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A-optimal Designs for Cubic Polynomial Models with Mixture Experiments in Three Components

Mahesh Kumar Panda and Rushi Prasad Sahoo
Department of Statistics, Central University of Odisha, Koraput 763004

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Abstract

This article discusses A-optimal minimum support designs for the three different forms of cubic polynomial mixture models *i.e.* full cubic, cubic without 3-way effect, and special cubic mixture models in three ingredients. The necessary and sufficient conditions for the proposed designs have been confirmed by the equivalence theorem.

Key words: A-optimal design; Mixture models; Equivalence theorem.

AMS Subject Classification: 62K05

1. Introduction

The importance of mixture experiments is increasing gradually, because it is utilized in many disciplines such as pharmaceutical science, food science, chemical science, and textile science, *etc*. Let us consider a mixture experiment having q ingredients with mixture proportions denoted by $x_1, x_2, ..., x_q$ then the factor space consisting of these ingredient proportions can be represented by a $(q-1)-$dimensional set χ given by

$$\chi = \left\{ \boldsymbol{x} = (x_1, x_2, ..., x_q)' \in R^q \mid \sum_{i=1}^{q} x_i = 1,\ 0 \le x_i \le 1,\ i = 1, 2, ..., q \right\}. \tag{1}$$

Let the observed response may be represented as $y = \eta(\boldsymbol{x}) + \varepsilon(\boldsymbol{x})$, where $\eta(\boldsymbol{x})$ is the expected response and $\varepsilon(\boldsymbol{x})$ is the random error observed at $\boldsymbol{x}$. We also assume that $\varepsilon(\boldsymbol{x})$ are *i.i.d.* random variables with mean 0 and variance σ^2. To describe the relationship between the response of interest and the ingredient proportions, in any mixture experiment, various mixture models have already been introduced in the literature *e.g.* Scheffè's canonical polynomial models, Becker's models, log contrast models, *etc*. Among these models, the canonical polynomial models are frequently used for the analysis of mixture data related to real-life problems.

In general, the optimal designs are constructed based on a certain optimality criterion to make the predicted response closer to the mean response over a certain region of interest. For the pioneering work on optimal designs for mixture experiments, one can refer to the work of Kiefer and Wolfowitz (1959), and Kiefer (1961). Afterward, many researchers have put their attention towards the discipline of optimal designs for mixture experiments [see Aggrawal *et*

Corresponding Author: Mahesh Kumar Panda
E-mail: mahesh2123ster@gmail.com

al. (2011), Singh and Panda (2011), Goos and Syafitri (2014), Mandal and Pal (2017), and Pal and Mandal (2021), *etc*.].

Kiefer (1961) obtained D-optimal designs for Scheffè's models of degrees one, two, and three. For Scheffè's linear model in q mixture ingredients, a saturated design that assigns a weight $1/q$ to each vertex of the simplex region is a D-optimal design. Again a minimum-point design supported by points of $\{q, 2\}$ simplex-lattice with equal mass assigned to each support point is D-optimum for Scheffè's quadratic mixture model. Kiefer (1961) obtained the saturated D-optimal designs for the full cubic model, the cubic model without 3-way effect, and the special cubic model when $q = 3$. Later on, Mikaeili (1989) obtained the D-optimal designs for the cubic model without 3-way effect. Farrell *et al*. (1967) and Lim (1990) derived the D-optimal designs for the general cubic polynomial model with two and three mixture components respectively. Mikaeli (1993) investigated the D-optimal designs for the full cubic model on the set χ.

For Scheffè's cubic canonical polynomial model in this effect, we see that most of the existing works focus solely on D-optimality. However, to date, no research work has been done concerning the A-optimal designs for the cubic polynomial models and it was still an open problem. The advantage of D-optimal design is that all the support points involved are associated with equal weight whereas in the case of A-optimality, the weights associated with different support points, in general, are different. Again, the weights vary when the number of mixture components varies. Thus, obtaining an A-optimal design for all the different forms of cubic mixture canonical polynomial models is comparatively much more complicated in comparison to the D-optimal design. In this article, we study the problem of finding A-optimal minimum support designs for the three different forms of cubic polynomial mixture models in three ingredients.

The article is structured as follows. In Section 2, a brief discussion on the A-optimal design and equivalence theorem is presented. Section 3 obtains A-optimal designs for the three different forms of the cubic model of mixture experiments *i.e.* full cubic model, cubic model without 3-way effect, and special cubic model when $q = 3$. The article ends with some discussions and conclusions in Section 4.

2. A-Optimal Design and Equivalence Theorem

Let us consider a regression model of the form

$$\eta(\boldsymbol{x}) = \boldsymbol{f}'(\boldsymbol{x})\boldsymbol{\beta}, \; \boldsymbol{x} \in \chi, \tag{2}$$

where $\eta(\boldsymbol{x})$ denotes the expected response, $\boldsymbol{x}$ is the input variable, and $\boldsymbol{f}(\boldsymbol{x})$ is the regression function.

Again, let us consider an approximate design (Kiefer, 1974) of the following form

$$\xi = \begin{Bmatrix} \boldsymbol{x}_{(1)} & \dots & \boldsymbol{x}_{(m)} \\ r_1 & \dots & r_m \end{Bmatrix}, \quad \boldsymbol{x}_{(i)} \in \chi, \quad 0 < r_i < 1, \; \sum_{i=1}^{m} r_i = 1,$$

where $\boldsymbol{x}_{(1)},...,\boldsymbol{x}_{(m)}$ are different design points over χ and r_i is the weight assigned to the point $\boldsymbol{x}_{(i)}$, $i=1,2,...,m$. Denote Δ as the set of all approximate designs with non-singular information matrix

$$\boldsymbol{M}(\xi)=\sum_{i=1}^{m} r_i \boldsymbol{f}(\boldsymbol{x}_{(i)})\boldsymbol{f}'(\boldsymbol{x}_{(i)})$$

on χ.

Definition 1: A design $\xi^* \in \Delta$ with an information matrix $\boldsymbol{M}(\xi)$ for model (2) is called A-optimal design if it minimizes Trace $(\boldsymbol{M}^{-1}(\xi))$ over Δ.

Definition 2:A minimum support design for any regression model having p parameters is supported on exactly p distinct support points [see Goos and Vandebroek (2001)].

The following equivalence theorem established by Fedorov (1971) provides the necessary and sufficient conditions for the determination of A-optimal design over the simplex region χ.

Theorem 1: A design $\xi^* \in \Delta$ is A-optimal for model (2) if and only if

$$\underset{\boldsymbol{x}\in\chi}{Max}\; d(\boldsymbol{x},\xi^*) = \text{Trace}(\boldsymbol{M}^{-1}(\xi^*)) \tag{3}$$

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

Selection of support points: Kiefer (1961) considered the design ξ_a (for $0<a<1/2$) which puts equal mass $\frac{1}{10}$ on each of the vertices $x_i=1, x_j=x_k=0$; each of the six points $x_i=1-x_j=a, x_k=0$, and $x_1=x_2=x_3=1/3$. He proved that the design ξ_a for $a=(1-5^{-\frac{1}{2}})/2$ is D-optimum for the full cubic model when $q=3$. Similarly, he showed that the design ξ_a (excluding the point $x_1=x_2=x_3=1/3$) in which each point is supported by a mass $\frac{1}{9}$ is D-optimum for the cubic model without 3-way effect in three ingredients for $a=(1-5^{-\frac{1}{2}})/2$. Further, he showed that the simplex centroid design which assigns mass $\frac{1}{7}$ to each of the support points is D-optimum for the special cubic model when $q=3$. We, therefore, propose the following subclasses (D_1, D_2, D_3) of designs ξ_a to find the minimum support A-optimal design.

Model (Subclass)	x_1	x_2	x_3	Weight
Full Cubic Model (D_1)	1	0	0	r_1
	0	1	0	
	0	0	1	
	a	$1-a$	0	r_2
	a	0	$1-a$	
($0 < a < 1/2$)	0	a	$1-a$	
	$1-a$	a	0	
	$1-a$	0	a	
	0	$1-a$	a	
	1/3	1/3	1/3	r_3
Cubic Model without 3-way effect (D_2)	1	0	0	r_1
	0	1	0	
	0	0	1	
	a	$1-a$	0	r_2
	a	0	$1-a$	
($0 < a < 1/2$)	0	a	$1-a$	
	$1-a$	a	0	
	$1-a$	0	a	
	0	$1-a$	a	
Special Cubic Model (D_3)	1	0	0	r_1
	0	1	0	
	0	0	1	
	a	$1-a$	0	r_2
	a	0	$1-a$	
	0	a	$1-a$	
	1/3	1/3	1/3	r_3

Here we assume that a weight of r_1 is associated with each of the vertices, a weight of r_2 is associated with each of the design points $x_i = 1 - x_j = a$, $x_k = 0$ (for full cubic and cubic model without 3-way effect) and $x_i = a$, $x_k = 0$ (for special cubic), and finally a weight of r_3 is associated with each of the midpoints of 2-dimensional faces such that the total weights add to unity. We can concentrate on the above class of designs because the A-optimality criterion is invariant for all three components. Consequently, the optimum design will also be invariant *w.r.t* x_1, x_2, and x_3.

In the next section, we obtain the A-optimal designs for the three different forms of Scheffè's cubic polynomial model when q =3.

3. A-Optimal Designs for Cubic Models for Mixture Experiments

3.1. Full cubic model

The expected response for a full cubic model (see Cornell (2002)) can be represented as

$$\eta_1 = \boldsymbol{f}_1'(\boldsymbol{x})\boldsymbol{\beta}_1 = \sum_{i=1}^{q}\beta_i x_i + \sum_{i<j=1}^{q}\beta_{ij}x_i x_j + \sum\sum_{i<j}^{q}\delta_{ij}x_i x_j(x_i - x_j) + \sum\sum_{i<j<k}\sum\beta_{ijk}x_i x_j x_k \tag{4}$$

where $\boldsymbol{f}_1(\boldsymbol{x})$ and $\boldsymbol{\beta}_1$ are column vectors of length $\frac{q(q+1)(q+2)}{6}$ and are defined by

$$\boldsymbol{f}_1(\boldsymbol{x}) = \big(x_1, x_2, ..., x_q, x_1x_2, x_1x_3, ..., x_{q-1}x_q, x_1x_2(x_1 - x_2), .x_1x_3(x_1 - x_3),$$

$$..., x_{q-1}x_q(x_{q-1} - x_q), x_1x_2x_3, x_1x_2x_4, ..., x_{q-2}x_{q-1}x_q\big)';$$

$$\boldsymbol{\beta}_1 = \big(\beta_1, \beta_2, ..., \beta_q, \beta_{12}, \beta_{13}, ..., \beta_{q-1q}, \delta_{12}, \delta_{13}, ..., \delta_{q-1q}, \beta_{123}, \beta_{124}, ..., \beta_{q-2q-1q}\big)'.$$

The non-singular information matrix for the model (4) is given by

$$\boldsymbol{M}(\xi) = \sum_{i=1}^{m} r_i\, \boldsymbol{f}_1(\boldsymbol{x}_{(i)})\, \boldsymbol{f}_1'(\boldsymbol{x}_{(i)}) \tag{5}$$

The next theorem obtains the A-optimal minimum support design for model (4) when q = 3.

Theorem 2: For q = 3, the design ξ_1 with support points from {3, 3} simplex-lattice that assigns a weight of 0.0612 to the 3 vertices (1, 0, 0), (0, 1, 0), (0, 0, 1); a weight of 0.0933 to the 6 points (1/3, 2/3, 0), (1/3, 0, 2/3), (0, 1/3, 2/3), (2/3, 1/3, 0), (2/3, 0, 1/3), (0, 2/3, 1/3); and a weight of 0.2567 to the centroid point (1/3, 1/3, 1/3) is the A-optimal minimum support design for the full cubic polynomial model with mixture experiments on χ .

Proof: According to the equivalence theorem in equation (3), if ξ^* is the A-optimal design then the infimum of Trace $(\boldsymbol{M}^{-1}(\xi))$ and the supremum of $d(\boldsymbol{x}, \xi)$ both exists at the support points of ξ^*. Based on this result, we search for support points of A-optimal design *i.e.* Min Trace $(\boldsymbol{M}^{-1}(\xi))$ for the full cubic model over the subclass D_1 by considering different values of 'a' subject to the linear constraint that the sum of the weights is equal to 1.

Let us consider the proposed design ξ_a for the full cubic model given in Section 2. The inverse of the information matrix of the form (5) for the design ξ_a is

$$\boldsymbol{M}^{-1}(\xi_a) = \begin{pmatrix} \frac{1}{r_1}\boldsymbol{I}_3 & \boldsymbol{A}_1' & \boldsymbol{A}_2' & g_6\boldsymbol{1}_3 \\ \boldsymbol{A}_1 & g_2\boldsymbol{I}_3 + g_3\boldsymbol{J}_3 & \boldsymbol{A}_3' & g_4\boldsymbol{1}_3 \\ \boldsymbol{A}_2 & \boldsymbol{A}_3 & \boldsymbol{A}_4 & 0.\boldsymbol{1}_3 \\ g_6\boldsymbol{1}_3' & g_4\boldsymbol{1}_3' & 0.\boldsymbol{1}_3' & g_7 \end{pmatrix} \tag{6}$$

where

$$g_1 = \frac{1}{2ar_1(1-a)},\ g_2 = \frac{2r_1+r_2}{4a^2(1-a)^2 r_1 r_2},\ g_3 = \frac{1}{4a^2(1-a)^2 r_1},$$

$$g_4 = -\frac{3(r_1+2r_2(3a(a-1)+1))}{2a^2(1-a)^2 r_1 r_2},\ g_5 = \frac{r_1+(1-2a)^2 r_2}{2a^2(2a^2-3a+1)^2 r_1 r_2},$$

$$g_6 = \frac{3(3a^2-3a+1)}{ar_1(1-a)},\ g_7 = \frac{27\left(54a^2(a-1)^2 r_1 r_2 + (2r_2(3a(a-1)+1)^2 + r_1)r_3\right)}{2a^2(1-a)^2 r_1 r_2 r_3},$$

and $\boldsymbol{I}_3$ is the identity matrix of order 3, $\boldsymbol{J}_3$ is a matrix of order 3×3 in which each entry is 1, $\boldsymbol{1}_3$ is a column vector of order 3×1,

$$\boldsymbol{A}_1 = \begin{pmatrix} -g_1 & -g_1 & 0 \\ -g_1 & 0 & -g_1 \\ 0 & -g_1 & -g_1 \end{pmatrix},\qquad \boldsymbol{A}_2 = \begin{pmatrix} -g_1 & g_1 & 0 \\ -g_1 & 0 & g_1 \\ 0 & -g_1 & g_1 \end{pmatrix},$$

$$\boldsymbol{A}_3 = \begin{pmatrix} 0 & g_3 & -g_3 \\ g_3 & 0 & -g_3 \\ g_3 & -g_3 & 0 \end{pmatrix},\qquad \boldsymbol{A}_4 = \begin{pmatrix} g_5 & g_3 & -g_3 \\ g_3 & g_5 & g_3 \\ -g_3 & g_3 & g_5 \end{pmatrix}.$$

Next, the trace of $\boldsymbol{M}^{-1}(\xi_a)$ is obtained as

$$\text{Trace}\,(\boldsymbol{M}^{-1}(\xi_a)) = \frac{3\left(2 + \frac{r_1+r_2}{(a-1)^2 a^2 r_2} + \frac{r_1+(1-2a)^2 r_2}{a^2(1-3a+2a^2)^2 r_2}\right)}{2r_1}$$
$$+ 27\left(\frac{54(a-1)^2 a^2 r_1 r_2 + (r_1 + 2(3a(a-1)+1)^2 r_2) r_3}{2a^2(a-1)^2 r_1 r_2 r_3}\right) \tag{7}$$

Now, the problem becomes minimizing equation (7) subject to the restriction of weights $3r_1 + 6r_2 + r_3 = 1$. To solve this problem, we use the Lagrangian multiplier method and set the Lagrangian function as

$$\psi = \text{Trace}\ (\boldsymbol{M}^{-1}(\xi_a)) + \lambda(3r_1 + 6r_2 + r_3 - 1).$$

By taking the partial derivatives of ψ *w.r.t* r_1, r_2, r_3, and λ, and set them equal to 0, we get

$$\frac{3a(a-1)\big(a(a-1)(\lambda r_1^2-82)-54\big)-30}{a^2(a-1)^2 r_1^2}=0, \tag{8}$$

$$-\frac{3(11+40a(a-1))}{2a^2(2a^2-3a+1)^2 r_2^2}+6\lambda=0, \tag{9}$$

$$-\frac{729}{r_3^2}+\lambda=0, \tag{10}$$

$$3r_1+6r_2+r_3=1. \tag{11}$$

The algebraic derivations for solving equations (8) – (11) are lengthy and tedious, thus we numerically compute possible optimal values of r_1, r_2, r_3 (rounded off to the fourth place of the decimal) and the corresponding value of Trace$(\boldsymbol{M}^{-1}(\xi_a))$ for different values of a, which are tabulated in Table 1.

Table 1:Trace$(\boldsymbol{M}^{-1}(\xi_a))$ and corresponding weights of full cubic model for different values of a

a	r_1	r_2	r_3	Trace$(\boldsymbol{M}^{-1}(\xi_a))$
0.01	0.1581	0.0853	0.0137	3.8758×10^6
0.05	0.1407	0.0854	0.0654	170599.0
0.10	0.1213	0.0856	0.1224	48687.3
0.20	0.0902	0.0867	0.2095	16614.4
*0.28	0.0724	0.0891	0.2484	11819.3
**0.33	0.0612	0.0933	0.2567	11061.0
0.40	0.0471	0.1048	0.2297	13817.8
0.45	0.0306	0.1248	0.1591	28810.3
0.49	0.0080	0.1557	0.0419	414412.0

*Corresponding D-optimal design, $\left(a=\frac{1-5^{-1/2}}{2}=0.276...\right)$

* *Simplex lattice design (a = 1/3)

From Table 1, we observe that the support points of simplex lattice design *i.e.* ξ_1 are the possible support points of the A-optimal design for the full cubic model.

The next step is to prove the necessary and sufficient condition *i.e.* $\underset{x \in \chi}{\text{Max}}\ d(\boldsymbol{x}, \xi_1) =$ Trace$(\boldsymbol{M}^{-1}(\xi_1))$ has been established as (A1) in Appendix A. In this case, we obtain the value of $\boldsymbol{M}^{-1}(\xi_1)$ by substituting a = 1/3 in equation (6).

We now obtain the A-optimal design for the cubic model without 3-way effect.

3.2. Cubic model without 3-way effect

The expected response for a cubic model without 3-way effect (see Cornell (2002)) is as follows:

$$\eta_2 = \boldsymbol{f}_2'(\boldsymbol{x})\boldsymbol{\beta}_2 = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j=1}^{q} \beta_{ij} x_i x_j + \sum\sum_{i<j}^{q} \delta_{ij} x_i x_j (x_i - x_j) \tag{12}$$

where $\boldsymbol{f}_2(\boldsymbol{x})$ and $\boldsymbol{\beta}_2$ are column vectors of length q^2 and are defined by

$$\boldsymbol{f}_2(\boldsymbol{x}) = \big(x_1, x_2, ..., x_q, x_1x_2, x_1x_3, ..., x_{q-1}x_q, x_1x_2(x_1 - x_2), x_1x_3(x_1 - x_3), \\ ..., x_{q-1}x_q(x_{q-1} - x_q)\big)'$$

$$\boldsymbol{\beta}_2 = \big(\beta_1, \beta_2, ..., \beta_q, \beta_{12}, \beta_{13}, ..., \beta_{q-1q}, \delta_{12}, \delta_{13}, ..., \delta_{q-1q}\big)'.$$

The non-singular information matrix for the model (12) is given by

$$\boldsymbol{M}(\xi) = \sum_{\text{i}=1}^{m} r_{\text{i}}\, \boldsymbol{f}_2(\boldsymbol{x}_{(\text{i})})\, \boldsymbol{f}_2'(\boldsymbol{x}_{(\text{i})}) \tag{13}$$

In the next theorem, we obtain an A-optimal minimum support design for the model (12) when q = 3.

Theorem 3: For q =3, the design ξ_2 with support points from the corresponding D-optimal design that assigns a weight of 0.0980 to the vertices (1, 0, 0), (0, 1, 0), (0, 0, 1); a weight of 0.1177 to the 6 points (a, 1- a, 0), (a, 0, 1-a),(0,a, 1- a), (1- a, a, 0), (1- a, 0, a),(0, 1 - a, a), with $a = (1 - 5^{-\frac{1}{2}})/2$ is the A-optimal minimum support design for the cubic polynomial model without 3-way effect on χ .

Proof: Following the similar arguments in Theorem 2, we search for support points of A-optimal design *i.e.* Min Trace$(\boldsymbol{M}^{-1}(\xi))$ for the cubic model without 3-way effect over the subclass D_2. Here we consider the proposed design ξ_a for the cubic model without 3-way effect given in Section 2. The inverse of the information matrix of the form (13) for the design ξ_a is

$$\boldsymbol{M}^{-1}(\xi_a)=\begin{pmatrix}\frac{1}{r_1}\boldsymbol{I}_3 & \boldsymbol{A}_1' & \boldsymbol{A}_2' \\ \boldsymbol{A}_1 & g_2\boldsymbol{I}_3+g_3\boldsymbol{J}_3 & \boldsymbol{A}_3' \\ \boldsymbol{A}_2 & \boldsymbol{A}_3 & \boldsymbol{A}_4\end{pmatrix} \tag{14}$$

which is again a submatrix of the information matrix in equation (6). Next, the trace of $\boldsymbol{M}^{-1}(\xi_a)$ is obtained as

$$\text{Trace}\,(\boldsymbol{M}^{-1}(\xi_a))=\frac{(6a(a-1)+3)r_1+3(1-2a)^2(a^2(a-1)^2+1)r_2}{a^2(2a^2-3a+1)^2 r_1 r_2}. \tag{15}$$

Now, the problem becomes minimizing equation (15) subject to the restriction of weights $3r_1+6r_2=1$. To solve this problem, we use the Lagrangian multiplier method and set the Lagrangian function as

$$\psi=\text{Trace }(\boldsymbol{M}^{-1}(\xi_a))+\lambda(3r_1+6r_2-1)$$

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

$$-\frac{3(a^2(a-1)^2+1)}{a^2(a-1)^2 r_1^2}+3\lambda=0, \tag{16}$$

$$\frac{-3-6a(a-1)}{a^2(2a^2-3a+1)^2 r_2^2}+6\lambda=0, \tag{17}$$

$$3r_1+6r_2=1. \tag{18}$$

Next, by solving equations (16) – (18), we numerically compute possible optimal values of r_1, r_2 (rounded off to the fourth place of the decimal) and the corresponding value of Trace $(\boldsymbol{M}^{-1}(\xi_a))$ for different values of a, which are tabulated in Table 2.

Table 2: Trace $(\boldsymbol{M}^{-1}(\xi_a))$ and corresponding weights of cubic model without 3-way effect for different values of a

a	r_1	r_2	Trace $(\boldsymbol{M}^{-1}(\xi_a))$
0.01	0.1372	0.0980	541681.0
0.05	0.1337	0.0998	24850.5
0.10	0.1285	0.1024	7539.0
0.20	0.1142	0.1096	3072.7
*0.28	0.0980	0.1177	2708.1

**0.33	0.0815	0.1259	3194.5
0.40	0.0560	0.1387	5866.4
0.45	0.0310	0.1512	18037.5
0.49	0.0067	0.1633	375443.0

*Corresponding D-optimal design, $\left(a = \frac{1-5^{-1/2}}{2} = 0.276... \right)$

** Simplex lattice design (a = 1/3) excluding the centroid

From Table 2, we observe that the support points of the corresponding D-optimal design *i.e.* ξ_2 are the possible support points of the A-optimal design for the cubic model without 3-way effect.

The next step is to prove the necessary and sufficient condition *i.e.* $\underset{\boldsymbol{x} \in \chi}{\text{Max}}\ d(\boldsymbol{x}, \xi_2) =$ Trace$(\boldsymbol{M}^{-1}(\xi_2))$ has been established as (A2) in Appendix A. In this case, we obtain the value of $\boldsymbol{M}^{-1}(\xi_2)$ by substituting a =0.276393 in equation (14).

In the next part, we obtain the A-optimal minimum support design for a special cubic model.

3.3. Special cubic model

The expected response for the special cubic model (see Cornell (2002)) is as follows:

$$\eta_3 = \boldsymbol{f}_3'(\boldsymbol{x})\boldsymbol{\beta}_3 = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j=1}^{q} \beta_{ij} x_i x_j + \sum \sum_{i<j<k} \sum \beta_{ijk} x_i x_j x_k \tag{19}$$

where $\boldsymbol{f}_3(\boldsymbol{x})$ and $\boldsymbol{\beta}_3$ are column vectors of length $\frac{q(q^2+5)}{6}$ and are defined as

$$\boldsymbol{f}_3(\boldsymbol{x}) = \left(x_1, x_2, ..., x_q, x_1x_2, x_1x_3, ..., x_{q-1}x_q, x_1x_2x_3, x_1x_2x_4, ..., x_{q-2}x_{q-1}x_q\right)';$$

$$\boldsymbol{\beta}_3' = \left(\beta_1, \beta_2, ..., \beta_q, \beta_{12}, \beta_{13}, ..., \beta_{q-1q}, \beta_{123}, \beta_{124}, ..., \beta_{q-2q-1q}\right)'.$$

The non-singular information matrix for the model (19) is as follows:

$$\boldsymbol{M}(\xi) = \sum_{i=1}^{m} r_i \boldsymbol{f}_3(\boldsymbol{x}_{(i)}) \boldsymbol{f}_3'(\boldsymbol{x}_{(i)}) \tag{20}$$

The next theorem obtains the A-optimal minimum support design for the model (19) when q = 3.

Theorem 4: For q = 3, the weighted simplex-centroid design ξ_3 that assigns a weight of 0.0546 to the vertices (1, 0, 0), (0, 1, 0), (0, 0, 1); a weight of 0.1629 to the barycentre of depth 1 *i.e.*(1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2); and a weight of 0.3476 to the centroid point (1/3, 1/3, 1/3) is the A-optimal minimum support design for the special cubic polynomial model with mixture experiments on χ .

Proof: Following the similar arguments in Theorem 2, we search for support points of A-optimal design *i.e.* Min Trace $(\boldsymbol{M}^{-1}(\xi))$ for the special cubic model over the subclass D_3. Here we consider the proposed design ξ_a for the special cubic model given in Section 2. The inverse of the information matrix of the form (20) for the design ξ_a is

$$\boldsymbol{M}^{-1}(\xi_a)=\begin{pmatrix} \frac{1}{r_1}\boldsymbol{I}_3 & \boldsymbol{A}_1' & \boldsymbol{\alpha} \\ \boldsymbol{A}_1 & \boldsymbol{A}_2 & \boldsymbol{\rho} \\ \boldsymbol{\alpha}' & \boldsymbol{\rho}' & h_3 \end{pmatrix} \tag{21}$$

where

$$h_1=\frac{r_1+r_2(2a(a-1)+1)}{(a-1)^2a^2r_1r_2},\ h_2=\frac{1}{(a-1)^2r_1},h_3=-\frac{3[r_1+r_2(a(5a-4)+1)]}{a^2(a-1)^2r_1r_2},$$

$$h_3=\frac{27r_1+9[5+a(a-1)(27a(a-1)+26)]r_2}{a^2(a-1)^2r_1r_2}+\frac{729}{r_3},\ h_4=\frac{1}{ar_1(1-a)},h_5=\frac{1}{a^2r_1},$$

$$\boldsymbol{A}_1=\begin{pmatrix} \frac{1}{(a-1)r_1} & -\frac{1}{a\,r_1} & 0 \\ \frac{1}{(a-1)r_1} & 0 & -\frac{1}{a\,r_1} \\ 0 & \frac{1}{(a-1)r_1} & -\frac{1}{a\,r_1} \end{pmatrix},\boldsymbol{A}_2=\begin{pmatrix} h_1 & h_2 & h_4 \\ h_2 & h_1 & h_5 \\ h_4 & h_5 & h_1 \end{pmatrix},$$

$$\boldsymbol{\alpha}=\begin{pmatrix} \frac{3(1-3a)}{(a-1)r_1} \\ \frac{3(3a^2-3a+1)}{ar_1(1-a)} \\ \frac{3(2-3a)}{ar_1} \end{pmatrix},\ \text{and}\qquad \boldsymbol{\rho}=\begin{pmatrix} -\frac{3[r_1+r_2(a(5a-4)+1)]}{a^2(a-1)^2r_1r_2} \\ -\frac{3[r_1+r_2(7a(a-1)+2)]}{a^2(a-1)^2r_1r_2} \\ -\frac{3[r_1+r_2(a(5a-6)+2)]}{a^2(a-1)^2r_1r_2} \end{pmatrix}.$$

Next, the trace of $\boldsymbol{M}^{-1}(\xi_a)$ is obtained as

$$\text{Trace}\,(\boldsymbol{M}^{-1}(\xi_a))=\frac{729}{r_3}+\frac{30r_1+6[8+a(a-1)(41a(a-1)+40)]r_2}{a^2(a-1)^2r_1r_2} \tag{22}$$

To minimize equation (22) subject to the restriction of weights $3r_1+3r_2+r_3=1$, we set the Lagrangian function as

$$\psi=\text{Trace}\ (\boldsymbol{M}^{-1}(\xi_a))\ +\lambda(3r_1+3r_2+r_3-1)$$

Now, taking the partial derivatives of ψ with respect to r_1, r_2, r_3 and λ, and set them equal to 0, we get

$$\frac{-48+3a(a-1)[-80+a(a-1)(-82+r_1^2\lambda)]}{a^2(a-1)^2 r_1^2}=0 \tag{23}$$

$$\frac{6[8+a(a-1)(41a(a-1)+40)]}{a^2(a-1)^2 r_1 r_2}$$

$$-\frac{30r_1+6[8+a(a-1)(41a(a-1)+40)]r_2}{a^2(a-1)^2 r_1 r_2^2}+3\lambda=0 \tag{24}$$

$$-\frac{729}{r_3^2}+\lambda=0 \tag{25}$$

$$3r_1+3r_2+r_3=1 \tag{26}$$

Next, by solving equations (23) – (26), we numerically compute possible optimal values of r_1, r_2, r_3 (rounded off to the fourth place of decimal) and corresponding value of Trace $(\boldsymbol{M}^{-1}(\xi_a))$ for different values of a, which are tabulated in Table 3.

Table 3:Trace $(\boldsymbol{M}^{-1}(\xi_a))$ and corresponding weights of special cubic model for different values of a

a	r_1	r_2	r_3	Trace $(\boldsymbol{M}^{-1}(\xi_a))$
0.01	0.1818	0.1474	0.0124	4.69727×10^6
0.05	0.1650	0.1483	0.0601	201592.0
0.10	0.1455	0.1495	0.1149	55204.2
0.20	0.1111	0.1527	0.2086	16758.6
0.28	0.0891	0.1556	0.2657	10322.6
0.33	0.0753	0.1580	0.2998	8106.8
0.40	0.0627	0.1608	0.3294	6716.7
0.45	0.0567	0.1623	0.3429	6199.2
*0.50	0.0546	0.1629	0.3476	6033.5

* Simplex centroid design and corresponding D-optimal design (a = 1/2)

From Table 3, we observe that the support points of simplex centroid design *i.e.* ξ_3 are the possible support points of the A-optimal design for the full cubic model.

The next step is to prove the necessary and sufficient condition *i.e.* $\underset{\boldsymbol{x}\in\chi}{\text{Max}}\, d(\boldsymbol{x},\, \xi_3)=$ Trace $(\boldsymbol{M}^{-1}(\xi_3))$ has been established as (A3) in Appendix A. In this case, we obtain the value of $\boldsymbol{M}^{-1}(\xi_3)$ by substituting a = 1/2 in equation (21).

4. Discussions and Conclusions

In comparison to D-optimal designs for models for mixture experiments, obtaining A-optimal designs for models with mixture experiments involves more challenges, as the support points in general, are associated with different weights. The present article obtains A-optimal minimum support designs for the three different forms of the cubic model of mixture experiments when the mixture involves three ingredients. We find that the design points of {3, 3} simplex- lattice and simplex-centroid designs are the support points of the obtained A-optimal designs for the full cubic and special cubic models respectively. In the case of the cubic model without 3-way effect, the support points of the corresponding D-optimal designs are the support points of A-optimal designs. One may apply this result to the case of mixture experiments having $q \geq 4$ ingredients. Of course, the task may be complicated for computing the inverse of the information matrix.

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APPENDIX A

Proof of Theorem 2:

$$d(\boldsymbol{x},\xi_1)=b_1\sum_{i=1}^{3}x_i^2+b_2\sum_{i<j}^{3}x_ix_j-b_3\left(\sum_{i<j}^{3}x_i^2x_j+\sum_{i<j}^{3}x_ix_j^2\right)+b_4\sum_{i<j}^{3}x_i^2x_j^2$$

$$-b_5\left(\sum_{i<j}^{3}x_i^3x_j+\sum_{i<j}^{3}x_ix_j^3\right)-b_6\sum_{i<j}^{3}x_i^3x_j^3+b_7\left(\sum_{i<j}^{3}x_i^4x_j^2+\sum_{i<j}^{3}x_i^2x_j^4\right)-b_8x_1x_2x_3$$

$$+b_9(x_1^2x_2x_3+x_1x_2^2x_3+x_1x_2x_3^2)+b_{10}(x_1^3x_2x_3+x_1x_2^3x_3+x_1x_2x_3^3)$$

$$+b_{11}(x_1^4x_2x_3+x_1x_2^4x_3+x_1x_2x_3^4)$$

$$-b_{11}(x_1^3x_2^2x_3+x_1^3x_2x_3^2+x_1x_2^3x_3^2+x_1^2x_2^3x_3+x_1^2x_2x_3^3+x_1x_2^2x_3^3)$$

$$-b_{12}(x_1^2x_2^2x_3+x_1^2x_2x_3^2+x_1x_2^2x_3^2)+b_{13}x_1^2x_2^2x_3^2$$

where

$b_1=11061$, $b_2=10794.5$, $b_3=129898$, $b_4=730343$,
$b_5=97276.5$, $b_6=2.67057\times10^6$, $b_7=1.33528\times10^6$, $b_8=289304$,
$b_9=2.04729\times10^6$, $b_{10}=473639$, $b_{11}=380398$, $b_{12}=9.93829\times10^6$,
$b_{13}=4.81873\times10^7$.

By using Matlab, the value of $d(\boldsymbol{x},\xi_1)$, at all the support points can be seen to be is equal to Trace$(\boldsymbol{M}^{-1}(\xi_1))$ = 11061. Again using the standard maximize function in Matlab, we find that

$$\underset{\boldsymbol{x}\in\chi}{Max}\ d(\boldsymbol{x},\xi_1)=11061 \qquad \text{(A1)}$$

over the simplex region χ. Thus equivalence theorem is verified and this proves Theorem 2.

Proof of Theorem 3:

$$d(\boldsymbol{x},\xi_2)=c_1\sum_{i=1}^{3}x_i^2-c_2\left(\sum_{i<j}^{3}x_i^2x_j+\sum_{i<j}^{3}x_ix_j^2\right)+c_3\left(\sum_{i<j}^{3}x_i^2x_j^2\right)-c_4\left(\sum_{i<j}^{3}x_i^3x_j+\sum_{i<j}^{3}x_ix_j^3\right)$$

$$+c_5\left(\sum_{i<j}^{3}x_i^4x_j^2+\sum_{i<j}^{3}x_i^2x_j^4\right)-c_6\sum_{i<j}^{3}x_i^3x_j^3+c_7\left(x_1^2x_2x_3+x_1x_2^2x_3+x_1x_2x_3^2\right)$$
$$+c_8\left(x_1^3x_2x_3+x_1x_2^3x_3+x_1x_2x_3^3-x_1^2x_2^2x_3-x_1^2x_2x_3^2-x_1x_2^2x_3^2\right)$$
$$+c_9\left(x_1^4x_2x_3+x_1x_2^4x_3+x_1x_2x_3^4-x_1^2x_2^3x_3-x_1^2x_2x_3^3-x_1x_2^2x_3^3-x_1^3x_2^2x_3\right.$$
$$\left.-x_1^3x_2x_3^2-x_1x_2^3x_3^2\right)+c_{10}x_1^2x_2^2x_3^2$$

where

$c_1=2708.1$, $c_2=18961$, $c_3=153524$, $c_4=40643.2$,
$c_5=451458$, $c_6=902917$, $c_7=60953.9$, $c_8=230319$,
$c_9=169365$, $c_{10}=508094$.

By using Matlab, the value of $d(\boldsymbol{x},\xi_2)$, at all the support points can be seen to be is equal to Trace$(\boldsymbol{M}^{-1}(\xi_2))$ = 2708.1. Again using standard maximize function in Matlab, we find that

$$\underset{\boldsymbol{x}\in\chi}{Max}\ d(\boldsymbol{x},\xi_2)=2708.1 \qquad \text{(A2)}$$

over the simplex region χ. Thus equivalence theorem is verified and this completes the proof of Theorem 3.

Proof of Theorem 4:

$$d(\boldsymbol{x},\xi_3)=a_1\sum_{i=1}^{3}x_i^2+a_2\sum_{i<j}^{3}x_ix_j-a_3\left(\sum_{i<j}^{3}x_i^2x_j+\sum_{i<j}^{3}x_ix_j^2\right)+a_4\sum_{i<j}^{3}x_i^2x_j^2-a_5x_1x_2x_3$$
$$+a_6\left(x_1^2x_2x_3+x_1x_2^2x_3+x_1x_2x_3^2\right)-a_7\left(x_1^2x_2^2x_3+x_1^2x_2x_3^2+x_1x_2^2x_3^2\right)+a_8x_1^2x_2^2x_3^2$$

where

a_1 = 6033.45, a_2 = 8714.99, $a_3=81138$, a_4 = 337960,
$a_5=201717$, $a_6=1.26788\times10^6$, $a_7=5.80653\times10^6$, $a_8=2.83064\times10^7$.

By using Matlab, the value of $d(\boldsymbol{x},\xi_3)$ at all the support points can be seen to be is equal to Trace$(\boldsymbol{M}^{-1}(\xi_3))$ = 6033.5. Again using the standard maximize function in Matlab, we find that

$$\underset{\boldsymbol{x}\in\chi}{Max}\ d(\boldsymbol{x},\xi_3)=6033.5 \qquad \text{(A3)}$$

over the simplex region χ. Thus equivalence theorem is verified and this proves Theorem 4.