may also be the robust D-optimal design for the three models. Again, we just use "Mathematica" to see whether design obtained satisfies the equivalence theorem by Dette(1990) for $q = 2, 3, 4$ at the selected points tested.

Taking $q = 2$ for instance, we have

$$r = \frac{2\left(-27+324\,\alpha_{r,k}{}^3+18\,\beta_{r,k}+5\,\beta_{r,k}{}^2+4\,\beta_{r,k}{}^3+9\,\alpha_{r,k}{}^2\left(65+28\,\beta_{r,k}\right)+\alpha_{r,k}\left(243+240\,\beta_{r,k}+57\,\beta_{r,k}{}^2\right)\right)}{207+324\,\alpha_{r,k}{}^3+240\beta_{r,k}+4\beta_{r,k}{}^2+4\beta_{r,k}{}^3+9\,\alpha_{r,k}{}^2\left(101+28\,\beta_{r,k}\right)+3\alpha_{r,k}\left(270+161\beta_{r,k}+19\beta_{r,k}{}^2\right)},$$

$$k = \frac{81-324\,\alpha_{r,k}{}^3+324\,\beta_{r,k}+99\,\beta_{r,k}{}^2-4\,\beta_{r,k}{}^3-9\,\alpha_{r,k}{}^2\left(9+28\,\beta_{r,k}\right)+\alpha_{r,k}\left(324+243\,\beta_{r,k}-57\,\beta_{r,k}{}^2\right)}{207+324\,\alpha_{r,k}{}^3+240\,\beta_{r,k}+49\,\beta_{r,k}{}^2+4\,\beta_{r,k}{}^3+9\,\alpha_{r,k}{}^2\left(101+28\,\beta_{r,k}\right)+3\,\alpha_{r,k}\left(270+161\,\beta_{r,k}+19\,\beta_{r,k}{}^2\right)}.$$

It is much more complicated than the previous case with only linear and quadratic models. So there are still many to be investigated.

In the previous context, we have tried to find through the class of the convex combination of the individual D-optimal designs for the candidate models considered. But there is still a situation that we have not discussed about,i.e. uncertaintes between the quadratic and cubic models without 3-way effect. For this case of quadratic and cubic models without 3-way effect, we are unable to find design $\xi_\alpha = \alpha\xi_2^* + (1-\alpha)\xi_3^* \in \Xi_c$ to satisfy the equivalence theorem at this moment. Therefore, the next effort will be trying to change the weights on the support points for cubic models without 3-way effect such that the dispersion function would equal to 1 and then check whether the obtained design, denoted as $\xi_{\hat{\alpha}_r}$, would satisfy the equivalence theorem. More precisely we find that for $q=2$, $\xi_{\hat{\alpha}_r}$ is the form

$$\begin{aligned}
\xi_{\hat{\alpha}} &= \alpha \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} & \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \\ \frac{1}{\binom{q+1}{2}} & \cdots & \frac{1}{\binom{q+1}{2}} & \frac{1}{\binom{q+1}{2}} & \cdots & \frac{1}{\binom{q+1}{2}} \end{pmatrix} \\
&\quad +(1-\alpha) \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} & \begin{pmatrix} \frac{1-\frac{1}{\sqrt{5}}}{2} \\ \frac{1+\frac{1}{\sqrt{5}}}{2} \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots \quad \cdots & \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \frac{1+\frac{1}{\sqrt{5}}}{2} \\ \frac{1-\frac{1}{\sqrt{5}}}{2} \end{pmatrix} \\ w_1 & \cdots & w_1 & w_2 & \cdots \quad \cdots & w_2 \end{pmatrix},
\end{aligned}$$

where

$$qw_1 + q(q-1)w_2 = 1,$$

and $(\hat{\alpha}_r, \hat{w}_{r,2})$ is a solution for equation

$$r = \frac{h_1(\alpha, w_2)}{h_2(\alpha, w_2)},$$

where

$$
\begin{aligned}
h_1(\alpha, w_2) \;=\; & -594\alpha - 54\; - 594\alpha - 54 - 594 - 594\alpha - 54\alpha^2 + 2520\alpha^3 - 1372\alpha^4 \\
& -1755w_2 + 1071\alpha w_2 + 24591\alpha^2 w_2 - 42135\alpha^3 w_2 + 18228\alpha^4 w_2 - 1512w_2^2 \\
& +78552\alpha w_2^2 - 243288\alpha^2 w_2^2 + 256968\alpha^3 w_2^2 - 90720\alpha^4 w_2^2 + 79488w_2^3 \\
& -438912\alpha w_2^3 + 839808\alpha^2 w_2^3 - 680832\alpha^3 w_2^3 + 200448\alpha^4 w_2^3 - 165888\, w_2^4 \\
& +663552\alpha w_2^4 - 995328\alpha^2 w_2^4 + 663552\alpha^3 w_2^4 - 165888\alpha^4 w_2^4.
\end{aligned}
$$

$$
\begin{aligned}
h_2(\alpha, w_2) \;=\; & -198\alpha + 1006\alpha^2 - 308\alpha^3 - 567w_2 + 6423\alpha w_2 - 8865\alpha^2 w_2 \\
& +3009\alpha^3 w_2 + 8568\, w_2^2 - 26856\alpha w_2^2 + 28008\alpha^2 w_2^2 - 9720\alpha^3 w_2^2 \\
& -10368w_2^3 + 31104\alpha w_2^3 - 31104\alpha^2 w_2^3 + 10368\alpha^3 w_2^3.
\end{aligned}
$$

Next, we list some results of (α_r, w_1, w_2) for $q = 2$ in the following table.

Table 2: The corresponding values of α,w_1 and w_2 for ξ_α under different r

r	α	w_1	w_2
0.379955	0	0.227391	0.272609
0.574861	0.25	0.228865	0.271135
0.739855	0.50	0.229980	0.270020
0.880065	0.75	0.230851	0.269149

Note that in the above table, it may happen that even if $r \neq 0$, we may end up with the optimal design for cubic model without 3-way effect only. This will be investigated in the future work.

References

[1] Atkinson, A.C., Cox, D.R. (1974). Planning experiments for discriminating between models (with discussion). *Journal of the Royal Statistical Society, Series B, Methodological*, 36, 321-348.

[2] Box, G.E.P., Draper, N.R. (1959). A basis for the selection of a response surface design. *Journal of the American Statistical Association*, 54, 622-654.

[3] Chan, L.Y. (2000). Optimal designs for experiments with mixtures: a surbvey. *Communications in statistics-theory and methods*, 29(9 &10), 2281-2312.

[4] Cornell, J.A., (1990). Experiments with mixtures. Designs, Models and Analysis of mixture data. 2nd ed. Wiley, New York.

[5] 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.

[6] Dette, H. (1991). A note on robust designs for polynomial regression. *Journal of Statistical Planning and Inference*, 28, 223-232.

[7] Dette, H. (1993). On a mixture of the D- and D_1-optimality criterion in polynomial regression. *Journal of Statistical Planning and Inference*, 35, 233-249.

[8] Dette, H. (1994). Robust designs for multivariate polynomial regression on the d-cube. *Journal of Statistical Planning and Inference*, 38, 105-124.

[9] Dette, H. (1995). Optimal designs in nonlinear regression models (STMA V38 4621). *Allgemeines Statistisches Archiv*, 29, 33-55.

[10] Draper, N.R., Pukelsheim,F. (1999). Kiefer ordering of simplex designs for first-And second-degree mixture models. *Journal of statistical planning and inference* 79, 325-348.

[11] Draper, N.R., Heiligers, B.,Pukelsheim, F. (2000). Kiefer ordering of simplex designs for second-degree mixture models with four or more ingredients. *The Annals of Statistics*, Vol. 28, No. 2, 578-590.

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

[13] Huang, M.-N. L., Studden, W.J. (1988). Model robust extrapolation designs. *Journal of Statistical Planning and Inference*, 18, 1-24.

[14] Huber, P.J. (1975). Robustness and designs. *Statistical Design and Linear Models*, 287-302.

[15] Kiefer, J. (1961). Optimal designs in regression problems, II. *Annals of mathematical Statistics*, Vol. 32, Issue 1, 298-325.

[16] Klein, T. (2002). Invariant symmetric block matrices for the design of mixture experiments. *Institut für Mathematik, Universität Augsburg, Report No. 443.*

[17] Lim, Y.B. (1990). D-optimal design for cubic polynomial regression on the q-simplex. *Journal of statistical planning and inference*, 25, 141-152.

[18] Mikaeili, F. (1989). D-optimal Design for cubic without 3-way effect on the simplex. *Journal of statistical planning and inference* 21, 107-115.

[19] Mikaeili, F. (1993). D-optimal Design for full cubic on q-simplex. *Journal of statistical planning and inference* 35, 121-130.

[20] Pukelsheim, F. (1993). Optimal design of experiments. Wiley, New York.

[21] Pukelsheim, F., Rosenberger, J.L. (1993). Experimental designs for model discrimination. *Journal of the American Statistical Association*, 88, 642-649.

[22] Sacks, J., Ylvisaker, D. (1984). Some model robust designs in regression. *The Annals of Statistics*, 12, 1324-1348.

[23] Stigler, S. M. (1971). Optimal experimental design for polynomial regression. *Journal of the American Statistical Association* 66, 311-318.

[24] Studden, W.J. (1982). Some robust-type D-optimal designs in polynomialregression . *Journal of the American Statistical Association*, 77, 916-921.

[25] Zen, M.M., Tsai. (2003). Criterion-robust designs for model discrimination and parameter estimation for polynomial models. To appear in Sankhya.

[26] Wolfram, S. (1999).The Mathematica Book *(Wolfram Media/Cambridge University Press, 4th ed.)*

A Scheffé models

In our study for the robust D-optimal designs, we must have a good grip in polynomial regression models and we are interested in mixture experiments. Therefore, the greatness models on mixture experiments are cited by Scheffé(1958). The following list is some polynomial regression models in q components on the simplex considered by Scheffé(1958) which we utilized in the research .

(i) Scheffé's Linear Model

$$\eta_{q,1}(x) = \sum_{1 \le i \le q} \beta_i x_i.$$

The design ξ assigns a weight $\frac{1}{q}$ to each of the points $x \leftrightarrow (1, 0, \cdots, 0)$ is the D-optimal design. We use the notation of ξ_1^* to represent the optimal design for linear model in section 4.

(ii) Scheffé's Quadratic Model

$$\begin{aligned} \eta_{q,2}(x) &= \sum_{1 \le i \le q} \beta_i x_i + \sum_{1 \le i < j \le q} \beta_{ij} x_i x_j \\ &= \eta_{q,1}(x) + \sum_{1 \le i < j \le q} \beta_{ij} x_i x_j. \end{aligned}$$

The design ξ assigns a weight $\frac{1}{\binom{q+1}{2}}$ to each of the points $x \leftrightarrow (1, 0, \cdots, 0)$ and $x \leftrightarrow (\frac{1}{2}, \frac{1}{2}, 0, \cdots, 0)$ is the D-optimal design(Kiefer (1961)). The notation of ξ_2^* to represent the optimal design for quadratic model we will take advantage of in section 4.

(iii) Scheffé's Special Cubic Model

$$\begin{aligned}\eta_{q,3}(x) &= \sum_{1\le i\le q}\beta_i x_i + \sum_{1\le i<j\le q}\beta_{ij}x_ix_j + \sum_{1\le i<j<k\le q}\beta_{ijk}x_ix_jx_k \\ &= \eta_{q,2}(x) + \sum_{1\le i<j<k\le q}\beta_{ijk}x_ix_jx_k.\end{aligned}$$

The design ξ assigns equal weight to each of the points $x \leftrightarrow (1, 0, \cdots, 0)$, $x \leftrightarrow (\frac{1}{2}, \frac{1}{2}, 0, \cdots, 0)$ and $x \leftrightarrow (\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0, \cdots, 0)$ is the D-optimal design.(Lim (1990))

(iv) Scheffé's Cubic Model Without 3-Way Effects

$$\begin{aligned}\eta_{q,3*}(x) &= \sum_{1\le i\le q}\beta_i x_i + \sum_{1\le i<j\le q}\beta_{ij}x_ix_j + \sum_{1\le i<j\le q}\gamma_{ij}x_ix_j(x_i - x_j) \\ &= \eta_{q,2}(x) + \sum_{1\le i<j\le q}\gamma_{ij}x_ix_j(x_i - x_j).\end{aligned}$$

The design ξ assigns a weight $\frac{1}{q^2}$ to each of the $\binom{q}{1}$ points $x \leftrightarrow (1, 0, \cdots, 0)$ and each of the $2\binom{q}{2}$ points $x \leftrightarrow (\frac{1-\frac{1}{\sqrt{5}}}{2}, \frac{1+\frac{1}{\sqrt{5}}}{2}, 0, \cdots, 0)$ is the D-optimal design.(Mikaeili (1989))

(v) Scheffé's Full Cubic Model

$$\begin{aligned}\eta_{q,3(full)}(x) &= \sum_{1\le i\le q}\beta_i x_i + \sum_{1\le i<j\le q}\beta_{ij}x_ix_j + \sum_{1\le i<j<k\le q}\beta_{ijk}x_ix_jx_k + \sum_{1\le i<j\le q}\gamma_{ij}x_ix_j(x_i - x_j) \\ &= \eta_{q,3}(x) + \sum_{1\le i<j\le q}\gamma_{ij}x_ix_j(x_i - x_j).\end{aligned}$$

The design ξ assigns a weight $\frac{1}{\binom{q+1}{3}}$ to each of the points $x \leftrightarrow (1, 0, \cdots, 0)$, $x \leftrightarrow (\frac{1-\frac{1}{\sqrt{5}}}{2}, \frac{1+\frac{1}{\sqrt{5}}}{2}, 0, \cdots, 0)$ and $x \leftrightarrow (\frac{1}{3}, \frac{1}{3}, 0, \cdots, 0)$ is the D-optimal design.(Mikaeili (1993))

B Example of exchangeable designs

Example 1. For $q = 2$, we have

$$\tau = \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \frac{1}{3} & \frac{2}{3} \end{pmatrix}.$$

The permutation group for $q = 2$ is given as

$$\text{Perm}(q) = \{R_1, R_2\} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}.$$

Therefore,

$$\begin{aligned} \tau^{R_2}\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) &= \tau\left(R_2^{-1}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) \\ &= \tau\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) \\ &= \tau\left(\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right) = \frac{2}{3}, \end{aligned}$$

but $\tau\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) = \frac{1}{3}$. Therefore,

$$\tau^{R_2}\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) \neq \tau\left(R_2^{-1}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right).$$

Hence, τ is not an exchangeable design. Otherwise, we can compute $\bar{\tau}$ as

$$\bar{\tau} = \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

Example 2. For $q = 2$, we have

$$\tau = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 \\ p_1 & p_2 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \\ \dfrac{1}{4} & \dfrac{3}{4} \end{pmatrix}.$$

The permutation group is the same one in Example 1. Then we can find the $\bar{\tau}$ as follows.

$$
\begin{aligned}
\bar{\tau}(\mathbf{x}_1) &= \frac{1}{q!}\sum_{R_i\in Perm(q)} \tau^{R_i}(\mathbf{x}_1) = \frac{1}{2}\sum_{R_i\in Perm(2)} \tau^{R_i}\left(\begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}\right) \\
&= \frac{1}{2}\left[\tau\left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}\right) + \tau\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}\right)\right] \\
&= \frac{1}{2}\left[\tau\begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix} + \tau\begin{pmatrix} \frac{2}{3} \\ \frac{1}{3} \end{pmatrix}\right] = \frac{1}{2}\left(\frac{1}{4}+0\right) = \frac{1}{8},
\end{aligned}
$$

by the same way, we can find the $\bar{\tau}$ below,

$$
\bar{\tau} = \begin{pmatrix} \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix} & \begin{pmatrix} \frac{2}{3} \\ \frac{1}{3} \end{pmatrix} & \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \\ \frac{1}{8} & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} \end{pmatrix}.
$$

C Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ for given $r' = 0.67$ at different q

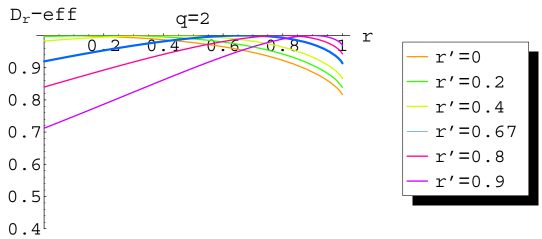

Figure 12: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 2$.

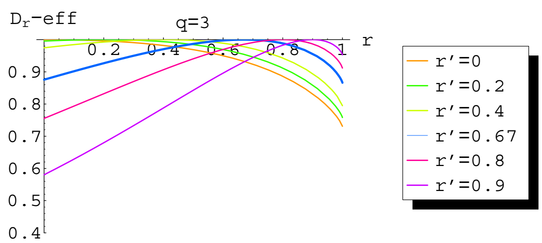

Figure 13: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 3$.

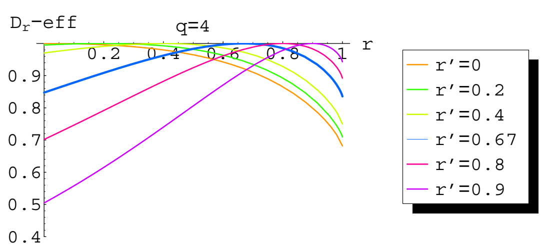

Figure 14: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 4$.

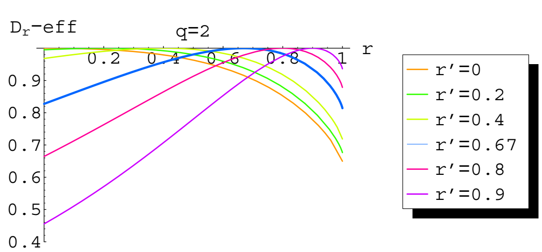

Figure 15: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 5$.

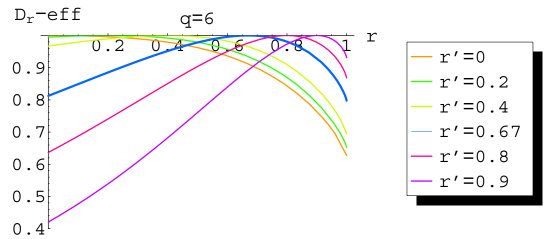

Figure 16: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 6$.

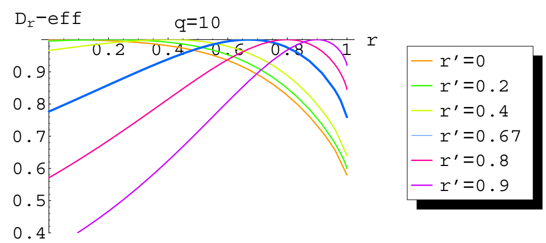

Figure 17: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 10$.

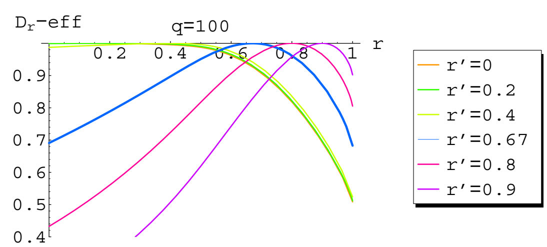

Figure 18: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 100$.

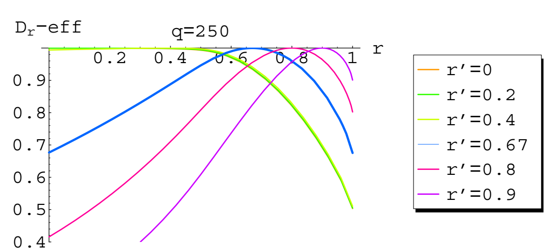

Figure 19: Plot of D_r-eff$(\xi_{\alpha^*_{0.67}})$ at $q = 250$.

D Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ under different r for $q = 2 \cdots, 250$

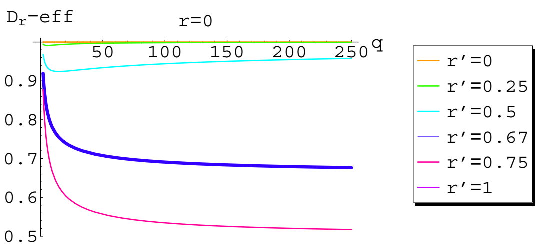

Figure 20: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r \approx 0$.

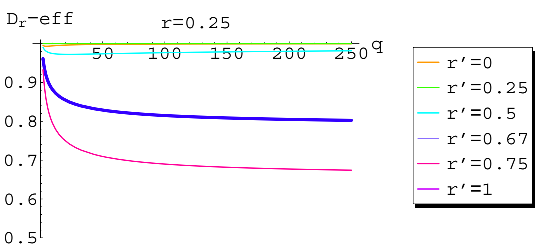

Figure 21: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r = 0.25$.

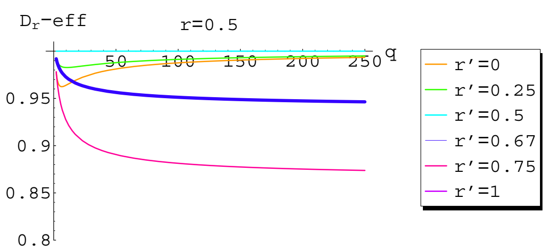

Figure 22: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r = 0.5$.

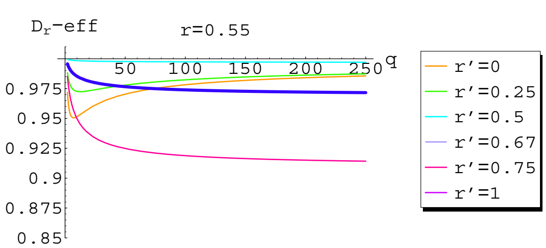

Figure 23: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r = 0.55$.

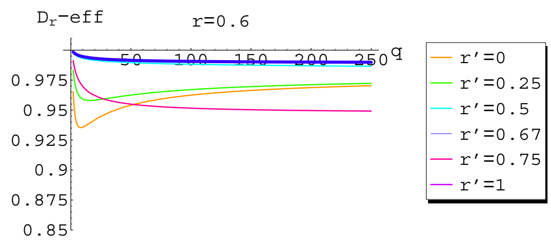

Figure 24: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r = 0.6$.

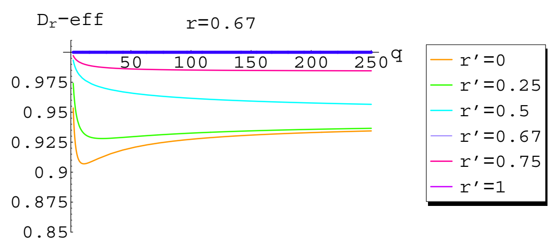

Figure 25: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r = 0.67$.

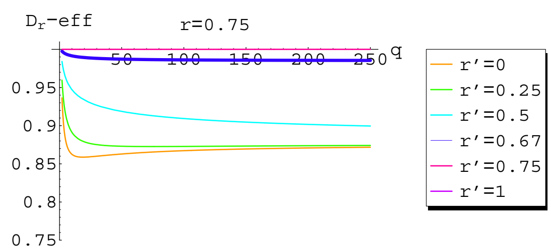

Figure 26: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r = 0.75$.

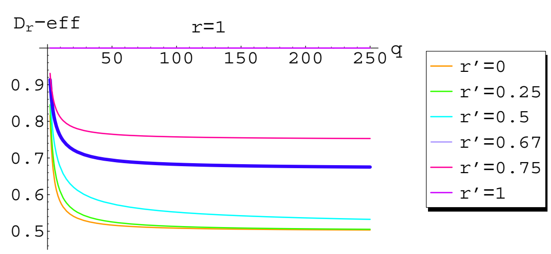

Figure 27: Plot of D_r-eff$(\xi_{\alpha^*_{r'}})$ at $r \approx 1$.