Statistics and Applications {**ISSN 2452-7395 (online)**}
Volume 17, No. 1, 2019 (New Series), pp 41–51

Optimum Repeated Measurement Mixture Designs

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Received: December 29, 2017; Revised September 24, 2018; Accepted September 24, 2018

Abstract

In agricultural experiments, we generally study the effect of manure on the yield of a crop, where the manure is applied on a single occasion. However, in real life, it is often observed that the farmer applies manure on the same plot at different time points. The composition of the manure may be same or may change depending on the growth of the plant at the intermediate time points. In this paper, we discuss a scenario where manure is applied at two time points – once at the time of sowing and next at some intermediate point before harvesting the crop. The composition of the manure applied at the second time point depends on the growth of the plant at that point. If the growth is found to be unsatisfactory, the manure is enriched with some additional components. We propose a linear model to describe the mean yield, which depends on the mixing proportions of the ingredients of the manure, and optimum designs are derived for the estimation of the model parameters. Examples are given for experiments with two/ three/ four component mixtures.

Key words: Mixture experiment; Repeated applications of manure; Quadratic yield model; Parameter estimation; D- and A- optimal designs.

AMS subject classification: 62K99; 62J05

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1 Introduction

A regression model describes the influence of various factors on the response under study. In agricultural experiments, regression models are used to study the effect of manure on the yield of a crop. In such experiments, the manure is generally applied on a single occasion. However, in real life, it is often observed that the farmer applies manure on the same plot at different time points. This is because repeated application on need basis is found to maintain good plant growth and crop production. Further, application in smaller amounts at frequent intervals may be more beneficial than a single application at a high rate, as some of the manure may be lost, say by leaching or in run-off due to heavy rains after it is applied, or a high rate of application may be harmful to the plant.

The composition of the manure in repeated applications may be same or may change depending on the growth of the plant at time points at which the manure is applied. Due to high cost or scarcity of certain organic substances used in the manure, the farmers may not be using

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them while applying manure before sowing of crop. However, if the crop growth is not found to be satisfactory at the time points of observation, they may be willing to enrich the manure with those ingredients. As the composition of the manure affects the growth and yield, one may be interested in modeling the mean yield of the crop as a function of the mixing proportions of the components used in the manure. For an updated account of mixture models and methods as also of optimality issues, we refer to a recent monograph by Sinha et al. (2014). In this paper, we assume that manure is applied to the soil twice before harvesting, once before sowing and then at some point before harvesting. We propose mixture models to describe the mean yield, which may vary with time, and optimum designs are derived for the estimation of the model parameters. Since manure is a mixture of a number of components, we have concentrated on mixture designs. Examples are given for experiments with two, three and four component mixtures. The study is, however, quite general, and can be applied to other areas as well, besides agricultural experimentation.

2 The Problem and Its Perspectives

Suppose the manure applied during sowing of the crop is a q-component mixture with mixing proportions given by $\boldsymbol{x} = (x_1, x_2, ..., x_q)$, where $\boldsymbol{x} \in \Xi_1 = \{(x_1, x_2, ..., x_q) \mid x_i \geq 0, 1 \leq i \leq q, \sum_{i=1}^{q} x_i = 1\}$. At an intermediate point t_0 before harvesting, the growth of the plant is measured. Let z denote the growth at t_0. If $z \geq z_0$, the manure with the same components is applied, while if $z < z_0$, the manure is enriched with r additional components. Let $\boldsymbol{x}^{(1)} = (x_1^{(1)}, x_2^{(1)}, ..., x_q^{(1)}) \in \Xi_1$ be the composition of the manure applied at t_0 when $z \geq z_0$, and $\boldsymbol{x}^{(2)} = (x_1^{(2)}, x_2^{(2)}, ..., x_q^{(2)}, x_{q+1}^{(2)}, x_{q+2}^{(2)}, ..., x_{q+r}^{(2)}) \in \Xi_2$ be its composition otherwise, where

$$\Xi_2 = \{(x_1^{(2)}, x_2^{(2)}, ..., x_q^{(2)}, x_{q+1}^{(2)}, ..., x_{q+r}^{(2)}) \mid x_i^{(2)} \geq 0, 1 \leq i \leq q+r, \sum_{i=1}^{q+r} x_i^{(2)} = 1\}.$$

Clearly, the domain of $\boldsymbol{x}^{(1)}$ is a subset of the domain of $\boldsymbol{x}^{(2)}$.

For $z \geq z_0$, let the mean yield be given by

$$\eta_{1\boldsymbol{x}^{(1)}} = \boldsymbol{f}_1(\boldsymbol{x}^{(1)})'\boldsymbol{\beta}, \text{if } z \geq z_0,$$

and

$$\eta_{1\boldsymbol{x}^{(2)}} = \boldsymbol{f}_2(\boldsymbol{x}^{(2)})'\boldsymbol{\gamma}, \text{if } z < z_0.$$

We consider the mean yield to be approximated by Scheffé's linear model:

$$\left.\begin{aligned} \eta_{1\boldsymbol{x}^{(1)}} &= \sum_{i=1}^{q} \beta_i x_i^{(1)}, \text{if } z \geq z_0, \\ \eta_{1\boldsymbol{x}^{(2)}} &= \sum_{i=1}^{q+r} \gamma_i x_i^{(2)}, \text{ if } z < z_0. \end{aligned}\right\} \quad (2.1)$$

As the manure applied at the time of sowing will be retained in the soil to certain extent at t_0, the effects of the old components used in the manure at t_0 will be enhanced. The coefficients of the mixing proportions of the old components in (2.1), are, therefore, expected to be functions of $\boldsymbol{x}$, the mixture applied at time 0. Let us approximate the regression coefficients in (2.1) by linear functions of $\boldsymbol{x}$ as given below:

$$\beta_i = \sum_{k=1}^{q} \alpha_{ik} x_k , 1 \le i \le q, \quad \gamma_i = \sum_{k=1}^{q} \delta_{ik} x_k , \ 1 \le i \le q, \tag{2.2}$$

Then, (2.1) becomes:

$$\eta_{1\boldsymbol{x}^{(1)}} \equiv \eta_{1\boldsymbol{x},\boldsymbol{x}^{(1)}} = \sum_{k=1}^{q}\sum_{i=1}^{q} \alpha_{ik} x_I^{(1)} x_k , \ \text{if } z \ge z_0 , \tag{2.3}$$

$$\eta_{1\boldsymbol{x}^{(2)}} \equiv \eta_{1\boldsymbol{x},\boldsymbol{x}^{(2)}} = \sum_{k=1}^{q}\sum_{i=1}^{q} \delta_{ik} x_i^{(2)} x_k + \sum_{i=1}^{r} \gamma_{q+i} x_{q+i}^{(2)} , \ \text{if } z < z_0 . \tag{2.4}$$

Suppose the experimenter has some idea about the proportion of times the growth of the plant at t_0 is less than z_0, and let it be p. Since the growth depends on the composition of the manure at time 0, we take p to be a function of $\boldsymbol{x}$. Let us assume that $p \equiv p(\boldsymbol{x}) = \sum_{i=1}^{q} \lambda_i x_i$.

Now, at time t_0, ideally we use a q-component mixture or a $(q+r)$-component mixture depending on the value of z. Essentially, considering the two situations, we are to use a $(q+r)$-component mixture. Let us denote the components as x_i^*, $i = 1,2, \ldots, q + r,$ satisfying $x_i^* \ge 0, 1 \le i \le q + r, \sum_{i=1}^{q+r} x_i^* = 1$. Then, we can write the mean yield

$$\begin{aligned} \eta_{\boldsymbol{x},\boldsymbol{x}^*} &= (1 - p(\boldsymbol{x})) \sum_{k=1}^{q}\sum_{i=1}^{q} \alpha_{ik} x_I^* x_k + p(\boldsymbol{x}) [\sum_{k=1}^{q}\sum_{i=1}^{q} \delta_{ik} x_i^* x_k + \sum_{i=1}^{r} \gamma_{q+i} x_{q+i}^*] \\ &= \sum_{i=1}^{q}\sum_{k=1}^{q} \mu_{iik} {x_i}^2 x_k^* + \sum_{i=1}^{q}\sum_{\substack{j=1 \\ i<j}}^{q}\sum_{k=1}^{q} \mu_{ijk} x_i x_j x_k^* + \sum_{i=1}^{q}\sum_{k=q+1}^{q+r} \mu_{ik}^* x_i x_k^* \\ &= \boldsymbol{f}'(\boldsymbol{x}, \boldsymbol{x}^*)\boldsymbol{\mu}, \ \text{say}, \quad \boldsymbol{x} \in \Xi_1 \text{ and } \boldsymbol{x}^* \in \Xi_2, \end{aligned} \tag{2.5}$$

where

$$\left. \begin{aligned} &\mu_{ijk} = \alpha_{ik} (1 - \lambda_j) + \delta_{ik} \lambda_j , \ 1 \le i, j, k \le q \\ &\mu_{ij}^* = \lambda_i \gamma_j , 1 \le i \le q, q + 1 \le j \le q + r \\ &\boldsymbol{\mu} = (\boldsymbol{\mu}'_{11}, \ldots, \boldsymbol{\mu}'_{qq}, \boldsymbol{\mu}'_{12}, \ldots, \boldsymbol{\mu}'_{1q}, \ldots, \boldsymbol{\mu}'_{q-1,q}, \boldsymbol{\mu}_{11}^{*\prime}, \ldots, \boldsymbol{\mu}_{qq}^{*\prime})' \\ &\boldsymbol{\mu}'_{ij} = (\mu_{ij1}, \mu_{ij2}, \ldots, \mu_{ijq}), \ \boldsymbol{\mu}_i^{*\prime} = (\mu_{i,q+1}^*, \mu_{i,q+2}^*, \ldots, \mu_{i,q+r}^*), \ 1 \le i \le j \le q \\ &\boldsymbol{f}'(\boldsymbol{x}, \boldsymbol{x}^*) = (f_1(\boldsymbol{x})' \otimes \boldsymbol{x}_{(1)}^{*\prime}, \boldsymbol{x}_{(2)}^{*\prime} \otimes \boldsymbol{x}') \\ &\boldsymbol{f}_1(\boldsymbol{x})' = (x_1^2, x_2^2, \ldots, x_q^2, x_1 x_2, x_1 x_3, \ldots, x_{q-1} x_q) \\ &\boldsymbol{x}_{(1)}^{*\prime} = (x_1^*, x_2^*, \ldots, x_q^*), \ \boldsymbol{x}_{(2)}^{*\prime} = (x_{q+1}^*, x_{q+2}^*, \ldots, x_{q+r}^*), \end{aligned} \right\} \tag{2.6}$$

and the experimental region is:

$$\Xi = \Xi_1 \cap \Xi_2 . \tag{2.7}$$

It is easy to note that model (2.5) is invariant w.r.t. the components within the sets $(x_1, x_2, ..., x_q)$, $(x_1^*, x_2^*, ..., x_q^*)$ and $(x_{q+1}^*, x_{q+2}^*, ..., x_{q+r}^*)$.

Our problem is to find optimum designs for estimating the parameters in (2.5).

3 Optimum Designs for Parameter Estimation

Consider the class $\mathcal{D}$ of all competing continuous designs, for which all the parameters of (2.5) are estimable. We want to find a design in $\mathcal{D}$ that can estimate the parameters with maximum accuracy.

For a linear model $\eta_x = \boldsymbol{f}'(\boldsymbol{x})\boldsymbol{\theta}$, a continuous design ξ is given by

$$\xi = \{ \boldsymbol{x_1}^{**}, \boldsymbol{x_2}^{**}, \ldots, \boldsymbol{x_N}^{**} ; w_1, w_2, \ldots, w_N \}, \tag{3.1}$$

with masses $w_1, w_2, \ldots, w_N$, at the points $\boldsymbol{x_1}^{**}, \boldsymbol{x_2}^{**}, \ldots, \boldsymbol{x_N}^{**}, \boldsymbol{x_i}^{**} \in \Xi$, where $w_i \geq 0$, $\sum w_i = 1$, and its information matrix is

$$M(\xi) = \sum w_i \boldsymbol{f}(\boldsymbol{x_i}^{**})\boldsymbol{f}(\boldsymbol{x_i}^{**})'.$$

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

$$\phi_D(M(\xi)) = \ln[\det .(M(\xi)^{-1})]$$

$$\phi_A(M(\xi)) = Trace[M(\xi)^{-1}], \tag{3.2}$$

which are convex in $M(\xi)$.

Let $\mathcal{B}_1$ and $\mathcal{E}_2$ denote, respectively the set of barycentres of Ξ_1 and the extreme points, that is, barycentres of depth 0 of Ξ_2. A point $\boldsymbol{x} \in \Xi_1$ is called a barycentre of depth j in Ξ_1 $(0 \leq j \leq q-1)$ if $j+1$ of its components are equal to $1/(j+1)$ and the remaining components are all equal to zero.

We show that the union of $\mathcal{B}_1$ and $\mathcal{E}_2$ are the only possible support points of the D-and A-optimal designs for estimating the parameters of the model (2.5).To do so, we shall first prove the following:

Theorem 3.1: *For a q-component full quadratic mixture model given by* $\eta_{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})'\boldsymbol{\theta}$, *where* $\boldsymbol{f}(\boldsymbol{x}) = (x_1^2, x_2^2, ..., x_q^2, x_1 x_2, x_1 x_3, ..., x_{q-1} x_q)'$, $\boldsymbol{x} \in \Xi_1$, and $\boldsymbol{\theta} = (\theta_{11}, ..., \theta_{qq}, \theta_{12}, ..., \theta_{1q}, ..., \theta_{q-1,q})$ *is the vector of unknown parameters,*

(a) *the D-optimal design for parameter estimation has support points at the barycentres of depth 0 and 1 of* Ξ_1 *each with mass* $1/{}^{q+1}C_2$,

(b) *the A-optimal design has support points at*

(i) *the barycentres of depth 0 each with mass 1/q, and the barycentres of depth 1, each with mass* $1/{}^{q+1}C_2$, *for* $q \neq 3$,

(ii) *the barycentres of depth 0 each with mass 0.1417, the barycentres of depth 1 each with mass0.1873 and the barycentre of depth 2 with mass 0.0130 forq= 3.*

Proof: Because of the natural restriction $\sum_{i=1}^{q} x_i = 1$, the full quadratic mixture model can be written as

$$\begin{aligned}\eta_{\boldsymbol{x}} &= \sum_{i=1}^{q}\theta_{ii}x_i^2 + \sum_{i<j=1}^{q}\theta_{ij}x_i x_j \\ &= \sum_{i=1}^{q}\theta_{ii}x_i\,(1-\sum_{\substack{j=1\\ j\neq i}}^{q}x_j) + \sum_{i<j=1}^{q}\theta_{ij}x_i x_j \\ &= \sum_{i=1}^{q}\theta_{ii}^{*}x_i + \sum_{i<j=1}^{q}\theta_{ij}^{*}x_i x_j \\ &= h(\boldsymbol{x})'\boldsymbol{\theta}^{*},\end{aligned}$$

where $h(\boldsymbol{x}) = (x_1, x_2, \ldots, x_q, x_1x_2, x_1x_3, \ldots, x_{q-1}x_q)'$, $\boldsymbol{\theta} = (\theta_{11}^{*}, \theta_{22}^{*}, \ldots, \theta_{qq}^{*}, \theta_{12}^{*}, \ldots, \theta_{1q}^{*}, \ldots, \theta_{q-1,q}^{*})'$, and

$$\theta_{ii}^{*} = \theta_{ii},\ \theta_{ij}^{*} = \theta_{ij}^{*},\ \forall\, i, j = 1(1)q,\ i<j. \tag{3.3}$$

From (3.3) it is evident that there is a one-to-one relation between $\boldsymbol{\theta}$ and $\boldsymbol{\theta}^{*}$. Hence, the design that is optimal for estimating $\boldsymbol{\theta}^{*}$ will also be optimal for estimating $\boldsymbol{\theta}$.

We note that $\eta_{\boldsymbol{x}} = h(\boldsymbol{x})'\boldsymbol{\theta}^{*}$ is the quadratic mixture model in the canonical form, due to Scheffé (1958), and (a) is the D-optimal design for estimating the parameters of the model, while (b) is the A-optimal design for parameter estimation (cf. Galil and Kiefer, 1977).The theorem therefore follows.

Theorem 3.2: *The support points of the D-optimal (A-optimal) design for estimating the parameters of the model (2.5) belong to the intersection of* $\mathcal{B}_1$ and $\mathcal{E}_2$.

The theorem can be proved using the Equivalence Theorem due to Kiefer (1974), which gives a necessary and sufficient condition for a design to be optimum in the entire class of competitive designs.In the present set-up, the theorem is given by:

Theorem 3.3 [Equivalence Theorem]: *A necessary and sufficient condition for a design* $\xi^{*} \in \mathcal{D}$ *to be D-optimal (A-optimal) for estimating the parameters of the model (2.5) is that*

$$f(x,x^*)'M^{-1}(\xi^*)f(x,x^*) \le \binom{q+1}{2}(q+r)\,((f(x,x^*)'M^{-2}(\xi^*)f(x,x^*) \le Trace\{M^{-1}(\xi^*)\})$$

*for all (**x, x***) $\in \Xi$., and equality holds at the support points of ξ*.*

Proof of Theorem 3.2: Consider $d(x,x^*) = f(x,x^*)'M^{-1}(\xi^*)f(x,x^*) - \binom{q+1}{2}(q+r)$. For given x^*, $d(x,x^*)$ is a fourth degree polynomial in x. Hence it can have atmost 3 maximal points with respect to each component of x, namely at the two extremes and one in-between. . Since $d(x,x^*)$ is invariant w.r.t. the components of x, the maximizing points will also be invariant w.r.t. the components of x, that is, they will be at the barycentres of Ξ. Again, for given x, $d(x,x^*)$ is a quadratic convex function in x, since $M(\xi)$ is positive definite. Hence it can have atmost 2 maximal points with respect to each component of x, namely at the two extremes. Thus, $d(x,x^*)$ is maximized at the extremes points of Ξ_2. Similar arguments confirm the support points of an A-optimal design.

For given x^*, η_{x,x^*} is a quadratic, invariant function in x, while for given x, η_{x,x^*} is a linear function in x^*. We know that for a quadratic response function the D-optimal design for parameter estimation has its support points at the barycentres of depth 0 and 1 of the simplex, and in a first degree model its support points are at the extreme points of the simplex. So, keeping in mind that the model (2.5) is invariant w.r.t. the components within the sets $(x_1, x_2,..., x_q), (x_1^*, x_2^*,..., x_q^*), (x_{q+1}^*, x_{q+2}^*,..., x_{q+r}^*)$, we first consider the subclass of designs $\mathcal{D}_1$ within $\mathcal{D}$, with support points and masses as follows:

i. $(\underbrace{1,0,...,0}_{x};\underbrace{1,0,...,0}_{x_{(1)}},\underbrace{0,0,...,0}_{x_{(2)}})$ and permutations respectively within the components of x and within those of $x_{(1)}$, each with mass w_1;

ii. $(\underbrace{1/2,1/2,...,0}_{x};\underbrace{1,0,...,0}_{x_{(1)}},\underbrace{0,0,...,0}_{x_{(2)}})$ and permutations respectively within the components of x and within those of $x_{(1)}$, each with mass w_2;

iii. $(\underbrace{1,0,...,0}_{x};\underbrace{0,0,...,0}_{x_{(1)}},\underbrace{1,0,...,0}_{x_{(2)}})$ and permutations respectively within the components of x and within those of $x_{(2)}$, each with mass w_3;

where $w_i \ge 0,\ 0 \le i \le 4,\ q^2 w_1 + qC(q,2)w_2 + qrw_3 = 1.$

It may be noted that the above design is a saturated design, that is, it as many design points as there are unknown parameters. The parameters μ_{iik} for $1 \le i, k \le q$ are estimated with the help of the design points in (i), while the parameters μ_{ik}^*, for $1 \le i \le q$, $q+1 \le k \le q+r$, are estimated with the help of the points in (iii). Once the parameters μ_{iik} for $1 \le i, k \le q$ are estimated, the parameters μ_{ijk}, $1 \le i, j, k \le q$, $i < j$, can be estimated with the help of the points in (ii). (See Sinha et al. (2010) for a better understanding of the aspect of estimability of model parameters based on a saturated design.)

The information matrix of any design $\xi \in \mathcal{D}_1$ is given by

$$M(\xi) = X \Lambda X',$$

where

$$X = \begin{bmatrix} I_{q^2} & \frac{1}{4} A \otimes I_q & 0 \\ 0 & \frac{1}{4} I_{qC(q,2)} & 0 \\ \hline 0 & 0 & I_{rq} \end{bmatrix} = \left(\begin{bmatrix} I_q & \frac{1}{4} A & 0 \\ 0 & \frac{1}{4} I_{C(q,2)} & 0 \\ \hline 0 & 0 & I_r \end{bmatrix} \otimes I_q \right) = \begin{bmatrix} B & 0 \\ 0 & I_r \end{bmatrix} \otimes I_q, \text{ say,} \tag{3.4}$$

$$\Lambda = Diag(w_1 I_{q^2}, w_2 I_{qC(q,2)}, w_3 I_{rq}) = Diag(w_1 I_q, w_2 I_{C(q,2)}, w_3 I_r) \otimes I_q, \tag{3.5}$$

$$A = \begin{bmatrix} \overbrace{1\ 1\ \dots\ 1}^{q\text{-1 elements}} & \overbrace{0\ 0\ \dots 0}^{q\text{-2 elements}} & 0 & \dots & \overbrace{0}^{\text{1 element}} \\ 1\ 0 \dots\ 0 & 1\ 1 \dots 1 & 0 & \dots & 0 \\ \dots\ \dots\ \dots & \dots\ \dots\ \dots & \dots & \dots & \dots \\ 0\ 0 \dots\ 1 & 0\ 0 \dots 1 & 0 & \dots & 1 \end{bmatrix}, \quad B = \begin{bmatrix} I_q & \frac{1}{4} A \\ 0 & \frac{1}{4} I_{C(q,2)} \end{bmatrix}. \tag{3.6}$$

Since the above design is a saturated one, the optimal allocation of the masses under the D-optimality criterion would be

$$w_1 = w_2 = w_3 = \frac{1}{q[C(q+1,2)+r]}. \tag{3.7}$$

Theorem 3.4: *The D-optimal design in $\mathcal{D}_1$ is D-optimal in $\mathcal{D}$.*

Proof: Let ξ_0 be the D-optimal design in $\mathcal{D}_1$. From (3.4)-(3.6), we can write the information matrix of the D-optimal design ξ_0 in $\mathcal{D}_1$ as

$$M(\xi_0) = \begin{bmatrix} (1/q - r w_{30}) B \Lambda^*_{(1)} B' & 0 \\ 0 & w_{30} I_r \end{bmatrix} \otimes I_q,$$

where $w_{30} = \frac{1}{q[C(q+1,2)+r]}$, $\Lambda_{(1)} = Diag(w^*_{10} I_q, w^*_{20} I_{C(q,2)})$, $w_{i0}{}^* = \frac{w_{i0}}{\frac{1}{q} - r w_{30}} = \frac{1}{C(q+1,2)}$,

$i = 1,2, \quad q w^*_{10} + C(q,2) w^*_{20} = 1.$

$B \Lambda^*_{(1)} B'$ is the information matrix of the D-optimal design $\xi_{(1)}$ for estimating the C(q+1,2) parameters of a q-component full quadratic mixture model, $\eta_{\boldsymbol{x}} = \boldsymbol{f}_1(\boldsymbol{x})'\boldsymbol{\theta}$, where $\boldsymbol{f}_1(\boldsymbol{x})$ is given in (2.6), and $\xi_{(1)}$ is given by Theorem 3.1. Hence, by Equivalence Theorem of Kiefer (1974),

$$\boldsymbol{f}_1(\boldsymbol{x})'(B\Lambda^*_{(1)}B')^{-1}\boldsymbol{f}_1(\boldsymbol{x}) \le C(q+1,2), \quad \text{for all } \boldsymbol{x}\in\Xi_1,$$

with equality holding at the support points.

Now, l.h.s. –r.h.s. of (3.3) gives

$$\boldsymbol{f}(\boldsymbol{x},\boldsymbol{x}^*)'M^{-1}(\xi^*)\boldsymbol{f}(\boldsymbol{x},\boldsymbol{x}^*) - q[C(q+1,2)+r]$$
$$= \frac{1}{\frac{1}{q} - rw_{30}}\boldsymbol{f}_1(\boldsymbol{x})'(B\Lambda^*_{(1)}B')^{-1}\boldsymbol{f}_1(\boldsymbol{x}) \times \boldsymbol{x}^{*\prime}_{(1)}\boldsymbol{x}^*_{(1)} + \frac{1}{w_{30}}\boldsymbol{x}^{*\prime}_{(2)}\boldsymbol{x}^*_{(2)} \times \boldsymbol{x}'\boldsymbol{x} - q[C(q+1,2)+r]$$
$$\le q[C(q+1,2)+r][\boldsymbol{x}^{*\prime}_{(1)}\boldsymbol{x}^*_{(1)} + \boldsymbol{x}^{*\prime}_{(2)}\boldsymbol{x}^*_{(2)} \times \boldsymbol{x}'\boldsymbol{x} - 1] \le 0,$$

since the maximum value of $\boldsymbol{x}'\boldsymbol{x}$ is 1, and because of the restrictions $0 \le x_i^* \le 1, i = 1(1)(q+r)$ and $\sum_{i=1}^{q+r} x_i^* = 1$, we have

$$\boldsymbol{x}^{*\prime}_{(1)}\boldsymbol{x}^*_{(1)} + \boldsymbol{x}^{*\prime}_{(2)}\boldsymbol{x}^*_{(2)} \times \boldsymbol{x}'\boldsymbol{x} = \sum_{i=1}^{q} x_i^{*2} + \sum_{i=q+1}^{q+r} x_i^{*2} \times \sum_{i=1}^{q} x_i^2 \le (\sum_{i=1}^{q} x_i^*)^2 + (\sum_{i=q+1}^{q+r} x_i^*)^2 \le 1 - 2(\sum_{i=1}^{q} x_i^*)(\sum_{i=q+1}^{q+r} x_i^*) \le 1.$$

Further, at each of the support points of ξ^*, $\boldsymbol{f}_1(\boldsymbol{x})'(B\Lambda^*_{(1)}B')^{-1}\boldsymbol{f}_1(\boldsymbol{x}) = C(q+1,2)$ and $\boldsymbol{x}^{*\prime}_{(1)}\boldsymbol{x}^*_{(1)} + \boldsymbol{x}^{*\prime}_{(2)}\boldsymbol{x}^*_{(2)} \times \boldsymbol{x}'\boldsymbol{x} = 1$, so that equality in (3.3) holds.

To get the A-optimal design, we note that for a quadratic response function in a s – component mixture experiment the optimal design for parameter estimation has its support points at the barycentres of depth 0 and 1 of the simplex for $s \ne 3$, and at the barycentres of depth 0, 1 and 2 for $s = 3$ (cf. Galil and Kiefer, 1977). On the other hand, in a first degree model its support points are at the extreme points of the simplex. We therefore, initially confine our search within the subclass $\mathcal{D}_1$ of $\mathcal{D}$ for $q \ne 3$, and within the subclass $\mathcal{D}_2$ of $\mathcal{D}$ for $q = 3$, where a typical design in $\mathcal{D}_2$ has the support points (i) – (iv) of designs in $\mathcal{D}_1$ and the support points

iv. $(\underbrace{1/3, 1/3, 1/3}_{\boldsymbol{x}}; \underbrace{1,0,0}_{\boldsymbol{x}_{(1)}}, \underbrace{0,0,...,0}_{\boldsymbol{x}_{(2)}})$ and permutations within the components of $\boldsymbol{x}_{(1)}$, each with mass w_4,

where $w_i \ge 0,\ 0 \le i \le 4,\ 9w_1 + 9w_2 + 3rw_3 + 3w_4 = 1.,$ ***or*** $3w_1 + 3w_2 + rw_3 + w_4 = \frac{1}{3}.$ (3.4)

Proceeding as before, it is easy to check that for any design $\xi \in \mathcal{D}_1$,

$$\text{Trace } [M(\xi)^{-1}] = \text{Trace}\left\{\begin{bmatrix} (1/q - rw_3)B\Lambda_{(1)}B' & 0 \\ 0 & w_3 I_r \end{bmatrix}^{-1} \otimes I_q\right\},$$

$$= q\text{Trace}\left[\frac{(B\Lambda_{(1)}B')^{-1}}{(1/q - rw_3)} + \frac{r^2}{rw_3}\right],$$

where $\Lambda_{(1)} = Diag(w_1^* I_q, w_2^* I_{C(q,2)})$, $w_i^* = \dfrac{w_i}{\frac{1}{q} - rw_3}$, $i = 1,2$, $qw_1^* + C(q,2)w_2^* = 1$.

$B\Lambda_1^* B'$ gives the information matrix of a design ξ^* for estimating the parameters of a full quadratic response function for a q-component mixture, with support points at the barycentres of depth 0 and 1 of the simplex and mass w_1^* for each barycentre of depth 0 and w_2^* for each barycentre of depth 1. From Theorem 3.1, ξ^* is the A-optimal design when $w_1^* = w_{10}^* = 1/q$, and $w_2^* = w_{20}^* = 1/{}^{q+1}C_2$.

Let, $A = \{Trace(B\Lambda_1^* B')^{-1} |_{w_{i0}, w_{ij0}}\}$. By Cauchy-Schwartz inequality,

$$Trace[M(\xi)^{-1}] \geq q\left[\frac{qA}{1 - rqw_3} + \frac{qr^2}{rqw_3}\right] \geq q(\sqrt{qA} + r\sqrt{q})^2,$$

with equality holding at $w_3 = \dfrac{1}{rq} \times \dfrac{r\sqrt{q}}{\sqrt{qA} + r\sqrt{q}} = \dfrac{1}{q(\sqrt{A} + r)} = w_{30}$, say.

Hence the optimal mass allocation is $w_i = w_{i0}$, $i = 1(1)4$, where $w_{i0} = w_{i0}^*[\frac{1}{q} - rw_{30}]$, $i = 1,2$.

For $q = 3$, the information matrix of any design $\xi \in \mathcal{D}_2$ is given by

$$M(\xi) = X\Lambda X',$$

where

$$X = \begin{bmatrix} I_3 & \frac{1}{4}M & \frac{1}{9}1_3 & 0 \\ 0 & \frac{1}{4}I_3 & \frac{1}{9}1_3 & 0 \\ 0 & 0 & 0 & I_r \end{bmatrix} \otimes I_3, \quad \Lambda = \begin{bmatrix} w_1 I_3 & 0 & 0 & 0 \\ 0 & w_2 I_3 & 0 & 0 \\ 0 & 0 & w_4 I_3 & 0 \\ 0 & 0 & 0 & w_3 I_r \end{bmatrix} \otimes I_3, \quad M = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

Hence,

$$Trace(X\Lambda X')^{-1} = 3[Trace(T\Lambda_1 T')^{-1} + \frac{r}{w_3}], \tag{3.5}$$

where $T = \begin{bmatrix} I_3 & \frac{1}{4}M_1 & \frac{1}{9}\underline{1} \\ 0 & \frac{1}{4}I_3 & \frac{1}{9}\underline{1} \end{bmatrix}$, $\Lambda_1 = \begin{bmatrix} w_1 I_3 & 0 & 0 \\ 0 & w_2 I_3 & 0 \\ 0 & 0 & w_4 \end{bmatrix} = (\frac{1}{3} - w_3)\begin{bmatrix} w_1^* I_3 & 0 & 0 \\ 0 & w_2^* I_3 & 0 \\ 0 & 0 & w_4^* \end{bmatrix}$,

$w_i^* = \dfrac{w_i}{\frac{1}{3} - w_3}$, $i = 1,2,4$, $w_1^* + w_2^* + w_4^* = 1$ (from (3.4)). Hence,

$$Trace(X\Lambda_1 X')^{-1} = 3\left[\frac{3Trace(T\Lambda_1^* T')^{-1}}{1-3w_3} + \frac{3r}{3w_3}\right], \text{ where } \Lambda_1^* = \begin{bmatrix} w_1^* I_3 & 0 & 0 \\ 0 & w_2^* I_3 & 0 \\ 0 & 0 & w_4^* I_r \end{bmatrix}.$$

$T\Lambda_1^* T'$ is the information matrix of a design ξ^* for estimating the parameters of a 3-component full quadratic mixture model, with support points at the barycentres of depth 0, 1 and 2 and mass w_1^* for each barycentre of depth 0 w_2^* for each barycentre of depth 1 and w_3^* for barycentre of depth 2. From Theorem 3.1, ξ^* is the A-optimal design when $w_1^* = w_{10}^* = 0.1417$, $w_2^* = w_{20}^* = 0.1873$ and $w_3^* = w_{30}^* = 0.0130$. (Cf. Galil and Kiefer, 1977).

Let,

$$A = Trace((T\Lambda_1^* T')^{-1} |_{w_i^* = w_{i0}^*, i=1,2,4}\}, \text{say.}$$

By Cauchy-Schwartz inequality,

$$Trace(X\Lambda_1 X')^{-1} \geq 3\left[\frac{3A}{1-3w_3} + \frac{3r}{3w_3}\right] \geq (\sqrt{3A} + \sqrt{3r})^2,$$

with equality holding at $w_3 = \frac{1}{3}[\frac{\sqrt{r}}{\sqrt{A} + \sqrt{r}}] = w_{30}$, say.

Hence the optimal mass allocation is $w_i = w_{i0}$, $i = 1(1)4$, where $w_{i0} = w_{i0}^*[\frac{1}{3} - w_{30}]$, $i = 1,2,4$,

As algebraic derivation is rather tedious, we have numerically checked, using several points in the domain (2.7), that the conditions of the Equivalence Theorem are satisfied by the above designs. The following table gives the A-optimal designs for some combinations of (q, r).

Table 3.1: The A-optimal designs for parameter estimation for some combinations of (q, r)

q	***r***	***w_1***	***w_2***	***w_3***	***w_4***
2	1	0.0984	0.1761	0.1271	-
3	1	0.0447	0.0591	0.0177	0.0041
3	2	0.0437	0.0578	0.0246	0.0040
4	2	0.0134	0.0174	0.0458	-

4 Concluding Remarks

The paper studies a very realistic situation observed in agricultural fields. Manure is used to make the soil fertile. For some crops it is added more than once to the soil at intermediate time points before harvesting. However, if a crop does not show satisfactory growth, the farmers may improve upon the manure by adding some new ingredients. This is done because good growth of crop is expected to result in good yield. In our study we treat manure as a mixture and suggest optimum designs for estimating the parameters of the yield function. While the D-optimal design is a saturated design, the A-optimal design needs one extra point, namely the overall centroid point, when there are three components in the manure used during sowing of the crop. However, the mass at the overall centroid point is pretty low (vide Table 3.1) so that it may be ignored unless the experiment is conducted for a large number of runs.

Acknowledgement

The authors thank the anonymous reviewer for the fruitful comments and suggestions, which have immensely helped to improve the paper.

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