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Research article

A-Optimal designs for mixture polynomial models with heteroscedastic errors

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Abstract: This paper searches A-optimal designs for mixture polynomial models when the errors are heteroscedastic. Sufficient conditions are given so that A-optimal designs for the complex mixture polynomial models can be constructed from the direct sum of A-optimal designs for their sub-mixture models with different structures of heteroscedasticity. Several examples are presented to further illustrate and check optimal designs based on A-optimality criterion.

Keywords: mixture experiments; heteroscedasticity; A-optimal design; mixture polynomial models; direct sum design
Mathematics Subject Classification: 62K05, 62K99

1. Introduction

Mixture experiment [1,2] is a special type of experiment in which two or more ingredients are mixed together in proportion and the response of interest depends not on the total amount of the mixture, but on the proportions of the ingredients. Mixture experiments have a wide range of applications in fields such as food science, blending gasoline, detergent formulation, pharmaceutical drugs, etc.

Mixture experiments are described by special multi-factor models defined on the regular simplex. Finding the optimal designs for various mixture models has always been a hot topic in the research of mixture experiment on the assumption that the errors are homoscedastic. Some excellent reviews of the developing for mixture models and designs can be found in Chan [3] and Cornell [4]. Recently, Huang et al. [5] proposed the D- and A-optimal designs for mixture experiments with linear and quadratic models. Goos et al. [6] investigated the I-optimal design with the Scheffé mixture models. Hao et al. [7] proposed the R-optimal design with the second-order Scheffé model and got the general expression for the weights. Ling et al. [8] considered the R-optimal design problem when the levels of the qualitative factor interact with the mixture factors.

What is worth attention is that the construction of optimal design for experiment will become more complicated once the assumption is invalid. Dette and Trampisch [9] derived the D-optimal designs for the common weighted univariate polynomial regression model with efficiency function. Wiens and Li [10] studied V-optimal designs for heteroscedastic linear regression when the structure of error variances does not follow any analytical function. Rodríguez et al. [11] and He and Yue [12] derived the construction of A- and R-optimal designs for Kronecker product and additive regression models with heteroscedastic errors, using the method of product designs, respectively. He and He [13] gave the construction of Bayesian Φ_q- and maximin D-optimal designs for the heteroscedastic multi-factor linear regression models, where the error variances depend on both the the covariate and unknown parameter. Some previous results based on the assumption of heteroscedastic errors in multi-factor models may refer to Wong [14], Montepiedra and Wong [15], Rodríguez and Ortiz [16], Graßhoff et al. [17] and others. The heteroscedastic mixture models have been less deeply studied. Yan et al. [18] used the method of direct sum design to investigate the construction of D- and A-optimal design for homogeneous additive mixture models when the efficiency function is exponential structure. Polynomial model is more useful than homogeneous model in mixture experiment. Optimal designs not only depend on the model selection, but also depend on the shapes of the efficiency function. The object of this paper is to study A-optimal designs for mixture polynomial models with two different efficiency functions using the previous research method. Mixture polynomial model and A-optimal criterion will be introduced in Section 2. A detailed introduction to the direct sum design can be found in Section 3. Our main results are shown in Section 4, in which we will apply the direct sum of the A-optimal designs for sub-mixture models into the investigation of the construction of A-optimal design for mixture polynomial model on the assumption of heteroscedastic errors under sufficient conditions. Finally, the conclusions are given in Section 5.

2. Preliminaries

For a p ingredient mixture in which $x_i (i = 1, \cdots, p)$ represents the proportion of the ith ingredient, these proportions are non-negative and sum to unity. Clearly, $\mathbf{x} \equiv (x_1, \cdots, x_p)^T$ belongs to the design space which is the $(p-1)$-dimensional regular simplex:

$$S^{p-1} = \{(x_1, \cdots, x_p)^T \in R^p : \sum_{i=1}^{p} x_i = 1, 0 \leq x_i \leq 1, i = 1, \cdots, p\}.$$

The response at $\mathbf{x}$ can be expressed by the mixture polynomial model:

$$\eta(\mathbf{x}) = \boldsymbol{\theta}^T f(\mathbf{x}) + \varepsilon / \sqrt{\lambda(\mathbf{x})}, \tag{2.1}$$

where $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_k)^T$ is k-dimensional vector of unknown parameters, $f(\mathbf{x}) = (f_1(\mathbf{x}), \cdots, f_k(\mathbf{x}))^T$ is a given vector of regression functions defined on S^{p-1} and each $f_i(\mathbf{x})$ satisfies (i) $f_i(\mathbf{0}) = 0$, (ii) $f_i(\alpha\mathbf{x}) = \alpha^{h_i} f_i(\mathbf{x})$ for any positive α, h_i is the degree of $f_i(\mathbf{x})$. The error ε is random noise with zero mean and constant variance σ^2. We assume all the errors are normal and independent. $\lambda(\mathbf{x})$, named efficiency function (Fedorov [19]), is a known, bounded, positive real-valued continuous function defined on S^{p-1}. The heteroscedastic structure is determined by the efficiency function. If $\lambda(\mathbf{x}) = 1$ for all $\mathbf{x}$ in S^{p-1}, then model (2.1) is a homoscedastic model.

Based on the model (2.1), an approximate design can be expressed as a probability distribution

$$\xi = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \\ w_1 & w_2 & \cdots & w_n \end{pmatrix},$$

where $\mathbf{x}_i \in S^{p-1}$ are finite support points and their weights $\xi(\mathbf{x}_i) = w_i$ satisfy $w_i > 0$ and $\sum_{i=1}^{n} w_i = 1$. The information contained in a design ξ for the parameter vector $\boldsymbol{\theta}$ is measured by its Fisher information matrix which is given by

$$M(\xi) = \int_{S^{p-1}} f(\mathbf{x}) f^T(\mathbf{x}) \lambda(\mathbf{x}) \xi(d\mathbf{x}).$$

Optimum experimental designs typically minimize some convex function of the inverse information matrix. The A-optimality criterion minimize the sum of the length of the axes in the confidence ellipsoid thereby minimizing the average of all the variances for the estimated parameters. Fedorov [19] presented the equivalence theorem of optimal design, which provides a methodology to check whether an arbitrary design ξ is optimal or not. If model (2.1) holds, then a design ξ_A is A-optimal if and only if

$$\phi(\mathbf{x}, \xi_A) = \lambda(\mathbf{x}) f^T(\mathbf{x}) M^{-2}(\xi_A) f(\mathbf{x}) \leq tr M^{-1}(\xi_A), \tag{2.2}$$

for all $\mathbf{x} \in S^{p-1}$. The equality holds if $\mathbf{x}$ belongs to the support of ξ_A. For simple problems, optimal designs may be determined first by guess work and afterward using the above equivalence theorem to verify if the candidate design is optimal. For complicated problems, algorithms are available to find some types of optimal designs sequentially. Recently, Zhang et al. [20] proposed a multi-stage differential evolution (MDE) algorithm to find the global approximated D-optimal design in an experimental region with linear or nonlinear constraints.

3. Direct sum design

We first consider two different mixture systems, in which the response variables of interest to the experimenter are modeled by the following two mixture polynomial models respectively:

$$\eta_1(\mathbf{x}) = \boldsymbol{\beta}_1^T f(\mathbf{x}) + \varepsilon / \sqrt{\lambda_1(\mathbf{x})}, \tag{3.1}$$

$$\eta_2(\mathbf{y}) = \boldsymbol{\beta}_2^T g(\mathbf{y}) + \varepsilon / \sqrt{\lambda_2(\mathbf{y})}, \tag{3.2}$$

where the two design spaces are

$$S^{p-1} = \{\mathbf{x} = (x_1, \cdots, x_p)^T \in R^p : x_1 + \cdots + x_p = 1, 0 \leq x_i \leq 1, i = 1, \cdots, p\},$$

$$S^{q-1} = \{\mathbf{y} = (y_1, \cdots, y_q)^T \in R^q : y_1 + \cdots + y_q = 1, 0 \leq y_j \leq 1, j = 1, \cdots, q\}.$$

$f(\mathbf{x}) = (f_1(\mathbf{x}), \cdots, f_{k_1}(\mathbf{x}))^T$ is a k_1-dimensional given vector of regression functions defined on S^{p-1} and each $f_i(\mathbf{x})$ has degree of h_i, $h = min(h_1, \cdots, h_{k_1})$. Meanwhile, $g(\mathbf{y}) = (g_1(\mathbf{y}), \cdots, g_{k_2}(\mathbf{y}))^T$ is a k_2-dimensional vector of regression functions defined on S^{q-1} and each $g_j(\mathbf{y})$ has degree of l_j, $l = min(l_1, \cdots, l_{k_2})$. $\boldsymbol{\beta}_i (i = 1, 2)$ is a k_i-dimensional vector of unknown parameters and $\lambda_i(\cdot)$ is an efficiency function.

Then, we consider a complex mixture experiment which is expressed by the sum of two sub-mixture models (3.1) and (3.2)

$$\eta(\mathbf{x},\mathbf{y}) = (\boldsymbol{\beta}_1^T, \boldsymbol{\beta}_2^T)\begin{pmatrix} f(\mathbf{x}) \\ g(\mathbf{y}) \end{pmatrix} + \varepsilon/\sqrt{\lambda(\mathbf{x},\mathbf{y})}, \tag{3.3}$$

where $(\mathbf{x}^T, \mathbf{y}^T)^T = (x_1, \cdots, x_p, y_1, \cdots, y_q)^T$ belongs to the $(p+q-1)$-dimensional regular simplex

$$\begin{aligned} S^{p+q-1} &= \{(x_1, \cdots, x_p, y_1, \cdots, y_q)^T \in R^{p+q} : \\ &\sum_{i=1}^{p} x_i + \sum_{j=1}^{q} y_j = 1, 0 \le x_i,\ y_j \le 1, i = 1, \cdots, p,\ j = 1, \cdots, q\}. \end{aligned}$$

- If $\lambda_1(\mathbf{x}) = u(\mathbf{x}), \lambda_2(\mathbf{y}) = v(\mathbf{y})$, where $u(\mathbf{x})$ and $v(\mathbf{y})$ are polynomials of $\mathbf{x}$ and $\mathbf{y}$ respectively, then the efficiency function in model (5) defined on S^{p+q-1} is determined by

$$\lambda(\mathbf{x},\mathbf{y}) = \lambda_1(\mathbf{x}) + \lambda_2(\mathbf{y}). \tag{3.4}$$

- If $\lambda_1(\mathbf{x}) = e^{u(\mathbf{x})}, \lambda_2(\mathbf{y}) = e^{u(\mathbf{y})}$, then the efficiency function is determined by

$$\lambda(\mathbf{x},\mathbf{y}) = \lambda_1(\mathbf{x}) \cdot \lambda_2(\mathbf{y}). \tag{3.5}$$

It is worth noting that model (3.3) is defined on S^{p+q-1} which contains $p+q$ ingredients in different proportions and the sum of these ingredients is 100%. When $\sum_{i=1}^{p} x_i \neq 0$ or $\mathbf{x} \neq \mathbf{0}$, $f^T\Big(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Big)$ defined on S^{p+q-1} can be equivalent to $f^T(\mathbf{x})$ defined on S^{p-1}. When $\sum_{i=1}^{p} x_i = 0$ or $\mathbf{x} = \mathbf{0}$, we have $f^T(\mathbf{0}) = \mathbf{0}$. Similarly, $g^T(\mathbf{0}) = \mathbf{0}$ when $\sum_{j=1}^{q} y_j = 0$ or $\mathbf{y} = \mathbf{0}$.

Let

$$\xi_1 : \begin{pmatrix} \begin{pmatrix} x_{11} \\ \vdots \\ x_{p1} \end{pmatrix} & \begin{pmatrix} x_{12} \\ \vdots \\ x_{p2} \end{pmatrix} & \cdots & \begin{pmatrix} x_{1n_1} \\ \vdots \\ x_{pn_1} \end{pmatrix} \\ \omega_1 & \omega_2 & \cdots & \omega_{n_1} \end{pmatrix}, \sum_{i=1}^{n_1} \omega_i = 1$$

and

$$\xi_2 : \begin{pmatrix} \begin{pmatrix} y_{11} \\ \vdots \\ y_{q1} \end{pmatrix} & \begin{pmatrix} y_{12} \\ \vdots \\ y_{q2} \end{pmatrix} & \cdots & \begin{pmatrix} y_{1n_2} \\ \vdots \\ y_{qn_2} \end{pmatrix} \\ \nu_1 & \nu_2 & \cdots & \nu_{n_2} \end{pmatrix}, \sum_{j=1}^{n_2} \nu_j = 1$$

be the designs for sub-models (3.1) and (3.2), respectively. The direct sum design

$$\xi = \alpha\xi_1 \oplus (1-\alpha)\xi_2 : \begin{pmatrix} \begin{pmatrix} x_{11} \\ \vdots \\ x_{p1} \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \cdots & \begin{pmatrix} x_{1n_1} \\ \vdots \\ x_{pn_1} \\ 0 \\ \vdots \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ \vdots \\ 0 \\ y_{11} \\ \vdots \\ y_{q1} \end{pmatrix} & \cdots & \begin{pmatrix} 0 \\ \vdots \\ 0 \\ y_{1n_2} \\ \vdots \\ y_{qn_2} \end{pmatrix} \\ \alpha\omega_1 & \cdots & \alpha\omega_{n_1} & (1-\alpha)\nu_1 & \cdots & (1-\alpha)\nu_{n_2} \end{pmatrix}$$

is defined for the complex mixture model (3.3), where $0 \leq \alpha \leq 1$ and the notation $\oplus$ stands for the direct sum.

Lemma 3.1. *Let $M(\xi_i)(i = 1, 2)$ be the information matrices of ξ_i for sub-models (3.1) and (3.2) with efficiency function $\lambda_i(\cdot)$. Then,*

$$M(\xi) = \alpha M(\xi_1) \oplus (1 - \alpha)M(\xi_2)$$

is the information matrix of the direct sum design $\xi = \alpha\xi_1 \oplus (1 - \alpha)\xi_2$ for model (3.3), if the efficiency function $\lambda(\mathbf{x}, \mathbf{y})$ is defined as (3.4) or (3.5).

4. Main results

Theorem 4.1. *Let ξ_1 and ξ_2 be A-optimal designs for the sub-mixture models (3.1) and (3.2), with the efficiency functions $\lambda_1(\mathbf{x}) = u(\mathbf{x})$ and $\lambda_2(\mathbf{y}) = v(\mathbf{y})$ mentioned above, respectively. If the following condition holds for all $(\mathbf{x}^T, \mathbf{y}^T)^T \in S^{p+q-1}$, when $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{y} \neq \mathbf{0}$:*

$$(\lambda_1(\mathbf{x}) + \lambda_2(\mathbf{y}))\left(\frac{\left(\sum\limits_{i=1}^{p} x_i\right)^{2h}}{\lambda_1\left(\frac{\mathbf{x}}{\sum\limits_{i=1}^{p} x_i}\right)} + \frac{\left(\sum\limits_{j=1}^{q} y_j\right)^{2l}}{\lambda_2\left(\frac{\mathbf{y}}{\sum\limits_{j=1}^{q} y_j}\right)}\right) \leq 1, \tag{4.1}$$

then the direct sum design $\xi = \alpha_0\xi_1 \oplus (1 - \alpha_0)\xi_2$ is A-optimal for the complex model (3.3) with the efficiency function (3.4), where

$$\alpha_0 = \frac{(trM^{-1}(\xi_1))^{\frac{1}{2}}}{(trM^{-1}(\xi_1))^{\frac{1}{2}} + (trM^{-1}(\xi_2))^{\frac{1}{2}}}.$$

Example 4.1. *Consider the four-factors polynomial mixture model*

$$\eta = \beta_1 x_1 + \beta_2 x_2 + \beta_{12}\sqrt{x_1 x_2} + \beta_3 x_3 + \beta_4 x_4 + \beta_{34} x_3 x_4 + \frac{\varepsilon}{\sqrt{2x_1 + x_2 + x_3 + 2x_4}},$$

where $(x_1, x_2, x_3, x_4)^T \in S^3$. This model could be decomposed into two sub-mixture models as follows:

$$Model\ I : \eta_1 = \beta_1 x_1 + \beta_2 x_2 + \beta_{12}\sqrt{x_1 x_2} + \frac{\varepsilon}{\sqrt{2x_1 + x_2}},$$

$$Model\ II : \eta_2 = \beta_3 x_3 + \beta_4 x_4 + +\beta_{34} x_3 x_4 + \frac{\varepsilon}{\sqrt{x_3 + 2x_4}}.$$

The A-optimal design for Model I is

$$\xi_{I_A} : \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 0.5673 \\ 0.4327 \end{pmatrix} \\ 0.2677 & 0.3307 & 0.4016 \end{pmatrix}, \ trM^{-1}(\xi_{I_A}) = 16.1191.$$

The A-optimal design for Model II is

$$\xi_{II_A} : \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 0.4602 \\ 0.5398 \end{pmatrix} \\ 0.2990 & 0.2402 & 0.4608 \end{pmatrix}, \ trM^{-1}(\xi_{II_A}) = 49.5712.$$

When $\mathbf{x} \neq \mathbf{0}$ *and* $\mathbf{y} \neq \mathbf{0}$*, condition (4.1) in this example is equivalent to*

$$X^3 + (1-X)^3 + ZX^2(1-X) + \frac{1}{Z}(1-X)^2 X \leq 1,$$

where $X = x_1 + x_2 \in (0,1),\ 1 - X = x_3 + x_4,\ Z = \frac{(x_3+2x_4)/(x_3+x_4)}{(2x_1+x_2)/(x_1+x_2)} \in (0.5, 2)$ *and it is easy to be confirmed by Figure 1. By calculating* $\alpha_0 = 0.36315$*, the direct sum design*

$$\xi_A = 0.36315\xi_{I_A} \oplus 0.63685\xi_{II_A} :$$

$$\left(\begin{array}{cccccc} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0.5673 \\ 0.4327 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0.4602 \\ 0.5398 \end{pmatrix} \\ 0.0972 & 0.1201 & 0.1458 & 0.1904 & 0.1530 & 0.2935 \end{array} \right)$$

is A-optimal for this four-factors mixture model and $trM^{-1}(\xi_A) = 122.2$*. We can prove that, for all* $(x_1, x_2, x_3, x_4)^T \in S^3$*,*

$$\phi(\mathbf{x}, \xi_A) = (2x_1 + x_2 + x_3 + 2x_4) \begin{pmatrix} x_1 \\ x_2 \\ \sqrt{x_1 x_2} \\ x_3 \\ x_4 \\ x_3 x_4 \end{pmatrix} M^{-2}(\xi_A)(x_1, x_2, \sqrt{x_1 x_2}, x_3, x_4, x_3 x_4) \leq 122.2,$$

the equality holds when (x_1, x_2, x_3, x_4) *are selected at the six points of* ξ_A*. Some values of* $\phi(\mathbf{x}, \xi_A)$ *at different experiment points are displayed in Table 1.*

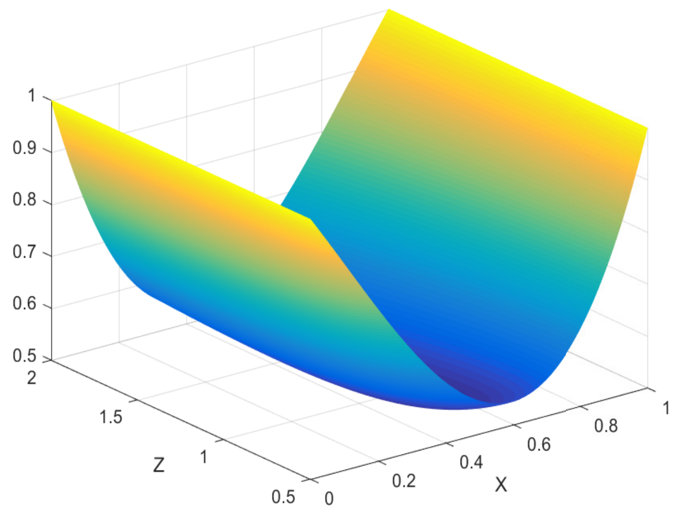

Figure 1. Plot of the checking condition in (4.1) confirms the A-optimality of the direct sum design in Example 4.1.

Table 1. The values of $\phi(\mathbf{x}, \xi_A)$ at different experiment points in Example 4.1.

x_1	x_2	x_3	x_4	$\phi(\mathbf{x}, \xi_A)$	x_1	x_2	x_3	x_4	$\phi(\mathbf{x}, \xi_A)$
1	0	0	0	122.2	0.5	0.25	0.25	0	69.2
0	1	0	0	122.2	0.5	0.25	0	0.25	74.1
0	0	1	0	122.2	0.5	0	0.25	0.25	27.9
0	0	0	1	122.2	0.25	0.5	0.25	0	55.9
0.5	0.5	0	0	118.8	0.25	0.5	0	0.25	61.3
0.5	0	0.5	0	68.8	0	0.5	0.25	0.25	39.0
0.5	0	0	0.5	61.1	0.25	0.25	0.5	0	63.0
0	0.5	0.5	0	61.1	0.25	0	0.5	0.25	14.9
0	0.5	0	0.5	68.8	0	0.25	0.5	0.25	17.2
0	0	0.5	0.5	119.3	0.25	0.25	0	0.5	61.4
0.4	0.3	0.2	0.1	60.7	0.25	0	0.25	0.5	20.3
0.5672	0.4327	0	0	122.2	0	0.25	0.25	0.5	23.1
0	0	0.4602	0.5398	122.2	0.25	0.25	0.25	0.25	30.7

Corollary 4.1. *For n heteroscedastic mixture polynomial models,*

$$\eta_i(\mathbf{x}_i) = \left(f_{i1}(\mathbf{x}_i), f_{i2}(\mathbf{x}_i), \cdots, f_{ik_i}(\mathbf{x}_i)\right)\begin{pmatrix} \beta_{i1} \\ \beta_{i2} \\ \vdots \\ \beta_{ik_i} \end{pmatrix} + \frac{\varepsilon}{\sqrt{\lambda_i(\mathbf{x}_i)}} = \mathbf{f}_i^{\mathrm{T}}(\mathbf{x}_i)\boldsymbol{\beta}_i + \frac{\varepsilon}{\sqrt{\lambda_i(\mathbf{x}_i)}},$$

where $\mathbf{x}_i = (x_{i1}, x_{i2}, \cdots, x_{ip_i})^{\mathrm{T}} \in S^{p_i-1}$, $i = 1, 2, \cdots, n$. h_i is the lowest degree of the ith sub-mixture model and the efficiency function $\lambda_i(\mathbf{x}_i)$ is polynomial. Let ξ_i be A-optimal design for the ith sub-mixture model. If the following condition holds for all $(\mathbf{x}_1^{\mathrm{T}}, \mathbf{x}_2^{\mathrm{T}}, \cdots, \mathbf{x}_n^{\mathrm{T}})^{\mathrm{T}} \in S^{p_1+p_2+\cdots+p_n-1}$ when $\mathbf{x}_i \neq \mathbf{0}(i = 1, 2, \cdots, n)$:

$$\sum_{i=1}^{n} \lambda_i(\mathbf{x}_i) \sum_{i=1}^{n} \frac{\left(\sum\limits_{j=1}^{p_i} x_{ij}\right)^{2h_i}}{\lambda_i\left(\frac{\mathbf{x}_i}{\sum\limits_{j=1}^{p_i} x_{ij}}\right)} \leq 1,$$

then the direct sum design $\xi = \alpha_1\xi_1 \oplus \alpha_2\xi_2 \oplus \cdots \oplus \alpha_n\xi_n$ is A-optimal for the complex model

$$\eta(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n) = (\mathbf{f}_1^{\mathrm{T}}(\mathbf{x}_1), \mathbf{f}_2^{\mathrm{T}}(\mathbf{x}_2), \cdots, \mathbf{f}_n^{\mathrm{T}}(\mathbf{x}_n))\begin{pmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \\ \vdots \\ \boldsymbol{\beta}_n \end{pmatrix} + \frac{\varepsilon}{\sqrt{\lambda(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n)}},$$

with the efficiency function $\lambda(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n) = \lambda_1(\mathbf{x}_1) + \lambda_2(\mathbf{x}_2) + \cdots + \lambda_n(\mathbf{x}_n)$, where

$$\alpha_i = \frac{(trM^{-1}(\xi_i))^{\frac{1}{2}}}{(trM^{-1}(\xi_1))^{\frac{1}{2}} + \cdots + (trM^{-1}(\xi_n))^{\frac{1}{2}}}.$$

Theorem 4.2. *Let ξ_1 and ξ_2 be A-optimal designs for the sub-mixture models (3.1) and (3.2), with the efficiency functions $\lambda_1(\mathbf{x}) = e^{u(\mathbf{x})}$ and $\lambda_2(\mathbf{y}) = e^{v(\mathbf{y})}$ mentioned above, respectively. If the following condition holds for all $(\mathbf{x}^T, \mathbf{y}^T)^T \in S^{p+q-1}$, when $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{y} \neq \mathbf{0}$:*

$$\lambda_1(\mathbf{x})\lambda_2(\mathbf{y}) \left(\frac{\Big(\sum_{i=1}^{p} x_i\Big)^{2h}}{\lambda_1\Big(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Big)} + \frac{\Big(\sum_{j=1}^{q} y_j\Big)^{2l}}{\lambda_2\Big(\frac{\mathbf{y}}{\sum_{j=1}^{q} y_j}\Big)} \right) \leq 1, \tag{4.2}$$

then the direct sum design $\xi = \alpha_0\xi_1 \oplus (1-\alpha_0)\xi_2$ is A-optimal for model (3.3) with the efficiency function (3.5), where $\alpha_0 = (trM^{-1}(\xi_1))^{\frac{1}{2}} / \Big((trM^{-1}(\xi_1))^{\frac{1}{2}} + (trM^{-1}(\xi_2))^{\frac{1}{2}}\Big)$.

Example 4.2. *Consider the four-factors polynomial mixture model*

$$\eta = \beta_1 x_1 + \beta_2 x_2 + \beta_{12}\sqrt{x_1 x_2} + \beta_3 x_3 + \beta_4 x_4 + \beta_{34} x_3 x_4 + \frac{\varepsilon}{\sqrt{e^{2x_1^2 + x_2 + 3x_3 + 2x_4^2}}},$$

where $(x_1, x_2, x_3, x_4)^T \in S^3$. This model could be decomposed into two sub-mixture models as follows:

$$Model\ 1: \eta_1 = \beta_1 x_1 + \beta_2 x_2 + \beta_{12}\sqrt{x_1 x_2} + \frac{\varepsilon}{\sqrt{e^{2x_1^2 + x_2}}},$$

$$Model\ 2: \eta_2 = \beta_3 x_3 + \beta_4 x_4 + +\beta_{34} x_3 x_4 + \frac{\varepsilon}{\sqrt{e^{3x_3 + 2x_4^2}}}.$$

The A-optimal design for Model 1 is

$$\xi_{1_A} : \left(\begin{array}{ccc} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 0.6328 \\ 0.3672 \end{pmatrix} \\ 0.2403 & 0.3018 & 0.4579 \end{array} \right), \ trM^{-1}(\xi_{1_A}) = 6.3827.$$

The A-optimal design for Model 2 is

$$\xi_{2_A} : \left(\begin{array}{ccc} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 0.4245 \\ 0.5755 \end{pmatrix} \\ 0.2510 & 0.1944 & 0.5546 \end{array} \right), \ trM^{-1}(\xi_{2_A}) = 8.6302.$$

When $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{y} \neq \mathbf{0}$, condition (4.2) in this example holds when the following inequality is satisfied,

$$X^2 Z^{X-1} + (1-X)^2 Z^X \leq 1,$$

where $X = x_1 + x_2 \in (0,1)$, $1 - X = x_3 + x_4$, $Z = \frac{e^{2(\frac{x_1}{x_1+x_2})^2 + (\frac{x_2}{x_1+x_2})}}{e^{3(\frac{x_3}{x_3+x_4}) + 2(\frac{x_4}{x_3+x_4})^2}} \in (e^{-\frac{17}{8}}, e^{\frac{1}{8}})$ and it is easy to be confirmed by Figure 2. By calculating $\alpha_0 = 0.46236$, the direct sum design

$$\xi_A = 0.46236\xi_{1_A} \oplus 0.53764\xi_{2_A} :$$

$$\left(\begin{array}{cccccc} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0.6328 \\ 0.3672 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0.4245 \\ 0.5755 \end{pmatrix} \\ 0.1111 & 0.1395 & 0.2117 & 0.1350 & 0.1045 & 0.2982 \end{array} \right)$$

is A-optimal for this four-factors mixture model and $trM^{-1}(\xi_A) = 29.8565$. *For all* $(x_1, x_2, x_3, x_4)^T \in S^3$,

$$e^{2x_1^2+x_2+3x_3+2x_4^2}\begin{pmatrix} x_1 \\ x_2 \\ \sqrt{x_1x_2} \\ x_3 \\ x_4 \\ x_3x_4 \end{pmatrix} M^{-2}(\xi_A)(x_1, x_2, \sqrt{x_1x_2}, x_3, x_4, x_3x_4) \leq 29.8565,$$

the equality holds when (x_1, x_2, x_3, x_4) *are selected at the six points of* ξ_A.

Similar to Corollary 4.1, the conclusion of Theorem 4.2 can also be generalized to n sub-models and is omitted.

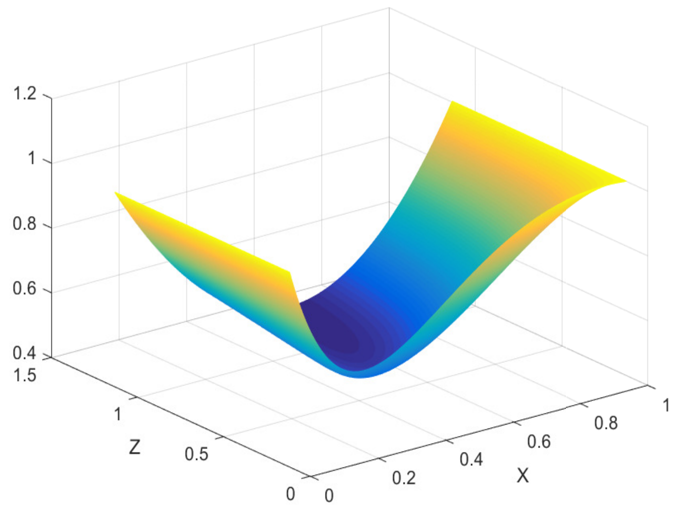

Figure 2. Plot of the checking condition in (4.2) confirms the A-optimality of the direct sum design in Example 4.2.

5. Conclusions

The method of constructing A-optimal designs for mixture polynomial models with two different heteroscedastic structures is presented in this paper. It is difficult to obtain the optimal designs for a complicated mixture model in a direct way. However, it becomes accessible with the assistance of the construction of optimal design for the corresponding sub-mixture models.

When the heteroscedastic structure is polynomials, the direct sum of A-optimal designs for two sub-mixture models is A-optimal for the complex mixture model with efficiency function defined as (3.4) if condition (4.1) is satisfied. When the heteroscedastic structure is exponential functions, the direct sum of A-optimal designs for two sub-mixture models is A-optimal for the complex mixture model with efficiency function defined as (3.5) if condition (4.2) holds. The conclusions of Theorems 4.1 and 4.2 can be generalized to n sub-models under very strict conditions. Further research should explore the generalization of the approaches for more complex efficiency functions.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that there is no conflict of interest.

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Appendix

A.1 Proof of Lemma 3.1.

If Eq (3.4) is hold, then the information matrix of the direct sum design ξ for model (3.3) is determined by

$$\begin{aligned}
M(\xi) &= \int_{S^{p+q-1}} \begin{pmatrix} f(\mathbf{x}) \\ g(\mathbf{y}) \end{pmatrix} (f^T(\mathbf{x}), g^T(\mathbf{y}))\lambda(\mathbf{x},\mathbf{y})\xi(d(\mathbf{x},\mathbf{y})) \\
&= \int_{S^{p+q-1}} \begin{pmatrix} f(\mathbf{x})f^T(\mathbf{x})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{y})) & f(\mathbf{x})g^T(\mathbf{y})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{y})) \\ g(\mathbf{y})f^T(\mathbf{x})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{y})) & g(\mathbf{y})g^T(\mathbf{y})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{y})) \end{pmatrix} \xi(d(\mathbf{x},\mathbf{y})) \\
&= \left(\begin{matrix} \int_{S^{p-1}} \alpha f(\mathbf{x})f^T(\mathbf{x})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{0}))\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)f(\mathbf{0})f^T(\mathbf{0})(\lambda_1(\mathbf{0})+\lambda_2(\mathbf{y}))\xi_2(d\mathbf{y}) \\ \int_{S^{p-1}} \alpha g(\mathbf{0})f^T(\mathbf{x})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{0}))\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)g(\mathbf{y})f^T(\mathbf{0})(\lambda_1(\mathbf{0})+\lambda_2(\mathbf{y}))\xi_2(d\mathbf{y}) \end{matrix} \right. \\
&\qquad \left. \begin{matrix} \int_{S^{p-1}} \alpha f(\mathbf{x})g^T(\mathbf{0})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{0}))\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)f(\mathbf{0})g^T(\mathbf{y})(\lambda_1(\mathbf{0})+\lambda_2(\mathbf{y}))\xi_2(d\mathbf{y}) \\ \int_{S^{p-1}} \alpha g(\mathbf{0})g^T(\mathbf{0})(\lambda_1(\mathbf{x})+\lambda_2(\mathbf{0}))\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)g(\mathbf{y})g^T(\mathbf{y})(\lambda_1(\mathbf{0})+\lambda_2(\mathbf{y}))\xi_2(d\mathbf{y}) \end{matrix} \right)
\end{aligned}$$

$$= \begin{pmatrix} \alpha M(\xi_1) & \mathbf{0} \\ \mathbf{0} & (1-\alpha)M(\xi_2) \end{pmatrix} = \alpha M(\xi_1) \oplus (1-\alpha)M(\xi_2).$$

If Eq (3.5) is hold, then the information matrix of the direct sum design ξ for model (3.3) is

$$\begin{aligned}
M(\xi) &= \int_{S^{p+q-1}} \begin{pmatrix} f(\mathbf{x}) \\ g(\mathbf{y}) \end{pmatrix} (f^T(\mathbf{x}), g^T(\mathbf{y}))\lambda(x,y)\xi(d(\mathbf{x},\mathbf{y})) \\
&= \int_{S^{p+q-1}} \begin{pmatrix} f(\mathbf{x})f^T(\mathbf{x})\lambda_1(\mathbf{x})\lambda_2(\mathbf{y}) & f(\mathbf{x})g^T(\mathbf{y})\lambda_1(\mathbf{x})\lambda_2(\mathbf{y}) \\ g(\mathbf{y})f^T(\mathbf{x})\lambda_1(\mathbf{x})\lambda_2(\mathbf{y}) & g(\mathbf{y})g^T(\mathbf{y})\lambda_1(\mathbf{x})\lambda_2(\mathbf{y}) \end{pmatrix} \xi(d(\mathbf{x},\mathbf{y})) \\
&= \left(\begin{matrix} \int_{S^{p-1}} \alpha f(\mathbf{x})f^T(\mathbf{x})\lambda_1(\mathbf{x})\lambda_2(\mathbf{0})\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)f(\mathbf{0})f^T(\mathbf{0})\lambda_1(\mathbf{0})\lambda_2(\mathbf{y})\xi_2(d\mathbf{y}) \\ \int_{S^{p-1}} \alpha g(\mathbf{0})f^T(\mathbf{x})\lambda_1(\mathbf{x})\lambda_2(\mathbf{0})\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)g(\mathbf{y})f^T(\mathbf{0})\lambda_1(\mathbf{0})\lambda_2(\mathbf{y})\xi_2(d\mathbf{y}) \end{matrix} \right. \\
&\qquad \left. \begin{matrix} \int_{S^{p-1}} \alpha f(\mathbf{x})g^T(\mathbf{0})\lambda_1(\mathbf{x})\lambda_2(\mathbf{0})\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)f(\mathbf{0})g^T(\mathbf{y})\lambda_1(\mathbf{0})\lambda_2(\mathbf{y})\xi_2(d\mathbf{y}) \\ \int_{S^{p-1}} \alpha g(\mathbf{0})g^T(\mathbf{0})\lambda_1(\mathbf{x})\lambda_2(\mathbf{0})\xi_1(d\mathbf{x}) + \int_{S^{q-1}} (1-\alpha)g(\mathbf{y})g^T(\mathbf{y})\lambda_1(\mathbf{0})\lambda_2(\mathbf{y})\xi_2(d\mathbf{y}) \end{matrix} \right) \\
&= \begin{pmatrix} \alpha M(\xi_1) & \mathbf{0} \\ \mathbf{0} & (1-\alpha)M(\xi_2) \end{pmatrix} = \alpha M(\xi_1) \oplus (1-\alpha)M(\xi_2).
\end{aligned}$$

A.2 Proof of Theorem 4.1.

Let ξ_1 and ξ_2 are A-optimal designs for model (3.1) and (3.2) respectively, according to the equivalence theorem (2.2) we find that

$$\lambda_1(\mathbf{x})f^T(\mathbf{x})M^{-2}(\xi_1)f(\mathbf{x}) \leq trM^{-1}(\xi_1), \quad \mathbf{x} \in S^{p-1},$$

$$\lambda_2(\mathbf{y})g^T(\mathbf{y})M^{-2}(\xi_2)g(\mathbf{y}) \leq trM^{-1}(\xi_2), \quad \mathbf{y} \in S^{q-1}.$$

Assume $\alpha_0 = a/(a+b)$, where $a = (trM^{-1}(\xi_1))^{\frac{1}{2}}, b = (trM^{-1}(\xi_2))^{\frac{1}{2}}$, then

$$\begin{aligned}
trM^{-1}(\xi) &= tr\Big(\frac{1}{\alpha_0}M^{-1}(\xi_1) \oplus \frac{1}{1-\alpha_0}M^{-1}(\xi_2)\Big) \\
&= \frac{1}{\alpha_0}trM^{-1}(\xi_1) + \frac{1}{1-\alpha_0}trM^{-1}(\xi_2) \\
&= \frac{a+b}{a} \cdot a^2 + \frac{a+b}{b} \cdot b^2 = (a+b)^2.
\end{aligned}$$

For all $(\mathbf{x}^T, \mathbf{y}^T)^T \in S^{p+q-1}$, When $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{y} \neq \mathbf{0}$,

$$f(\mathbf{x}) \leq f\Bigg(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Bigg) \cdot \Big(\sum_{i=1}^{p} x_i\Big)^h, \quad g(\mathbf{y}) \leq g\Bigg(\frac{\mathbf{y}}{\sum_{j=1}^{q} y_j}\Bigg) \cdot \Big(\sum_{j=1}^{q} y_j\Big)^l,$$

$$\lambda_1\Bigg(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Bigg)f^T\Bigg(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Bigg)M^{-2}(\xi_1)f\Bigg(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Bigg) \leq tr(M^{-1}(\xi_1)), \quad \mathbf{x} \in S^{p+q-1},$$

$$\lambda_2\Big(\frac{\mathbf{y}}{\sum\limits_{j=1}^{q} y_j}\Big)g^T\Big(\frac{\mathbf{y}}{\sum\limits_{j=1}^{q} y_j}\Big)M^{-2}(\xi_2)g\Big(\frac{\mathbf{y}}{\sum\limits_{j=1}^{q} y_j}\Big) \le tr(M^{-1}(\xi_2)), \quad \mathbf{y} \in S^{p+q-1}.$$

If condition (4.1) is satisfied, for the direct sum $\xi = \alpha_0\xi_1 \oplus (1-\alpha_0)\xi_2$,

$$\begin{aligned}
&\lambda(\mathbf{x},\mathbf{y})(f^T(\mathbf{x}), g^T(\mathbf{y}))M^{-2}(\xi)\begin{pmatrix} f(\mathbf{x}) \\ g(\mathbf{y}) \end{pmatrix} \\
=\;& \lambda(\mathbf{x},\mathbf{y})(f^T(\mathbf{x}), g^T(\mathbf{y}))\Big(\frac{1}{\alpha_0^2}M^{-2}(\xi_1) \oplus \frac{1}{(1-\alpha_0)^2}M^{-2}(\xi_2)\Big)\begin{pmatrix} f(\mathbf{x}) \\ g(\mathbf{y}) \end{pmatrix} \\
=\;& (\lambda_1(\mathbf{x}) + \lambda_2(\mathbf{y}))\Big(\frac{1}{\alpha_0^2}f^T(\mathbf{x})M^{-2}(\xi_1)f(\mathbf{x}) + \frac{1}{(1-\alpha_0)^2}g^T(\mathbf{y})M^{-2}(\xi_2)g(\mathbf{y})\Big) \\
\le\;& (\lambda_1(\mathbf{x}) + \lambda_2(\mathbf{y}))\Big(\frac{1}{\alpha_0^2}f^T\Big(\frac{\mathbf{x}}{\sum\limits_{i=1}^{p} x_i}\Big)M^{-2}(\xi_1)f\Big(\frac{\mathbf{x}}{\sum\limits_{i=1}^{p} x_i}\Big)\Big(\sum_{i=1}^{p} x_i\Big)^{2h} \\
&+\frac{1}{(1-\alpha_0)^2}g^T\Big(\frac{\mathbf{y}}{\sum\limits_{j=1}^{q} y_j}\Big)M^{-2}(\xi_2)g\Big(\frac{\mathbf{y}}{\sum\limits_{j=1}^{q} y_j}\Big)\Big(\sum_{j=1}^{q} y_j\Big)^{2l}\Big) \\
\le\;& (\lambda_1(\mathbf{x}) + \lambda_2(\mathbf{y}))\left(\frac{trM^{-1}(\xi_1)}{\alpha_0^2}\cdot\frac{\Big(\sum\limits_{i=1}^{p} x_i\Big)^{2h}}{\lambda_1\Big(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Big)} + \frac{trM^{-1}(\xi_2)}{(1-\alpha_0)^2}\cdot\frac{\Big(\sum\limits_{j=1}^{q} y_j\Big)^{2l}}{\lambda_2\Big(\frac{\mathbf{y}}{\sum_{j=1}^{q} y_j}\Big)}\right) \\
=\;& (a+b)^2(\lambda_1(\mathbf{x}) + \lambda_2(\mathbf{y}))\left(\frac{\Big(\sum\limits_{i=1}^{p} x_i\Big)^{2h}}{\lambda_1\Big(\frac{\mathbf{x}}{\sum_{i=1}^{p} x_i}\Big)} + \frac{\Big(\sum\limits_{j=1}^{q} y_j\Big)^{2l}}{\lambda_2\Big(\frac{\mathbf{y}}{\sum_{j=1}^{q} y_j}\Big)}\right) \\
=\;& (a+b)^2 = trM^{-1}(\xi).
\end{aligned}$$

When $\mathbf{x} = \mathbf{0}$,

$$\lambda(\mathbf{x},\mathbf{y})(f^T(\mathbf{x}), g^T(\mathbf{y}))M^{-2}(\xi)(f^T(\mathbf{x}), g^T(\mathbf{y}))^T = \frac{1}{(1-\alpha_0)^2}\lambda_2(\mathbf{y})g^T(\mathbf{y})M^{-2}(\xi_2)g(\mathbf{y}) \le trM^{-1}(\xi).$$

When $\mathbf{y} = \mathbf{0}$,

$$\lambda(\mathbf{x},\mathbf{y})(f^T(\mathbf{x}), g^T(\mathbf{y}))M^{-2}(\xi)(f^T(\mathbf{x}), g^T(\mathbf{y}))^T = \frac{1}{\alpha_0^2}\lambda_1(\mathbf{x})f^T(\mathbf{x})M^{-2}(\xi_1)f(\mathbf{x}) \le trM^{-1}(\xi).$$

By the equivalence theorem (2.2), the design ξ is A-optimal for model (3.3).

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