Hacettepe Journal of
Mathematics & Statistics

Hacet. J. Math. Stat.
Volume 53 (6) (2024), 1759 – 1773
DOI : 10.15672/hujms.1374974

Research Article

A-optimal design for cubic model without a 3-way effect for mixture experiment

Mahesh Kumar Panda

Department of Statistics, Ravenshaw University, Cuttack 753003, India

Abstract

In this article, we obtain a saturated A-optimal design for the cubic model without a 3-way effect for mixture experiment and get a general formula of the weights. The necessary and sufficient condition of the A-optimality criterion is confirmed by using the corresponding equivalence theorem.

Mathematics Subject Classification (2020). 62K05

Keywords. Saturated design, A-optimal design, cubic model, mixture experiment, equivalence theorem

1. Introduction

A mixture experiment is typically used in formulation and blending experiments. In a mixture experiment, the response is a function of the proportion and not the amount of the ingredients. If a mixture consists of q number of components and proportions of the ingredients are denoted by $x_1, x_2, \ldots, x_q$, then the experimental region containing these mixture components becomes a $(q-1)$-dimensional simplex represented as

$$S^{q-1} = \left\{ \mathbf{x} = (x_1, x_2, \ldots, x_q)^T \in R^q | \sum_{i=1}^{q} x_i = 1, 0 \leq x_i \leq 1, i = 1, 2, \ldots, q \right\}. \tag{1.1}$$

The construction of an optimal design aims to improve the statistical inference about a particular quantity of interest by appropriately selecting the value of the predictors. These values are so chosen as to minimize the variability of the estimators of the unknown parameters based on a specific criterion. In the literature, different optimal designs are defined like D-, A-, E-, R-, and others. Research work on optimal designs for mixture experiment continued to be an interest to many researchers across the globe. In the last decade, several articles on the construction of optimal designs for mixture models were published [1, 13–17, 19].

The canonical polynomial models are widely used for analyzing mixture data. In particular, Scheffès quadratic model is quite useful in analyzing agricultural and industrial problems [18]. Nevertheless, if the goal is to model the curvature in the interior of a factor space, cubic polynomial models are preferable than quadratic models. Three different

Email address: mahesh2123ster@gmail.com
Received: 12.10.2023; Accepted: 29.09.2024

forms of cubic polynomial models are proposed in the literature i.e., full cubic model, cubic model without a 3-way effect, and special cubic model [2].

In case of D-optimal design, equal weights are allocated to all the support points. In contrast, weights associated with different support points, in general, are not same in case of A-optimal design. Further, the weights assigned to these support points vary with change in the value of q. Therefore, construction of an A-optimal design for higher-degree mixture models involves much more difficulty than the D-optimal design.

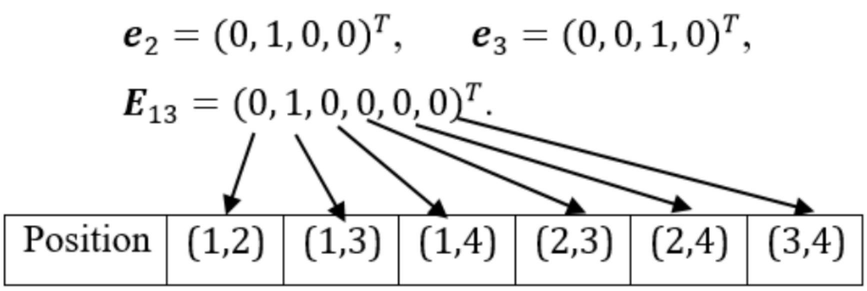
Kiefer [7] derived saturated D-optimal designs for full cubic, cubic without a 3-way effect, and special cubic models for a three-component mixture. For other works related to optimal designs for cubic canonical polynomial models for mixture experiment, we can refer to the work of Farrell et al. [3], Mikaeili [11,12], and Lim [10]. Panda and Sahoo [16] obtained a saturated A-optimal design for the full cubic model, cubic model without a three-way effect, and special cubic model for mixture experiment, where $q = 3$. Recently, Zhu and Hao [20] investigated an A-optimal design for the special cubic mixture model. Notwithstanding such works, the problem of constructing A-optimal design for cubic model without a 3-way effect has not yet been solved. That motivated us to work on the same problem. In this work, we prove that the saturated A-optimal design is supported by the design points of the corresponding D-optimal design. However, the weights assigned to all these design points are not same.

This article is structured as follows: In Section 2, we provide some preliminaries. Section 3 presents a brief discussion on A-optimal design and corresponding equivalence theorem. Section 4 obtains an A-optimal design for the cubic model without a 3-way effect. In Section 5, we obtain the A- efficiency of the corresponding D-optimal design for the discussed model to compare both A-, and D-optimal designs. Finally, we infer the conclusions in Section 6.

2. Preliminaries

In this section, some vectors and matrices are defined that we will use to define the information matrix of the proposed model. These are as follows:

For $q \geq 2$, denote the canonical unit vectors in R^q by $\mathbf{e}_1, \ldots, \mathbf{e}_q$ and those in $R^{\binom{q}{2}}$ by $\mathbf{E}_{ij}$ with lexicographically ordered index pairs $(i, j), 1 \leq i < j \leq q$. Here R^q and $R^{\binom{q}{2}}$ are the the sets of q- and $\binom{q}{2}$-dimensional vectors respectively. In the vector $\mathbf{e}_i$, the i^{th} element is 1 for $i = 1, 2, \ldots, q$, and the remaining elements are 0. Similarly, in the vector $\mathbf{E}_{ij}$ the element at (i, j)th-position is 1 for $1 \leq i < j \leq q$, and the rest of the elements of the vector are 0. For instance, when $q = 4$:



We denote the identity matrices of dimension q and $\binom{q}{2}$ by $\mathbf{U}_1$ and $\mathbf{W}_1$, respectively. We also denote the vector $\mathbf{1}_q \in R^q$ as $\mathbf{1}_q = (1, \ldots, 1)^\top$. Furthermore, we define

$$\mathbf{U_2} = \mathbf{1_q 1_q^\top} - \mathbf{I_q} \in Sym(q),$$

$$\mathbf{V_1} = \sum_{\substack{i,j=1\\ i<j}}^{\mathbf{q}} \mathbf{E_{ij}}(\mathbf{e}_i + \mathbf{e}_j)^\top \in R^{\binom{q}{2}\times q},$$

$$\mathbf{V_2} = \sum_{\substack{i,j=1\\ i<j}}^{\mathbf{q}} \sum_{\substack{k=1\\ k\notin\{i,j\}}}^{q} \mathbf{E_{ij}}\mathbf{e}_k^\top \in R^{\binom{q}{2}\times q},$$

$$\mathbf{X_1} = \sum_{\substack{i,j=1\\ i<j}}^{\mathbf{q}} \mathbf{E_{ij}}(\mathbf{e}_j - \mathbf{e}_i)^\top \in R^{\binom{q}{2}\times q}.$$

Here $Sym(q)$ and $R^{\binom{q}{2}\times q}$ are the set of symmetric matrices of order q and the set of matrices of order $\binom{q}{2} \times q$, respectively [9].

3. A-optimal design and equivalence theorem

Let us consider a regression model of the form

$$\eta(\mathbf{x}) = \mathbf{f}^\top(\mathbf{x})\boldsymbol{\beta}, \quad \mathbf{x} \in S^{q-1}, \tag{3.1}$$

where $\eta(\mathbf{x})$, $\mathbf{x}$, $\mathbf{f(x)}$ are the expected response, input variable, and regression function respectively. Here we assume that all the responses are independent of each other and have a constant variance. A continuous design $\xi \in \Delta$ have the following form [8]:

$$\xi = \begin{Bmatrix} \mathbf{x}_{(1)} & \mathbf{x}_{(2)} & \dots & \mathbf{x}_{(m)} \\ r_1 & r_2 & \dots & r_m \end{Bmatrix}, \mathbf{x}_{(j)} \in S^{q-1}, 0 < r_j < 1, \sum_{j=1}^{m} r_j = 1,$$

where $\mathbf{x}_{(1)}, \mathbf{x}_{(2)}, \dots, \mathbf{x}_{(m)}$ are different design points defined over S^{q-1}; r_j is the weight associated with the point $x_{(j)}$, $j = 1, 2, , m$. Here Δ is defined as the set of all continuous designs. A non-singular information matrix for a design $\xi \in \Delta$ can be defined as

$$\mathbf{M}(\xi) = \sum_{j=1}^{m} r_j \mathbf{f}(\mathbf{x_{(j)}})\mathbf{f}^\top(\mathbf{x_{(j)}})$$

over S^{q-1}.

Definition 3.1. A design $\xi^* \in \Delta$ with an information matrix $\mathbf{M}(\xi^*)$ for model Equation (3.1) is called A-optimal design if it minimizes Trace$(\mathbf{M^{-1}}(\xi))$ over the set Δ.

Definition 3.2. A saturated design for any regression model (with p number of parameters) is a design which is supported on exactly p distinct support points [5].

The following equivalence theorem examines the necessary and sufficient conditions of A-optimality over the simplex region S^{q-1} [4].

Theorem 3.3. *A continuous design $\xi^* \in \Delta$ is said to be an A-optimal design for the model Equation* (3.1) *if and only if*

$$Max_{\mathbf{x}\in S^{q-1}} d(\mathbf{x}, \xi^*) = Trace[\boldsymbol{M}^{-1}(\xi^*)], \tag{3.2}$$

where $d(\mathbf{x}, \xi) = \mathbf{f}^\top(\mathbf{x})\boldsymbol{M}^{-2}(\xi)\mathbf{f}(\mathbf{x})$. Furthermore, the supremum exists at the support point of ξ^*.

Selection of support points: The pioneer work on the construction of D-optimal design for the cubic polynomial model without a 3-way effect was due to Kiefer [7]. He considered the initial design $\xi_a\left(0 < a < \dfrac{1}{2}\right)$ and obtained the D-optimal design for the cubic model without a 3-way effect for the three-component mixture. The design $\xi_a\left(a = \dfrac{(1-5^{-1/2})}{2}\right)$ that puts equal mass 1/9 to each of the three vertices $\mathbf{x} \longleftrightarrow (1, 0, 0)$

and six points of the form $\mathbf{x} \longleftrightarrow (a, 1-a, 0)$ is D-optimal design for the cubic model without a 3-way effect. Here $\mathbf{x} \longleftrightarrow (1, 0, 0)$ means the design point $(1, 0, 0)$ and its permutations i.e., $(0, 1, 0)$,$(0, 0, 1)$. Similarly, $\mathbf{x} \longleftrightarrow (a, 1-a, 0)$ means the design point $(a, 1-a, 0)$ and its permutations i.e., $(a, 0, 1-a)$, $(0, a, 1-a)$, $(1-a, a, 0)$, $(1-a, 0, a)$, $(0, 1-a, a)$.

We, therefore, consider the design $\xi_a \left(0 < a < \dfrac{1}{2}\right)$ that assign weight r_1 to each of the vertices i.e., $\mathbf{x} \longleftrightarrow (1, 0, \ldots, 0)$ and weight r_2 to each of the points i.e., $\mathbf{x} \longleftrightarrow (a, 1-a, \ldots, 0)$ to construct a saturated A-optimal design for the cubic model without a 3-way effect.

4. A-optimal design for cubic model without a 3-way effect

In this Section, we obtain A-optimal design for the cubic model without a 3-way effect that can be represented as

$$\begin{aligned}\eta_1 &= \mathbf{f_1}^\top(\mathbf{x})\boldsymbol{\beta_1} \\ &= \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{i<j}^{q} \delta_{ij} x_i x_j (x_i - x_j), \end{aligned} \tag{4.1}$$

where $\mathbf{f_1}(\mathbf{x})$ and $\boldsymbol{\beta_1}$ are column vectors of length q^2 and are defined as

$$\mathbf{f_1}(\mathbf{x}) = (x_1, x_2, \ldots, x_q, x_1x_2, x_1x_3, \ldots, x_{q-1}x_q, x_1x_2(x_1 - x_2),$$
$$x_1x_3(x_1 - x_3), \ldots, x_{q-1}x_q(x_{q-1} - x_q))^\top,$$
$$\beta_\mathbf{1} = (\beta_1, \beta_2, \ldots, \beta_q, \beta_{12}, \beta_{13}, \ldots, \beta_{q-1q}, \delta_{12}, \delta_{13}, \ldots, \delta_{q-1q})^\top.$$

The information matrix for the model Equation (4.1) is given by

$$\mathbf{M}(\xi) = \sum_{i=1}^{m} r_i \mathbf{f_1}(\mathbf{x_{(i)}})\mathbf{f_1}^\top(\mathbf{x_{(i)}}). \tag{4.2}$$

In the next theorem, we obtain the A-optimal allocation ξ_a for the model Equation (4.1).

Theorem 4.1. *The design ξ_a that allocates weight $\dfrac{\sqrt{g_1(a,q)}}{\theta}$ to the support points $\mathbf{x} \longleftrightarrow (1, 0, \ldots, 0)$ and allocates weight $\dfrac{\sqrt{g_2(a,q)}}{\theta}$ to the support points $\mathbf{x} \longleftrightarrow (a, 1-a, 0, \ldots, 0)$ is the A-optimal allocation, where*

$$g_1(a, q) = 1 + \frac{q-1}{2}\frac{1}{a^2(1-a)^2},$$

$$g_2(a, q) = \frac{2a^2 + 1 - 2a}{2a^2(1-a)^2(1-2a)^2},$$

and

$$\theta = q\sqrt{g_1(a,q)} + 2\binom{q}{2}\sqrt{g_2(a,q)}.$$

Proof. The information matrix of model Equation (4.1) for the design ξ_a is given by

$$\mathbf{M}(\xi_a) = \begin{bmatrix} a_1\mathbf{U_1} + a_2\mathbf{U_2} & \dfrac{a_2}{2}\mathbf{V_1^\top} + 0\mathbf{V_2^\top} & a_3\mathbf{X_1}^\top \\ \dfrac{a_2}{2}\mathbf{V_1} + 0\mathbf{V_2} & \dfrac{a_2^2}{2r_2}\mathbf{W_1} & \mathbf{0} \\ a_3\mathbf{X_1} & \mathbf{0} & a_4\mathbf{W_1} \end{bmatrix}, \tag{4.3}$$

where $\mathbf{0}$ is a $\binom{q}{2} \times \binom{q}{2}$ square matrix having each entry equal to 0. Here the coefficients are given by

$$\left.\begin{array}{l} a_1 = r_1 + (q-1)(1+2a(a-1))r_2 \\ a_2 = -2a(a-1)r_2 \\ a_3 = a(a-1)(1-2a)^2 r_2 \\ a_4 = 2a^2(1-3a+2a^2)^2 r_2 \end{array}\right\}. \tag{4.4}$$

The computation of the inverse of the information matrix i.e., $\mathbf{M}^{-1}(\xi_a)$ for the model Equation (4.1) is a quite difficult job. Thus, we compute $Trace(\mathbf{M}^{-1}(\xi_a))$ by considering the sum of the variance of least square estimates of the unknown parameters of the cubic model without a 3-way effect. The least square estimate (LSE) of the parameters of the cubic model without a 3-way effect [2,6] based on design ξ_a are

$$\left.\begin{array}{l} \hat{\beta}_i = \hat{\eta}_i; \quad i = 1, 2, \ldots, q, \\ \hat{\beta}_{ij} = -\dfrac{1}{2a(1-a)}(\hat{\eta}_i + \hat{\eta}_j) + \dfrac{1}{2a(1-a)}(\hat{\eta}_{ij} + \hat{\eta}_{ji}), \quad i < j, \\ \hat{\delta}_{ij} = \dfrac{1}{2a(1-a)}(\hat{\eta}_j - \hat{\eta}_i) + \dfrac{1}{2a(1-a)(1-2a)}(\hat{\eta}_{ji} - \hat{\eta}_{ij}), \quad i < j \end{array}\right\}, \tag{4.5}$$

where η_i is response to $x_i = 1$, $x_j = 0$, $j \neq i$; $i = 1, 2, \ldots, q$; η_{ij} is response to $x_i = a$, $x_j = 1 - a$, $x_k = 0$, $k \neq i, j$; $i \neq j$.

The variances of the LSEs given in Equation (4.5) are

$$\left.\begin{array}{l} var(\hat{\beta}_i) = \dfrac{\sigma^2}{r_1}, \\ var(\hat{\beta}_{ij}) = \dfrac{1}{2a^2(1-a)^2}\left(\dfrac{1}{r_1} + \dfrac{1}{r_2}\right)\sigma^2, \\ var(\hat{\delta}_{ij}) = \left(\dfrac{1}{2a^2(1-a)^2}\dfrac{1}{r_1} + \dfrac{1}{2a^2(1-a)^2(1-2a)^2}\dfrac{1}{r_2}\right)\sigma^2 \end{array}\right\}. \tag{4.6}$$

Here the real-valued function $Trace(\mathbf{M}^{-1}(\xi_a))$ is proportional to the sum of the variances of LSEs as given in Equation (4.6). Hence, we get

$$\begin{aligned} T &= Trace(\mathbf{M}^{-1}(\xi_a)) \\ &= q var(\hat{\beta}_i) + \binom{q}{2} var(\hat{\beta}_{ij}) + \binom{q}{2} var(\hat{\delta}_{ij}) \\ &\propto q g_1(a,q)\frac{1}{r_1} + 2\binom{q}{2} g_2(a,q)\frac{1}{r_2}, \end{aligned} \tag{4.7}$$

where

$$g_1(a,q) = 1 + \frac{q-1}{2}\frac{1}{a^2(1-a)^2},$$

$$g_2(a,q) = \frac{2a^2+1-2a}{2a^2(1-a)^2(1-2a)^2}.$$

Now, the problem is to minimize Equation (4.7) subject to the restriction of weights

$$q r_1 + 2\binom{q}{2} r_2 = 1.$$

To solve this problem, we use the Lagrangian multiplier method and set the Lagrangian function as

$$\Psi = Trace(\mathbf{M}^{-1}(\xi_a)) + \lambda\left[q r_1 + 2\binom{q}{2} r_2 - 1\right].$$

By taking the partial derivatives of Ψ w.r.t r_1, r_2, and λ and set them equal to 0, we get

$$\left.\begin{array}{l} -\dfrac{qg_1(a,q)}{r_1^2}+\lambda q=0, \\ -2\binom{q}{2}g_2(a,q)\dfrac{1}{r_1^2}+2\lambda\binom{q}{2}=0, \\ qr_1+2\binom{q}{2}r_2-1=0 \end{array}\right\}. \tag{4.8}$$

Solving the system of Equation (4.8), we get

$$r_1=\frac{\sqrt{g_1(a,q)}}{\theta}, \quad r_2=\frac{\sqrt{g_2(a,q)}}{\theta}. \tag{4.9}$$

Hence the theorem is proved. □

Next, we find the optimal values of r_1, r_2 (rounded off to the fourth place of the decimal) and the corresponding value of the $Trace(\mathbf{M}^{-1}(\xi_a))$ for different values of a using Equations (4.7) and (4.9). These values are provided in Table 2 (Appendix I) for different values of q when $3 \leq q \leq 20$. From Table 2, we observe that the design $\xi_a\left(a=\dfrac{1-5^{-1/2}}{2}=0.276393\right)$ is a candidate design for the cubic model without a 3-way effect. Let us denote this design by ξ^*.

In the next theorem, we shall prove that the design ξ^* is the A-optimal design for the model Equation (4.1).

Theorem 4.2. *The design ξ^* is the A-optimal design for the cubic model without a three-way effect.*

Proof. We use appropriate Matlab code by following the steps of Algorithm 1 (Appendix I) and demonstrate numerically that

$$Max_{\mathbf{x}\in S^{q-1}}d(\mathbf{x},\xi^*)=Trace(\mathbf{M}^{-1}(\xi^*)).$$

We also find that equality hold at the support points of the design ξ^* only. The values of $Max_{\mathbf{x}\in S^{q-1}}d(\mathbf{x},\xi^*)$ for different values of q for $3 \leq q \leq 20$ are provided in column (11) of Table 2 (Appendix I). This proves that the design ξ^* is the A-optimal design for the model Equation (4.1) in the class of all designs Δ. □

In the next Section, we calculate the A-efficiency of the D-optimal design for different values of q to make a comparison between the A-optimal and D-optimal designs.

5. A-efficiency

Let us denote the A- and D-optimal designs for model Equation (4.1) by ξ_A^* and ξ_D^* respectively. To compare the efficiency, we compute the A- efficiency of the design ξ_D^* for various values of q. Here the A-efficiency of the design ξ_D^* is defined as

$$\Delta_A(\xi_D^*)=\frac{Trace(\mathbf{M}^{-1}(\xi_A^*))}{Trace(\mathbf{M}^{-1}(\xi_D^*))}.$$

These efficiency values are displayed in Table 1.

Table 1 shows that the A-efficiency of the D-optimal design continuously decreases as q increases except when $q = 4$. This indicates that ξ_A^* can significantly improve the ability of parameter estimation.

Table 1. Values of $\Delta_A(\xi_D^*)$ for the cubic model without a 3-way effect for various values of q.

q	$\Delta_A(\xi_D^*)$
3	99.31%
4	99.99%
5	99.58%
7	98.08%
10	95.91%
12	94.70%
15	93.21%
20	91.32%
30	88.84%
40	87.24%
50	86.09%

6. Conclusions

The present article obtains a saturated A-optimal design for the cubic model without a 3-way effect with mixture experiment. It is established that the support points of the corresponding D-optimal design are the support points of A-optimal design. Further, the A-optimal design has higher efficiency than the corresponding D-optimal design and this increase in efficiency becomes significant as the number of mixture components increases. For the three-component mixture, we also examine that the derived A-optimal design for the cubic model without a three-way effect are similar to the result obtained by Panda and Sahoo [16].

Finding D- and A-optimal designs for the quartic mixture polynomial model will be interesting. Work in this direction is currently under progess, and we hope to report these findings in a future paper.

Acknowledgements

The author is very grateful to the editor and two anonymous referees for their valuable suggestions.

Author contributions. Not applicable.

Conflict of interest statement. There is no conflict of interest.

Funding. No funding.

Data availability. Not applicable.

References

[1] M.L. Aggrawal, P. Singh and M.K. Panda, *A-optimal designs for an additive cubic model*, Stat. Probab. Lett. **81** (2), 259-266, 2011.

[2] J.A. Cornell, *Experiments with Mixtures: Designs, Models, and the Analysis of Mixture Data*, John Wiley & Sons, New York, 2002.

[3] R.H. Farrell, J. Kiefer and J. Walbran, *Optimum multivariate designs*, Proc. 5th Berkeley Symp. Math. Stat. Probab. **1**, 113-139, University of California Press, 1967.

[4] V.V. Fedorov, *Design of experiments for linear optimality criteria*, Theory Probab. Appl. **16** (1), 189-195, 1971.
[5] P. Goos and M. Vandebroek, *D-optimal response surface designs in the presence of random block effects*, Comput. Stat. Data Anal. **37** (4), 433-453, 2001.
[6] J.W. Gorman and J. Hinman, *E Simplex lattice designs for multicomponent systems*, Technometrics **4** (4), 463-487, 1962.
[7] J. Kiefer, *Optimal designs in regression problems II*, Ann. Math. Stat. **32** (1), 298-325, 1961.
[8] J. Kiefer, *General equivalence theory for optimum designs (approximate theory)*, Ann. Statist. **2**, 849-879, 1974.
[9] T. Klein, *Invariant symmetric block matrices for the design of mixture experiments*, Linear Algebra Appl. **388**, 261-278, 2004.
[10] Y.B. Lim, *D-optimal design for cubic polynomial regression on the q-simplex*, J. Stat. Plan. Infer. **25** (2), 141-152, 1990.
[11] F. Mikaeili, *D-optimum design for cubic without 3-way effect on the simplex*, J. Stat. Plan. Infer. **21** (1), 107-115, 1989.
[12] F. Mikaeili, *D-optimum design for full cubic on q-simplex*, J. Stat. Plan. Infer. **35** (1), 121-130, 1993.
[13] M. Pal and N.K. Mandal, *Optimum designs for parameter estimation in mixture experiments with group synergism*, Commun. Stat. Theory Methods **50** (9), 2001-2014, 2021.
[14] M.K. Panda, *R-optimal designs for canonical polynomial models with mixture experiments*, Calcutta Stat. Assoc. Bull. **73** (2), 146-161, 2021.
[15] M.K. Panda and R.P. Sahoo, *D-optimal designs for Scheffès quadratic mixture model with spline involving two insensitive components*, Int. J. Stat. Reliab. Eng. **9** (1), 108-117, 2022a.
[16] M.K. Panda and R.P. Sahoo, *A-optimal designs for cubic polynomial models with mixture experiments in three components*, Stat. Appl. **20** (2), 41-55, 2022b.
[17] M.K. Panda and R.P. Sahoo, *R-optimal designs for linear log contrast model with mixture experiments*, Commun. Stat. Theory Methods **53** (7), 2355-2368, 2024.
[18] H. Scheffé, *Experiments with mixtures*, J. R. Stat. Soc. Ser. B. **20** (2), 344-360, 1958.
[19] P. Singh and M.K. Panda, *Optimal design for second degree K-model for mixture experiments based on weighted simplex centroid design*, Metron **69** (3), 251-263, 2011.
[20] X. Zhu and H. Hao, *A-optimal design for the special cubic mixture model*, Commun. Stat. Theory Methods **53** (3), 1081-1090, 2024.

APPENDIX I

Algorithm 1. Algorithm to demonstrate Equivalence theorem
Input:

Step 1. Set the value of q and $a = 0.276393$.
Step 2. Input the values of r_1 from Column (4) and r_2 from Column (7) using Table 2 for the value $a = 0.276393$.
Step 3. Input the column vector

$$\mathbf{f_1}(\mathbf{x}) = (x_1, x_2, \ldots, x_q, x_1x_2, x_1x_3, \ldots, x_{q-1}x_q, x_1x_2(x_1 - x_2),$$

$$x_1x_3(x_1 - x_3), \ldots, x_{q-1}x_q(x_{q-1} - x_q))^\top,$$

$$\mathbf{1}_q = (1, \ldots, 1)^\top.$$

Step 4. Read the matrices $\mathbf{U_1} = \mathbf{I_q}$, $\mathbf{W_1} = \mathbf{I}_{\binom{\mathbf{q}}{\mathbf{2}}}$, $\mathbf{U_2} = \mathbf{1_q}\mathbf{1_q}^\top - \mathbf{I_q}$,

$$\mathbf{V_1} = \sum_{\substack{i,j=1\\ i<j}}^{\mathbf{q}} \mathbf{E_{ij}}(\mathbf{e}_i + \mathbf{e}_j)^\top,$$

$$\mathbf{V_2} = \sum_{\substack{i,j=1\\ i<j}}^{\mathbf{q}} \sum_{\substack{k=1\\ k\notin\{i,j\}}}^{q} \mathbf{E_{ij}}\mathbf{e}_k^\top,$$

$$\mathbf{X_1} = \sum_{\substack{i,j=1\\ i<j}}^{\mathbf{q}} \mathbf{E_{ij}}(\mathbf{e}_j - \mathbf{e}_i)^\top.$$

Computation:

Step 5. Determine the values of a_1, a_2, a_3, and a_4 by using the following formulae:

$$a_1 = r_1 + (q-1)(1 + 2a(a-1))r_2,$$
$$a_2 = -2a(a-1)r_2,$$
$$a_3 = a(a-1)(1-2a)^2 r_2,$$
$$a_4 = 2a^2(1 - 3a + 2a^2)^2 r_2.$$

Step 6. Obtain the matrix

$$\mathbf{M}(\xi_a) = \begin{bmatrix} a_1\mathbf{U_1} + a_2\mathbf{U_2} & \frac{a_2}{2}\mathbf{V_1}^\top + 0\mathbf{V_2}^\top & a_3{\mathbf{X_1}}^\top \\ \frac{a_2}{2}\mathbf{V_1} + 0\mathbf{V_2} & \frac{a_2^2}{2r_2}\mathbf{W_1} & \mathbf{0} \\ a_3\mathbf{X_1} & \mathbf{0} & a_4\mathbf{W_1} \end{bmatrix}.$$

Step 7. Find the functional form $d(\mathbf{x}, \xi^*)$ where $\mathbf{d}(\mathbf{x}, \xi) = \mathbf{f}^\top(\mathbf{x})\mathbf{M}^{-\mathbf{2}}(\xi)\mathbf{f}(\mathbf{x})$.
Step 8. Estimate the value of $d(\mathbf{x}, \xi^*)$ at the support points of the design ξ^*.
Step 9. Find $Max_{x\in S^{q-1}} d(\mathbf{x}, \xi^*)$.

Table 2. Optimal values of r_1, r_2, Trace$[M^{-1}(\xi_a)]$, and $Max_{x\in S^{q-1}}d(\mathbf{x},\boldsymbol{\xi}^*)$ based on the A-optimality criterion.

(1)	**(2)**	**(3)**	**(4)**	**(5)**	**(6)**	**(7)**	**(8)**	**(9)**	**(10)**	**(11)**
q	a	n_1	r_1	n_1r_1	n_2	r_2	n_2r_2	n	Trace$[M^{-1}(\xi_a)]$	$Max_{x\in S^{q-1}}d(\mathbf{x},\boldsymbol{\xi}^*)$
3	0.01	3	0.1373	0.4119	6	0.098	0.588	9	541680.92	2708.1
	0.05	3	0.1337	0.4011	6	0.0998	0.5988	9	24850.52	
	0.1	3	0.1285	0.3855	6	0.1024	0.6144	9	7539	
	0.2	3	0.1141	0.3423	6	0.1096	0.6576	9	3072.69	
	*0.276393	3	0.0979	0.2937	6	0.1177	0.7062	9	2708.09	
	0.33	3	0.0815	0.2445	6	0.1259	0.7554	9	3194.52	
	0.4	3	0.0559	0.1677	6	0.1387	0.8322	9	5866.44	
	0.45	3	0.0309	0.0927	6	0.1512	0.9072	9	18037.5	
	0.49	3	0.0067	0.0201	6	0.1633	0.9798	9	375443.08	
4	0.01	4	0.0909	0.3636	12	0.053	0.636	16	1.8517×10^6	9663.7
	0.05	4	0.0883	0.3532	12	0.0539	0.6468	16	85285.46	
	0.1	4	0.0845	0.338	12	0.0552	0.6624	16	26017.24	
	0.2	4	0.0744	0.2976	12	0.0585	0.702	16	10767.32	
	*0.276393	4	0.0631	0.2524	12	0.0623	0.7476	16	9663.68	
	0.33	4	0.052	0.208	12	0.066	0.792	16	11618	
	0.4	4	0.0351	0.1404	12	0.0716	0.8592	16	21985.81	
	0.45	4	0.0191	0.0764	12	0.077	0.924	16	69604.85	
	0.49	4	0.0041	0.0164	12	0.082	0.984	16	1.49018×10^6	
5	0.01	5	0.0662	0.331	20	0.0334	0.668	25	4.65444×10^6	25021.43
	0.05	5	0.0643	0.3215	20	0.0339	0.678	25	214974.27	
	0.1	5	0.0614	0.307	20	0.0346	0.692	25	65838.9	
	0.2	5	0.0657	0.3285	20	0.0336	0.672	25	1.20456×10^6	
	*0.276393	5	0.0452	0.226	20	0.0387	0.774	25	25021.42	
	0.33	5	0.037	0.185	20	0.0407	0.814	25	30454.69	
	0.4	5	0.0247	0.1235	20	0.0438	0.876	25	58730.21	
	0.45	5	0.0134	0.067	20	0.0466	0.932	25	189277	
	0.49	5	0.0028	0.014	20	0.0493	0.986	25	4.12063×10^6	

	0.01	6	0.0511	0.3066	30	0.0231	0.693	36	9.75318×10^6	
	0.05	6	0.0495	0.297	30	0.0234	0.702	36	451409.14	
	0.1	6	0.0472	0.2832	30	0.0239	0.717	36	138664.42	
	0.2	6	0.041	0.246	30	0.0251	0.753	36	58473.41	
6	*0.276393	6	0.0345	0.207	30	0.0264	0.792	36	53603.29	53603.3
	0.33	6	0.028	0.168	30	0.0277	0.831	36	65825.11	
	0.4	6	0.0185	0.111	30	0.0296	0.888	36	128644.14	
	0.45	6	0.01	0.06	30	0.0313	0.939	36	419749.48	
	0.49	6	0.0022	0.0132	30	0.0329	0.987	36	9.24303×10^6	
	0.01	7	0.0412	0.2884	42	0.0169	0.7098	49	1.81077×10^7	
	0.05	7	0.0398	0.2786	42	0.0172	0.7224	49	839468.86	
	0.1	7	0.0379	0.2653	42	0.0175	0.735	49	258483.15	
	0.2	7	0.0329	0.2303	42	0.0183	0.7686	49	109696.08	
7	*0.276393	7	0.0275	0.1925	42	0.0192	0.8064	49	101264.61	101264.6
	0.33	7	0.0222	0.1554	42	0.0201	0.8442	49	125204.2	
	0.4	7	0.0146	0.1022	42	0.0214	0.8988	49	247173.06	
	0.45	7	0.0078	0.0546	42	0.0225	0.945	49	813967.75	
	0.49	7	0.0016	0.0112	42	0.0235	0.987	49	1.80756×10^7	
	0.01	8	0.034	0.272	56	0.013	0.728	64	3.08316×10^7	
	0.05	8	0.0329	0.2632	56	0.0132	0.7392	64	1.43128×10^6	
	0.1	8	0.0313	0.2504	56	0.0134	0.7504	64	441572.17	
	0.2	8	0.027	0.216	56	0.014	0.784	64	188374.89	
8	*0.276393	8	0.0225	0.18	56	0.0146	0.8176	64	174881.29	174881.3
	0.33	8	0.0181	0.1448	56	0.0153	0.8568	64	217407.97	
	0.4	8	0.012	0.096	56	0.0161	0.9016	64	432645.07	
	0.45	8	0.0063	0.0504	56	0.017	0.952	64	1.43509×10^6	
	0.49	8	0.0013	0.0104	56	0.0177	0.9912	64	3.20784×10^7	
	0.01	9	0.0288	0.2592	72	0.0103	0.7416	81	4.91897×10^7	
	0.05	9	0.0278	0.2502	72	0.0104	0.7488	81	2.28612×10^6	
	0.1	9	0.0264	0.2376	72	0.0106	0.7632	81	706465.16	
	0.2	9	0.0228	0.2052	72	0.011	0.792	81	302698.93	
9	*0.276393	9	0.019	0.171	72	0.0115	0.828	81	282340.29	282340.3

	0.33	9	0.0152	0.1368	72	0.012	0.864	81	352583.53	
	0.4	9	0.01	0.09	72	0.0126	0.9072	81	706257.02	
	0.45	9	0.0054	0.0486	72	0.0132	0.9504	81	2.35648×10^6	
	0.49	9	0.0011	0.0099	72	0.0138	0.9936	81	5.29534×10^7	
10	0.01	10	0.0248	0.248	90	0.0084	0.756	100	7.45967×10^7	432531.9
	0.05	10	0.0239	0.239	90	0.0085	0.765	100	3.47031×10^6	
	0.1	10	0.0227	0.227	90	0.0086	0.774	100	1.07393×10^6	
	0.2	10	0.0196	0.196	90	0.0089	0.801	100	461870.9	
	*0.276393	10	0.0162	0.162	90	0.0093	0.837	100	432531.89	
	0.33	10	0.013	0.13	90	0.0097	0.873	100	542201	
	0.4	10	0.0085	0.09	90	0.0102	0.918	100	1.09206×10^6	
	0.45	10	0.0045	0.05	90	0.0106	0.954	100	3.66164×10^6	
	0.49	10	0.0009	0.01	90	0.011	0.99	100	8.2644×10^7	
11	0.01	11	0.0217	0.2387	110	0.0069	0.759	121	1.08615×10^8	635343.5
	0.05	11	0.0209	0.2299	110	0.007	0.77	121	5.05719×10^6	
	0.1	11	0.0199	0.2189	110	0.0071	0.781	121	1.56694×10^6	
	0.2	11	0.017	0.187	110	0.0074	0.814	121	676099.37	
	*0.276393	11	0.014	0.154	110	0.0076	0.836	121	635343.49	
	0.33	11	0.0113	0.1243	110	0.008	0.88	121	799047.08	
	0.4	11	0.0073	0.0803	110	0.0084	0.924	121	1.61697×10^6	
	0.45	11	0.0039	0.0429	110	0.0087	0.957	121	5.44426×10^6	
	0.49	11	0.0008	0.0088	110	0.0091	1.001	121	1.23335×10^8	
12	0.01	12	0.0191	0.2292	132	0.0059	0.7788	144	1.52955×10^8	901654.4
	0.05	12	0.0184	0.2208	132	0.0059	0.7788	144	7.12701×10^6	
	0.1	12	0.0175	0.21	132	0.006	0.792	144	2.21067×10^6	
	0.2	12	0.0175	0.21	132	0.006	0.792	144	2.21067×10^6	
	*0.276393	12	0.0123	0.1476	132	0.0065	0.858	144	901654.39	
	0.33	12	0.0099	0.1188	132	0.0066	0.8712	144	1.13722×10^6	
	0.4	12	0.0064	0.0768	132	0.007	0.924	144	2.31071×10^6	
	0.45	12	0.0034	0.0408	132	0.0073	0.9636	144	7.80814×10^6	
	0.49	12	0.0008	0.0096	132	0.0075	0.99	144	1.77454×10^8	

	0.01	13	0.017	0.221	156	0.005	0.78	169	2.0947×10^8	
	0.05	13	0.0169	0.2197	156	0.005	0.78	169	5.43339×10^7	
	0.1	13	0.0157	0.2041	156	0.0051	0.7956	169	3.03247×10^6	
	0.2	13	0.0133	0.1729	156	0.0053	0.8268	169	1.31555×10^6	
13	*0.276393	13	0.011	0.143	156	0.0055	0.858	169	1.24333×10^6	1.2434×10^6
	0.33	13	0.0088	0.1144	156	0.0057	0.8892	169	1.57212×10^6	
	0.4	13	0.0057	0.0741	156	0.006	0.936	169	3.20588×10^6	
	0.45	13	0.003	0.039	156	0.0061	0.9516	169	1.08672×10^7	
	0.49	13	0.0006	0.0078	156	0.0063	0.9828	169	2.47667×10^8	
	0.01	14	0.0154	0.2156	182	0.0043	0.7826	196	2.80162×10^8	
	0.05	14	0.0148	0.2072	182	0.0044	0.8008	196	1.3071×10^7	
	0.1	14	0.0141	0.1974	182	0.0044	0.8008	196	4.06186×10^6	
	0.2	14	0.012	0.168	182	0.0046	0.8372	196	1.76617×10^6	
14	*0.276393	14	0.0098	0.1372	182	0.0048	0.8736	196	1.67322×10^6	1.6733×10^6
	0.33	14	0.0079	0.1106	182	0.0049	0.8918	196	2.12046×10^6	
	0.4	14	0.0051	0.0714	182	0.0051	0.9282	196	4.33788×10^6	
	0.45	14	0.0026	0.0364	182	0.0053	0.9646	196	1.47456×10^7	
	0.49	14	0.0005	0.007	182	0.0055	1.001	196	3.36885×10^8	
	0.01	15	0.0139	0.2085	210	0.0038	0.798	225	3.67175×10^8	
	0.05	15	0.0134	0.201	210	0.0038	0.798	225	1.71399×10^7	
	0.1	15	0.0127	0.1905	210	0.0039	0.819	225	5.33052×10^6	
	0.2	15	0.0108	0.162	210	0.004	0.84	225	2.32262×10^6	
15	*0.276393	15	0.0089	0.1335	210	0.0042	0.882	225	2.20516×10^6	2.206×10^6
	0.33	15	0.0071	0.1065	210	0.0043	0.903	225	2.80024×10^6	
	0.4	15	0.0046	0.069	210	0.0045	0.945	225	5.74494×10^6	
	0.45	15	0.0024	0.036	210	0.0046	0.966	225	1.95774×10^7	
	0.49	15	0.0005	0.0075	210	0.0048	1.008	225	4.48259×10^8	
	0.01	16	0.0127	0.2032	240	0.0034	0.816	256	4.72795×10^8	
	0.05	16	0.0123	0.1968	240	0.0034	0.816	256	2.20813×10^7	
	0.1	16	0.0117	0.1872	240	0.0034	0.816	256	6.87227×10^6	
	0.2	16	0.0099	0.1584	240	0.0035	0.84	256	3.00005×10^6	
16	*0.276393	16	0.0081	0.1296	240	0.0037	0.888	256	2.85396×10^6	2.854×10^6

	0.33	16	0.0065	0.104	240	0.0037	0.888	256	3.63077×10^6	
	0.4	16	0.0041	0.0656	240	0.0039	0.936	256	7.46811×10^6	
	0.45	16	0.0021	0.0336	240	0.0041	0.984	256	2.55068×10^7	
	0.49	16	0.0004	0.0064	240	0.0042	1.008	256	5.85179×10^8	
17	0.01	17	0.0117	0.1989	272	0.0029	0.7888	289	5.99454×10^8	3.636×10^6
	0.05	17	0.0112	0.1904	272	0.003	0.816	289	2.80096×10^7	
	0.1	17	0.0107	0.1819	272	0.003	0.816	289	8.72308×10^6	
	0.2	17	0.0091	0.1547	272	0.0031	0.8432	289	3.81461×10^6	
	*0.276393	17	0.0074	0.1258	272	0.0032	0.8704	289	3.63539×10^6	
	0.33	17	0.006	0.102	272	0.0033	0.8976	289	4.63263×10^6	
	0.4	17	0.0038	0.0646	272	0.0035	0.952	289	9.55126×10^6	
	0.45	17	0.002	0.034	272	0.0036	0.9792	289	3.26884×10^7	
	0.49	17	0.0004	0.0068	272	0.0037	1.0064	289	7.5128×10^8	
18	0.01	18	0.0108	0.1944	306	0.0026	0.7956	324	7.49723×10^8	4.566×10^6
	0.05	18	0.0104	0.1872	306	0.0027	0.8262	324	3.50457×10^7	
	0.1	18	0.0098	0.1764	306	0.0027	0.8262	324	1.0921×10^7	
	0.2	18	0.0083	0.1494	306	0.0028	0.8568	324	4.78341×10^6	
	*0.276393	18	0.0068	0.1224	306	0.0029	0.8874	324	4.56621×10^6	
	0.33	18	0.0054	0.0972	306	0.003	0.918	324	5.82772×10^6	
	0.4	18	0.0035	0.063	306	0.0031	0.9486	324	1.20411×10^7	
	0.45	18	0.0018	0.0324	306	0.0032	0.9792	324	4.12864×10^7	
	0.49	18	0.0003	0.0054	306	0.0033	1.0098	324	9.50436×10^8	
19	0.01	19	0.0099	0.1881	342	0.0024	0.8208	361	9.26317×10^8	5.665×10^6
	0.05	19	0.0095	0.1805	342	0.0024	0.8208	361	4.33175×10^7	
	0.1	19	0.009	0.171	342	0.0025	0.855	361	1.35064×10^7	
	0.2	19	0.0077	0.1463	342	0.0025	0.855	361	5.92452×10^6	
	*0.276393	19	0.0063	0.1197	342	0.0026	0.8892	361	5.66414×10^6	
	0.33	19	0.005	0.095	342	0.0027	0.9234	361	7.2392×10^6	
	0.4	19	0.0032	0.0608	342	0.0028	0.9576	361	1.4987×10^7	
	0.45	19	0.0017	0.0323	342	0.0028	0.9576	361	5.14754×10^7	
	0.49	19	0.0003	0.0057	342	0.0029	0.9918	361	1.18676×10^9	

	0.01	20	0.0093	0.186	380	0.00214	0.8132	400	1.13209×10^9	
	0.05	20	0.0089	0.178	380	0.0022	0.836	400	5.29593×10^7	
	0.1	20	0.0084	0.168	380	0.0022	0.836	400	1.65214×10^7	
	0.2	20	0.0071	0.142	380	0.0023	0.874	400	7.25699×10^6	
20	*0.276393	20	0.0058	0.116	380	0.0023	0.874	400	6.94789×10^6	6.948×10^6
	0.33	20	0.0046	0.092	380	0.0024	0.912	400	8.89153×10^6	
	0.4	20	0.0029	0.058	380	0.0025	0.95	400	1.84415×10^7	
	0.45	20	0.0015	0.03	380	0.0026	0.988	400	6.344×10^7	
	0.49	20	0.0004	0.008	380	0.0026	0.988	400	1.46462×10^9	

* Corresponding D-optimal design $\xi_a \left(a = \dfrac{1 - 5^{-1/2}}{2} = 0.276393\ldots \right)$.