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Optimum Designs for Mixture Experiments With Relational Constraints on the Mixing Components

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Abstract

In a mixture experiment, the mean response is expressed as a function of the mixing proportions of the ingredients. Often the ingredients can be grouped into classes, depending on their degree of usefulness or similarity in use. Each such class is called a major component and the members of a class are termed as its minor components. In a major component, the minor components are generally subjected to a relational constraint, which gives a range of acceptable values for each proportion. In this presentation, we discuss the optimum designs suggested by Pal et al. (2018)[*] for the estimation of the parameters of a mixture model in an experiment with major and minor components

Key words: Mixture experiment; Major and minor components; Relational constraints; D-optimality criterion.

1 Introduction

Mixture experiments are commonly encountered in formulation of industrial products, like pharmaceutical drugs, textile fibers, food processing, etc. They also find usefulness in agricultural research. For example, a mixture experiment may be conducted to model the yield of a crop as a function of the mixture combination of fertilizers or pesticides, when the same amount is applied. Many situations arise in agriculture where an overall mixture response is more useful than the traditional individual responses, *e.g.*, monoculture vs. multicultural cultivars, soil mixtures, seed mixtures, feed mixtures for animals, etc.

In experiments with mixtures, it is often possible to group the ingredients of the mixture into distinct classes, based on their degree of usefulness or similarity in usefulness. For example, in an agricultural experiment, the growth of a plant depends on a number of nutrients. The nutrients like Nitrogen (N), Phosphorus (P), Potassium (K), Magnesium (Mg), Calcium (Ca) and Hydrogen (H), which are required in abundance, may be put in a class, while the nutrients that are required in small quantities can be put in another class. These classes are referred to as major components, and for each major component there is generally a restriction on the proportion of

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the component to be used in the mixture. This automatically imposes a relational constraint on the mixing proportions of the minor components. In fact, the relational constraint gives a range of acceptable values of the proportion of each minor component. Again, in a pharmaceutical experiment, the two important components affecting the mean dissolution time of an oral tablet are the polymer and diluent. As more than one polymer and one diluent are usually used in a tablet, we may define polymer and diluent as the major components, and their minor components are respectively the different polymers and diluents used. The relational constraints on the minor components are defined by the constraints on the proportions of polymer and diluent.

Pal and Mandal (2013) studied a problem with two major components A and B and discussed optimum designs for parameter estimation and also for estimating the optimum mixing proportions of minor components in A. The model considered was

$$\eta_x = \sum_{i=1}^{m} \beta_1 x_1 + \sum_{i<j=1}^{m} \beta_{ij} x_i x_j, \tag{1.1}$$

where m and n denote the number of minor components in A and B, respectively, $\beta_{\mathrm{i}} = \sum_{k=1}^{n} \alpha_{ik} y_k, i = 1(1)m, \beta_{ij} = \sum_{k=1}^{n} \alpha_{ijk} y_k, 1 \le i, j \le m, i < j,$ and $(x_1, x_2, ..., x_m)$ and $(y_1, y_2, ..., y_n)$ are the mixing proportions of the minor components in A and B, respectively, with $0 \le x_i, y_k \le 1, i = 1(1)m, k = 1(1)n, \sum_{i=1}^{m} x_i = c, \sum_{k=1}^{n} y_k = 1 - c, 0 < c < 1,$ c specified.

The present study reflects on the major-minor component problem addressed by Pal et al. (2018). The problem had two major components, and their proportions in the mixture are subject to specified lower and upper bounds. D-optimality criterion is used to estimate the parameters of the response model.

2 The Models

Consider a mixture of two major components M_1 and M_2 there being m minor components in M_1 with proportions $\boldsymbol{x}_{(1)} = (x_1, x_2, ..., x_m)$ and n minor components in M_2 with proportions $\boldsymbol{x}_{(2)} = (x_{m+1}, x_{m+2}, ..., x_{m+n})$, where $0 \le x_i \le 1,$ $\sum_{\boldsymbol{i}=\boldsymbol{1}}^{\boldsymbol{m}+\boldsymbol{n}} x_i = 1.$ Suppose the proportions in the major component $M_1$are required to satisfy $\delta_1 \le \sum_{\boldsymbol{i}=1}^{\boldsymbol{m}} x_i \le \delta_2,$ $0 < \delta_1 < \delta_2 < 1.$

2.1 Consider the mean response $\eta_{\boldsymbol{x}}$ given by

$$\eta_x = \sum_{i=1}^{m+n} \beta_i x_i + \sum_{i<j=1}^{m} \beta_{ij} x_i x_j, \tag{2.1}$$

where the experimental region is

$$\Xi = \{(x_1, x_2, \ldots x_{m+n}) \mid 0 \le x_i \le 1, i = 1,2,\ldots, m+n, \delta_1 \le \sum_{i=1}^{m} x_i \le \delta_2,\ 0 < \delta_1 < \delta_2 < 1\}. \tag{2.2}$$

We can write $\Xi = \Xi_1 \cap \Xi_2$, where

$$\Xi_1 = \{(x_1, x_2, \ldots x_m) \mid 0 \le x_i \le 1, i = 1,2,\ldots, m,\ \delta_1 \le \sum_{i=1}^{m} x_i \le \delta_2\}, (2.3)$$

$$\Xi_2 = \{(x_{m+1}, x_{m+2}, \ldots x_{m+n}) \mid 0 \le x_i \le 1, i = m+1, m+2, \ldots, m+n, 1-\delta_2 \le \sum_{i=m+1}^{m+n} x_i \le 1-\delta_1,$$
$$0 < \delta_1 < \delta_2 < 1.\}, \tag{2.4}$$

Clearly, Ξ_1 and Ξ_2 denote the experimental regions of M_1 and M_2, respectively.

The response model can be re-written as

$$\eta_x = \boldsymbol{f}(\boldsymbol{x})'\boldsymbol{\beta},$$

where $\boldsymbol{f}(\boldsymbol{x}) = \begin{pmatrix} \boldsymbol{f}_1(\boldsymbol{x}_{(1)}) \\ \boldsymbol{x}_{(2)} \end{pmatrix}$, $\boldsymbol{f}_1(\boldsymbol{x}_{(1)}) = (x_1, x_2, \ldots, x_m, x_1x_2, x_1x_3, \ldots, x_{m-1}x_m)'$, $\boldsymbol{\beta} = \begin{pmatrix} \boldsymbol{\beta}_{(1)} \\ \boldsymbol{\beta}_{(2)} \end{pmatrix}$,

$\boldsymbol{\beta}_{(1)} = (\beta_1, \beta_2, \ldots, \beta_m, \beta_{12}, \ldots, \beta_{m-1,m})'$, $\boldsymbol{\beta}_{(2)} = (\beta_{m+1}, \beta_{m+2}, \ldots, \beta_{m+n})'$.

Let $\mathcal{D}$ be the class of all competing continuous designs, for which all the parameters of (2.1) are estimable. We want to find a design ξ in $\mathcal{D}$ that can estimate the parameters with maximum accuracy.

For a continuous design $\xi \in \mathcal{D}$:

$$\xi = \{ \boldsymbol{x_1}^*, \boldsymbol{x_2}^*, \ldots, \boldsymbol{x_N}^* ; w_1, w_2, \ldots, w_N \}, \tag{2.5}$$

with masses $w_1, w_2, \ldots, w_N$, $w_i > 0$, $\sum w_i = 1$, at points $\boldsymbol{x_1}^*, \boldsymbol{x_2}^*, \ldots, \boldsymbol{x_N}^*$,

the information (moment) matrix is given by $M(\xi) = \sum w_i \boldsymbol{f}(\boldsymbol{x_i}^*)\boldsymbol{f}(\boldsymbol{x_i}^*)'$.

Design optimality aims at minimizing some function of $M^{-1}(\xi)$, or maximizing some function of $M(\xi)$. For comparing different designs in $\mathcal{D}$, consider the D-optimality criterion, given by

$$\text{Maximize}\ \phi_D(\xi), \text{ where } \phi_D(\xi) = \text{Det.}(M(\xi)).$$

(2.6)

The above criterion is invariant with respect to the components of $x_{(1)}$ and $x_{(2)}$.

In order to find the design points, it is argued that when the mean response has quadratic dependence on the mixing proportions, a reasonable choice for the experimental points would be the extreme points of the design space and mid-points of the edges of the space when the optimality criterion is invariant with respect to the proportions; while in case of linear dependence, only the extreme points of the design space seem to be the reasonable choice. Thus, in the present situation, where the model (2.1) is linear in $x_{(2)}$ and quadratic in $x_{(1)}$, it seems only logical to start with a class $\mathcal{D}_1$ of designs with support points given by

(i) $(\delta_i, 0,...,0; 1-\delta_i, 0,...,0)$ and all possible permutations within the first m co-ordinates and within the last n co-ordinates each with mass v_i, $i = 1,2$;

(ii) $(\delta_0, 0,0,...,0; 1-\delta_0, 0,0,...,0)$ and all possible permutations within the first m co-ordinates and within the last n co-ordinates each with mass v_0;

(iii) $(\delta_i/2, \delta_i/2, 0,...,0; 1-\delta_i, 0,...,0)$ and all possible permutations within the first m co-ordinates and within the last n co-ordinates, each with mass w_i, , $i = 1,2$,

where the extreme points of Ξ_1 and Ξ_2 are respectively $(\delta_1, 0,...,0)$ and $(\delta_2, 0,...,0)$ and all possible permutations within these, and $(1-\delta_1, 0,...,0)$ and $(1-\delta_2, 0,...,0)$ and all possible permutations within these, while the mid-points of the edges of Ξ_1 are $(\delta_1/2, \delta_1/2, 0,...,0)$, $(\delta_2/2, \delta_2/2, 0,...,0)$, $(\delta_0, 0,0,...,0)$ and all possible permutations within these, with $\delta_0 = (\delta_1 + \delta_2)/2$.

Pal and Mandal (2013) defined the support points in (i) and (ii) as pure type support points and those in (iii) as mixed type support points. For any design $\xi \in \mathcal{D}_1$, there are mn points of the type (i) and (ii), and $m(m\text{-}1)n$ points of the type (iii), for each i= 1, 2 The masses assigned to the support points, therefore, satisfy $mn(v_0 + v_1 + v_2) + C(m,2)n(w_1 + w_2) = 1,$ where $C(s,t) = \binom{s}{t}$.

As noted, the number of support points in $\xi \in \mathcal{D}_1$ is very large compared to the number of parameters to be estimated, and the difference between the two increases as m and n increase. To reduce the number of support points, Lewis et al. (2010), for the case of m = 2 and n = 3, used the exchange algorithm. However, the optimum design they derived lack the invariance property though the criterion function used, namely D-optimality criterion, is invariant with respect to the minor components within each of M_1 and M_2. This contradicts the well-established fact that *in an invariant optimality design problem, the support points of the optimum design must be invariant with respect to its components* (*cf.* Pukelsheim, 1993). Further, they have assigned equal masses to the design points.

The example considered by Lewis et al. (2010) assumes δ_1= 0.1 and δ_2= 0.5. They used the exchange algorithm to choose a 9- point design with equal masses, which they claim to be the D-optimal design. The 9 points are:

(0.1, 0; 0.9, 0, 0), (0, 0.5; 0.5, 0 0), (0.5, 0; 0, 0.5, 0),

(0, 0.5; 0, 0.5, 0), (0, 0.1; 0, 0, 0.9), (0.5, 0; 0, 0, 0.5),

(0.25, 0.25; 0.5, 0, 0), (0.25, 0.25; 0, 0, 0.5), (0.05, 0.05; 0, 0.9, 0),

and the determinant of the information matrix is 1.50366×10^{-09}.

Pal et al. (2018) proposed the following ways to reduce the number of support points, while retaining the property of invariance.

2.1.1 Consider a class of designs $\mathcal{D}_2$ having the following support points:

(a) all the pure support points in (i) with the stated masses,

(b) mixed support points of the form $(\delta/2, \delta/2, 0, \ldots, 0; 1-\delta, 0, \ldots, 0)$ and all possible permutations within the first *m* co-ordinates and within the last *n* co-ordinates, for some $\delta \in [\delta_1, \delta_2]$, each with mass *w*.

The number of support points of a design in $\mathcal{D}_2$ is thus $2mn + C(m,2)n$.

For $m = 2, n = 3$, $\delta_1 = 0.1$, $\delta_2 = 0.5$, and equal masses for all design points, the determinant of the information matrix is maximum (4.32709×10^{-09}) for a 15-point design with $\delta = \delta_2$. A comparison of this design with that having 18 support points given by (i) and (iii) with equal masses shows this design to be better as the determinant of the information matrix of the 18-point design is 3.91969×10^{-09}. However, this design may not be a D-optimal design since the number of design points is more than the number of parameters to be estimated, and in that case the optimum masses allocated to the design points may not be equal. To find the D-optimal design within $\mathcal{D}_2$ for $m = 2$, $n = 3$, consider any $\xi \in \mathcal{D}_2$. The determinant of the information matrix of ξ is given by

$$Det.[M(\xi)] = \frac{27}{16}\delta^4 w(\delta_1^2 v_1 + \delta_2^2 v_2)^2 [2(1-\delta_1)^2 v_1 + 2(1-\delta_2)^2 v_2 + (1-\delta)^2 w]^3 . \qquad (2.7)$$

The D-optimal design within $\mathcal{D}_2$ is obtained by determining the optimal values of δ, v_1, v_2 and w that maximize (2.7), subject to $6(v_1 + v_2) + 3w = 1$.

2.1.2 To maintain invariance among the minor components within the major components, the minimum number of design points required is $r = mn + C(m, 2)n$. So, consider the sub-class $\mathcal{D}_3$ of *r* point designs with support points as follows.

(a) $(\delta_3, 0, 0, \ldots, 0; 1-\delta_3, 0, 0, \ldots, 0)$ and all possible permutations within the first *m* co-ordinates and within the last *n* co-ordinates each with mass *v*;

(b) $(\delta_4/2, \delta_4/2, 0, \ldots, 0; 1-\delta_4, 0, \ldots, 0)$ and all possible permutations within the first *m* co-ordinates and within the last *n* co-ordinates, each with mass *w*, where $\delta_1 \le \delta_3, \delta_4 \le \delta_2$.

The determinant of the information matrix of $\xi \in \mathcal{D}_3$ is

$$\text{Det.}\, M(\xi) = \{m(1\text{-}\delta_3)^2 v + C(m,2)(1-\delta_4)^2 w\}^n \left(\frac{n\delta_4{}^4 w}{16}\right)^{C(m,2)} |M_{11}| \times |I_{C(m,2)} - \frac{n\delta_4^2 w}{4} Q' M_{11}^{-1} Q|, \tag{2.8}$$

$$\text{where}\, M_{11} = n\delta_3^2 v I_m + \frac{n\delta_4^2 w}{4} 1_m 1_m{}', \quad Q^{m\times C(m,2)} = \begin{bmatrix} \overbrace{1\,1\ldots1}^{m\text{-}1}\ \overbrace{0\,0\ldots0}^{m-2}\,\overbrace{0\,0\ldots0}^{m-3}\ldots\overbrace{0}^{1} \\ 1\ 0\ldots0\,1\ 1\ldots1\ \ 0\,0\ldots0\ldots0 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ 0\,0\ldots1\,0\,0\ldots1\,0\,0\ldots1\ldots\ 1 \end{bmatrix}.$$

For $m = 2, n = 3$, we have $r = 9$, and

$$\text{Det.}\ M(\xi) = \frac{27}{16}\delta_3^4\delta_4^4 v^2 w[2(1\text{-}\delta_3)^2 v + (1-\delta_4)^2 w]^3, \tag{2.9}$$

where $w = 1/3 - 2v, \quad v, w > 0$.

2.1.3 For $\xi \in \mathcal{D}_4$, where $\mathcal{D}_4$ is a sub-class of $\mathcal{D}_3$ with $\delta_3 = \delta_4 = \delta$,

$$\text{Det.}\, M(\xi) = \frac{1}{16}\delta^8 (1\text{-}\delta)^6 v^2 w,$$

which is a concave function of δ and is maximized at $\delta = 4/7$ and $v = w = 1/9$.

Since $\delta_1 \le \delta \le \delta_2$, the optimal value of δ is given by

(a) $\delta = 4/7$ if $\delta_1 \le 4/7 \le \delta_2$,

(b) $\delta = \delta_1$ if $\delta_1 \ge 4/7$,

(c) $\delta = \delta_2$ if $\delta_2 \le 4/7$.

The D-optimal designs within $\mathcal{D}_2$, $\mathcal{D}_3$ and $\mathcal{D}_4$ have been given by Pal et al. (2018) for some combinations of (δ_1, δ_2), when $m = 2$, $n = 3$, and are shown in Table 2.1.

Table 2.1: D-optimal designs within $\mathcal{D}_2$, $\mathcal{D}_3$ and $\mathcal{D}_4$ for some combinations of (δ_1, δ_2) when m = 2, n = 3.

(δ_1, δ_2)	**Sub-class**	**δ_1 / δ_3**	**δ_2 / δ_4**	**δ**	**v_1**	**v_2**	**v**	**w**	**Det.**
(0.1,0.4)	$\mathcal{D}_2$	0.1	0.4	0.4	0.02774	0.0116	-	0.0459	1.7308×10^{-8}
	$\mathcal{D}_3$	0.4	0.4	-	-	-	1/9	1/9	1.6384×10^{-8}
	$\mathcal{D}_4$	-	-	0.4	-	-	1/9	1/9	1.6384×10^{-8}
(0.1,0.5)	$\mathcal{D}_2$	0.1	0.5	0.5	0.0398	0.0876	-	0.0788	3.4684×10^{-8}
	$\mathcal{D}_3$	0.5	0.5	-	-	-	1/9	1/9	2.0931×10^{-8}
	$\mathcal{D}_4$	-	-	0.5	-	-	1/9	1/9	2.0931×10^{-8}
(0.2,0.6)	$\mathcal{D}_2$	0.2	0.6	0.6	.07186	.06288		0.06418	4.6625×10^{-8}
	$\mathcal{D}_3$	0.2896	0.6	-	-	-	0.0702	0.1931	3.0188×10^{-8}
	$\mathcal{D}_4$	-	-	4/7	-	-	1/9	1/9	1.8606×10^{-8}
(.3,.7)	$\mathcal{D}_2$	0.3	0.7	0.6872	0.0644	0.0639	-	0.0770	4.6903×10^{-8}
	$\mathcal{D}_3$	0.7	0.3616	-	-	-	0.0702	0.1931	4.2936×10^{-8}
	$\mathcal{D}_4$	-	-	4/7	-	-	1/9	1/9	1.8606×10^{-8}
(.6,.8)	$\mathcal{D}_2$	0.6	0.8	0.6	1/9	0	-	1/9	1.6481×10^{-8}
	$\mathcal{D}_3$	0.6	0.6	-	-	-	1/9	1/9	1.6481×10^{-8}
	$\mathcal{D}_4$	-	-	0.6	-	-	1/9	1/9	1.6481×10^{-8}

2.2 Consider the response function given by

$$\left.\begin{aligned} \eta_x &= \sum_{i=1}^{m} \beta_i x_i + \sum_{\substack{i,j=1\\ i<j}}^{m} \beta_{ij} x_i x_j, \\ \text{where } \beta_i &= \sum_{k=m+1}^{m+n} \theta_{ik} x_k,\ i = 1(1)m,\ \ \beta_{ij} = \sum_{k=m+1}^{m+n} \theta_{ijk} x_k,\ i<j=1(1)m. \end{aligned}\right\} \quad (2.10)$$

It can be re-written as

$$\eta_{\boldsymbol{x}} = \sum_{i=1}^{m} \sum_{k=m+1}^{m+n} \theta_{ik} x_i x_k + \sum_{i<j=1}^{m} \sum_{k=m+1}^{m+n} \theta_{ijk} x_i x_j x_k, \quad (2.11)$$

The experimental region will be, as before, given by $\Xi = \Xi_1 \cap \Xi_2$.

2.2.1 Because of invariance among the components in $x_{(1)}$ and $x_{(2)}$, one can start with a class of designs $\mathcal{D}_1$ defined in sub-section 2.1.For m =2, n = 3, the determinant of the information matrix of $\xi \in \mathcal{D}_1$ is obtained as

$$\text{Det. } [M(\xi)] = (a+b)^3 [d(a-b) - 2c^2]^3,$$

where

$$a = \sum_{i=0}^{2} \delta_i^2 (1-\delta_i)^2 v_i + b, \quad b = \sum_{i=1}^{2} \frac{\delta_i^2 (1-\delta_i)^2}{4} w_i,$$
$$c = \sum_{i=1}^{2} \frac{\delta_i^3 (1-\delta_i)^2}{8} w_i, \quad d = \sum_{i=1}^{2} \frac{\delta_i^4 (1-\delta_i)^2}{16} w_i.$$

2.2.2 As the number of support points of designs in $\mathcal{D}_1$ is very large compared to the number of parameters to be estimated, one can consider the class $\mathcal{D}_2^*$ of designs with all support points of (i) and (ii), and mixed support points of the type $(\delta/2, \delta/2, 0, \ldots, 0; 1-\delta, 0, \ldots, 0)$ and all possible permutations within the first m co-ordinates and within the last n co-ordinates, for some $\delta \in [\delta_1, \delta_2]$, each with mass w. The information matrix for any $\xi \in \mathcal{D}_2^*$ has the determinant given by

$$\text{Det.}[M(\xi_1)] = \left(\frac{\delta^4 (1-\delta)^2}{16} w \right)^{C(m,2)n} \left(\sum_{i=0}^{2} \delta_i^2 (1-\delta_i)^2 v_i \right)^{mn}, \ \delta \in [\delta_1, \delta_2].$$

For given δ_i, v_i, i= 1, 2 and w, det. $[M(\xi_1)]$ is a concave function of δ with maximum at δ= 2/3. Since δ should belong to $[\delta_1, \delta_2]$, the optimal value of δ is

δ= 2/3 if $\delta_1 \le 2/3 \le \delta_2$,

= δ_1 if $\delta_1 \ge 2/3$,

= δ_2 if $\delta_2 \le 2/3$,

which is independent of m and n.

2.2.3 Another way suggested to reduce the number of support points is to consider the class of saturated designs $\mathcal{D}_3^*$. Consider $\delta \in [\delta_1, \delta_2]$, and confine to designs with support points (i) $(\delta, 0, \ldots, 0; 1-\delta, 0, \ldots, 0)$ and all possible permutations within the first m co-ordinates and within the last n co-ordinates each with mass v;(ii) $(\delta/2, \delta/2, 0, \ldots, 0; 1-\delta_i, 0, \ldots, 0)$ and all possible permutations within the first m co-ordinates and within the last n co-ordinates, each with mass w, such that $mnv + C(m,2)nw = 1$. In this case, for any design $\xi \in \mathcal{D}_3^*$,

$$\text{Det. } [M(\xi)] = \delta^{2(m+2C(m,2))n}(1-\delta)^{2(m+C(m,2))n}\frac{v^{mn}w^{C(m,2)n}}{16^{C(m,2)n}}.$$

For given v and w, Det. $[M(\xi)]$ is a concave function of δ with maximum value at $\delta = \frac{2m}{3m+1}$. Thus, the experiment should be conducted with

$$\delta = \frac{2m}{3m+1} \text{ if } \delta_1 \le \frac{2m}{3m+1} \le \delta_2,$$

$$= \delta_1 \text{ if } \delta_1 \ge \frac{2m}{3m+1},$$

$$= \delta_2 \text{ if } \delta_2 \le \frac{2m}{3m+1},$$

which is dependent on m but independent of n.

Table 2.2, reproduced from Pal et al. (2018), shows the optimum designs in the sub-classes $\mathcal{D}_1$, $\mathcal{D}_2^*$ and $\mathcal{D}_3^*$ for some combinations of (δ_1, δ_2) when (m, n)= (2, 3).

Table 2.2: D-optimal designs within $\mathcal{D}_1$, $\mathcal{D}_2^*$ and $\mathcal{D}_3^*$ for some combinations of (δ_1, δ_2) when (m, n)= (2, 3).

(δ_1, δ_2)	Sub-class	δ_0	δ_1	δ_2	δ	v_0	v_1	v_2	w_1	w_2	v	w	Det.
(0.1,0.5)	$\mathcal{D}_1$	0.3	0.1	0.5	-	0.034	0.015	0.053	0.049	0.080	-	-	1.08119×10^{-12}
	$\mathcal{D}_2^*$	-	-	-	0.5	-	0.055	0.055	-	-	-	0.088	1.36482×10^{-12}
	$\mathcal{D}_3^*$	-	-	-	0.5	-	-	-	-	-	1/9	1/9	4.27219×10^{-12}
(0.3,0.7)	$\mathcal{D}_1$	0.5	0.3	0.7	-	0.035	0.055	0.040	0.0012	0.072	-	-	$2.29991\times10^{--12}$
	$\mathcal{D}_2^*$	-	0.3	0.7	2/3	-	0.055	0.055	-	-	-	0.088	3.78612×10^{-12}
	$\mathcal{D}_3^*$	-	-	-	4/7	-	-	-	-	-	1/9	1/9	8.38711×10^{-12}
(0.6,0.8)	$\mathcal{D}_1$	0.7	0.6	0.8	-	0.019	0.039	0.086	0.001	0.044	-	-	2.27387×10^{-13}
	$\mathcal{D}_2^*$	-	0.6	0.8	2/3	-	0.055	0.055	-	-	-	0.088	3.78229×10^{-12}
	$\mathcal{D}_3^*$	-	-	-	0.6	-	-	-	-	-	1/9	1/9	8.65667×10^{-12}

Remark: It is observed that the D-optimal design within $\mathcal{D}_3^*$ performs better than those within $\mathcal{D}_1$ and $\mathcal{D}_2^*$.

3 Conclusion

The study is along the lines of Lewis et al. (2010) involving mixture designs with major and minor components subject to relational constraints. Pal et al. (2018) endeavored to exploit symmetry and invariance of the model parameters towards identification of D-optimal designs within suitably defined subclasses of admissible mixture designs.

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