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D-Optimal Designs and Model Uncertainty in Mixture Experiments

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Abstract

The problem of determining the optimal design to examine the degree of the polynomial that well approximates the response function has been studied by many authors. Stigler (1971) suggested optimal designs for polynomial regressions that enable efficient inferences to be made about the fitted model and, at the same time, check its adequacy in defining the mean response. In this paper we consider a mixture experiment and investigate the optimal design that can estimate the parameters of a first degree mixture model and also check the model adequacy as against the presence of one or more interaction terms.

Keywords and Phrases: Mixture experiment, model adequacy, D-optimality criterion, optimal design, power constraint.

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1 Introduction

A standard design problem is concerned with choosing the values of the independent variables so as to come up with the best experiment. To define a "best design" or an 'optimum design', several optimality criteria have been proposed and discussed by many authors in the past several decades, (see, for example, Kiefer (1959, 1961, 1974), Karlin and Studden (1966), Atwood (1969)). However, these criteria have a serious drawback, namely they are model dependent. As such, if the assumed model is inadequate in approximating the response function, they fail to detect this departure, no matter how large the sample size is. One attempt to address this drawback has been made by Box and Draper (1959, 1963), who suggested that a design should minimize $V + B$, where V is the error due to sampling variation and B is the error due to inadequate modeling, and at the same time maximize the power of a goodness-of-fit test for some class of alternative models. The main weakness of the approach is that it depends on the alternative model whose parameters are unknown. A further suggestion by Box and Draper to overcome this difficulty was to minimize B alone. However, as Stigler (1971) observed, "minimum bias designs, while they are an important attempt to meet realistically the problem of checking the representational adequacy of the model, may often be inappropriate, inefficient, or both". This observation reduces the appeal of the approach of Karson et al. (1969), who proposed to choose the estimator by minimizing B, rather than by minimizing V.

Stigler (1971) suggested two optimality criteria, which "can be considered as compromises between the incompatible goals of inference about the regression function under an assumed model and of checking the model's adequacy" (quote Stigler, 1971). He called them *restricted D- and G-optimality criteria* and studied them for the problem of estimating a regression function which can be well-approximated by a polynomial. He imposed the condition that the independent variable lies in the interval [-1, 1], and illustrated the use of the criteria by assuming a first degree polynomial model as against a second degree polynomial. His study yielded optimum designs which were superior to designs proposed by others, including the minimum bias designs. An algorithm for constructing these designs was suggested by Mikulecka (1983). Using a technique involving canonical moments, Studden (1982) investigated the problem of design construction under a generalization of Stigler's criterion. Later, Lee (1987, 1988) introduced several constrained optimality criteria and provided necessary and sufficient conditions for a design to be optimal.

In this paper, we adopt the approach of Stigler (1975) to suggest optimum designs in mixture experiments that would permit efficient inferences to be made about the assumed model while still allowing the model to be checked for adequacy. We assume a first degree mixture model and attempt to design an experiment which allows to check the competence of the model as against a quadratic mixture model, and also tests hypotheses like $\beta_{ij} = 0$, with some specified degree of precision. The paper is organized as follows. Section 2 discusses the problem and its perspectives. Optimal designs are studied in Section 3. Optimum designs in some specific situations are computed in Section 4. Finally, in Section 5, concluding remarks on the study are made.

2 The problem and its perspectives

For the sake of completeness, we start with model adopted by Stigler (1971). He considered the standard univariate regression set-up, where an experiment is conducted with n fixed values of the independent variable $x, x \in [-1, 1]$, and the response Y is measured. He assumed that the response function is sufficiently smooth over the range of interest and is adequately represented by an m-th degree polynomial

$$P_m : E(Y \mid x) = \beta_0 + \beta_1 + \beta_2 x^2 + \ldots + \beta_m x^m,$$

where β_i's are unknown.

In order to find an optimum design which (i) checks for the adequacy of the fitted model P_m, (ii) enables to make reasonably efficient inferences concerning the model (parameters) if it is adequate, and (iii) does not depend on the unknown parameters, he proposed a restricted D-optimality criterion which maximizes $\mid M_m(\xi) \mid$, where $M_m(\xi)$ is the information matrix of a design ξ when the fitted model is P_m, subject to the constraint $\mid M_m(\xi) \mid \leq C \mid M_{m+1}(\xi) \mid$.

Stigler (1971) attempted to provide a justification for imposing this constraint. This refers to the estimation of the 'extra' parameter β_{m+1} for which an expression for the variance of the least square estimator $\hat{\beta}_{m+1}$ is given by Var $(\hat{\beta}_{m+1}) = \sigma^2 \mid M_m(\xi) \mid . \mid M_{m+1}(\xi) \mid^{-1}$. Next he argues "minimize the generalized variance of the least squares estimators $\hat{\beta}_1, \hat{\beta}_2, \ldots \hat{\beta}_m$ for the model P_m subject to the constraint that $\text{Var}(\hat{\beta}_{m+1}) \leq \sigma^2 C$."

At this stage, it seems imperative to assume a prior knowledge about the error variance σ^2 as otherwise it is impractical to attach any meaning to the constraint $\sigma^2 C$. Henceforth, we will assume without any loss that $\sigma^2 = 1$.

Stigler (1971) further indicated that in the event of finding an optimum design to test the null hypothesis $H_0 : \beta_{m+1} = 0$ against the alternative $H_A : \beta_{m+1} 0$, for a given level of significance and the power at a stated alternative not below a specified value, the restricted D- optimality criterion can be made to meet the requirement.

Following Stigler (1971), we attempt to investigate optimum designs with the properties (i) - (iii) above in the mixture set-up.

Consider a mixture experiment that is run under the assumption that the first degree model is adequate to approximate the response function:

$$E(Y \mid \boldsymbol{x}) = \zeta_{\boldsymbol{x}}^{(1)} = \sum_i \beta_i x_i, \tag{1}$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_q)$ denotes the mixing proportions defined in the experimental region

$$\Xi = \{(x_1, x_2, \ldots, x_q) \mid x_i \geq 0, i = 1, 2, \ldots, q, \Sigma x_i = 1\}.$$

Several optimum designs have been suggested for estimation of β_is using different optimality criteria. (Cf. Sinha, et al., 2014). However, these designs fail to check whether the assumed model provides an adequate fit to the true response function, no matter how large the sample size is.

Suppose the experimenter suspects that there might be interaction between the first and some of the other components and considers a quadratic model of the form

$$E(Y \mid \boldsymbol{x}) = \zeta_{\boldsymbol{x}}^{(2)} = \sum_i \beta_i x_i + \sum_{2 \leq j \leq s} \beta_{1j} x_1 x_j, \tag{2}$$

where $s \leq q$.

There exist optimum designs for testing the significance of the parameters β_{1j}s or estimating them. However, such designs will not be optimum for estimating the parameters of (1) in case model (1) is true. Also, even if β_{1j}s are significant, these designs will not be optimal for making global inferences about the response function (2).

It would, therefore, be worthwhile to design a mixture experiment which allows efficient estimation of the parameters of model (1), and also tests hypotheses of the form $\beta_{1j} = 0, j = 2, 3, \ldots, s, 2 \leq s \leq q$, with some specified degree of precision. Following Stigler (1971), we define a criterion that *minimizes the generalized variance of the least squares estimators of β_is of the model (1) subject to the constraint that the minimum power of the test for testing $\beta_{1j} = 0$ for $j = 2, 3, \ldots, s$ attains at least a specified value C (in units of σ^2, the error variance).*

The choice of C reflects a compromise between two conflicting goals: precise inference about β_{1j}s and precise inference about the parameters of model (1). While C should be small to yield efficient designs for model (1), sufficiently large C will detect departures from the model with a specified power of the test for $\beta_{1j} = 0, j \geq 2$. We note that for $C = 0$, the above criterion gives the D-optimal design for estimating the parameters of model (1). On the other hand, when C attains its maximum value, we get the optimal design for testing $\beta_{1j} = 0, j \geq 2$.

3 Restricted D-optimal design for efficient estimation of $\boldsymbol{\beta_i}$'s subject to testing $\boldsymbol{\beta_{1j} = 0}$ for $\boldsymbol{2 \leq j \leq s (s \leq q)}$ with specified degree of precision

In consideration of the model fitting issue, the experimenter wishes to examine whether the interactions in model (2) influence the mean response or not, i.e. he wants to test the null hypothesis

$$H_0 : \beta_{12} = \beta_{13} = \ldots = \beta_{1s} = 0. \tag{3}$$

Let us write the models (1) and (2) as

$$\zeta_x^{(1)} = f_1'(x)\beta^{(1)}$$
$$\zeta_x^{(2)} = f_1'(x)\beta^{(1)} + f_2'(x)\beta^{(2)},$$

where

$$\boldsymbol{f}_1(\boldsymbol{x}) = (x_1, x_2, \ldots, x_q)', \boldsymbol{f}_2(\boldsymbol{x}) = (x_1x_2, x_1x_3, \ldots, x_1x_s)',$$
$$\boldsymbol{\beta}^{(1)} = (\beta_1\beta_2, \ldots, \beta_q)', \boldsymbol{\beta}^{(2)} = (\beta_{12}, \beta_{13}, \ldots, \beta_{1s})'.$$

The hypothesis (3) is tested using the classical F-test.

For any given design ξ, let $M(\xi)$ denote the information matrix for $\boldsymbol{\beta} = (\boldsymbol{\beta}^{(1)'}, \boldsymbol{\beta}^{(2)'})'$, which may be partitioned as

$$M(\xi) = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}, \tag{4}$$

where $M_{ij} = E_\xi[\boldsymbol{f}_i(\boldsymbol{x})\boldsymbol{f}_j(\boldsymbol{x})'], i, j = 1, 2$.

M_{11} is the information matrix for $\boldsymbol{\beta}^{(1)}$ in model (1). The power of the test for (3) is a non-decreasing function of the non-centrality parameter

$$\delta = \boldsymbol{\beta}^{(2)'}[Disp\ (\hat{\boldsymbol{\beta}}^{(2)})]^{-1}\boldsymbol{\beta}^{(2)} = \frac{1}{\sigma^2}\boldsymbol{\beta}^{(2)'}M_{22,1}\boldsymbol{\beta}^{(2)},$$

where, σ^2 is the error variance, $M_{22,1} = M_{22} - M_{21}M_{11}^{-1}M_{12}$ and $Disp(\hat{\boldsymbol{\beta}}^{(2)}) = \sigma^2 M_{22,1}^{-1}$.

Here under a non-null hypothesis, $\boldsymbol{\beta}^{(2)}$ is unknown. Let us assume that $\boldsymbol{\beta}^{(2)}$ is such that $\Omega = \{\boldsymbol{\beta}^{(2)} : \boldsymbol{\beta}^{(2)'}\boldsymbol{\beta}^{(2)} = D\}$, for some $D > 0$ and known.

So, the statement "power of the test is at least equal to C for $\boldsymbol{\beta}^{(2)}$ belonging to Ω'' is equivalent to the statement" $\boldsymbol{\beta}^{(2)'} M_{22,1} \boldsymbol{\beta}^{(2)} \geq C_0$ for $\boldsymbol{\beta}^{(2)}$ belonging to Ω'', for some function C_0 of C. It is tacitly assumed that the bounds are expressed in units of σ^2. Now,

$$\boldsymbol{\beta}^{(2)'} M_{22,1} \boldsymbol{\beta}^{(2)} \geq C_0, \textit{ for all } \boldsymbol{\beta}^{(2)} \in \Omega$$

$$\Leftrightarrow \min_{\boldsymbol{\beta}^{(2)} \ni \boldsymbol{\beta}^{(2)} \boldsymbol{\beta}^{(2)} = D} \boldsymbol{\beta}^{(2)'} M_{22,1} \boldsymbol{\beta}^{(2)} \geq C_0$$

$$\Leftrightarrow \lambda_{\min}(M_{22,1}) \geq C_0 D, \tag{5}$$

where $\lambda_{\min}$ denotes the minimum eigen value of $M_{22,1}$.

WOLG, we can take $D = 1$.

Hence our problem reduces to finding a design ξ_0 for the problem

$$\begin{aligned} &\text{maximize } \phi_2(\xi) = \log \mid M_{11}(\xi) \mid \\ &\text{subject to } \phi_1(\xi) = \lambda_{\min}(M_{22,1}(\xi)) \geq C_0. \end{aligned} \tag{6}$$

Let, $\mathcal{D}(C_0)$ denote the class of all designs ξ satisfying the restriction $\phi_1(\xi) \geq C_0$, and Δ_{C_0} be the set of all constrained optimal designs for a specific choice of C_0, that is, $\Delta_{C_0} = \{\xi \mid \xi \text{ maximizes } \phi_2(\xi) \text{ subject to the constraint } \phi_1(\xi) \geq C_0\}$. If there be a choice between designs in Δ_{C_0}, then we select the design that does the best on the primary criterion $\phi_1(\xi)$. Arguing as in Stigler (1971), it is easy to show that $\mathcal{D}(C_0)$ is a convex set and the set of restricted D-optimal designs Δ_{C_0} forms a convex subset of $\mathcal{D}(C_0)$.

Let ξ_1 be a restricted D-optimal design. Let us define $\xi_P \in \mathcal{D}(C_0)$ such that $\xi_P(x) = \xi_1(Px)$, where P is a permutation matrix. The matrix P depends on the model and the hypothesis considered as is evident from the examples considered below.

Example 3.1: Let $s = 2$ in (2). The model is, therefore,

$$E(Y \mid \boldsymbol{x}) = \zeta_x^{(2)} = \sum_i \beta_i x_i + \beta_{12} x_1 x_2,$$

and the hypothesis to be tested is $H_0 : \beta_{12} = 0$. In this case, the problem is invariant with respect to x_1 and x_2, and with respect to $x_3, x_4, \ldots, x_q$ and the permutation matrix is

$$P = \left[\begin{array}{cc|cc} 0 & 1 & 0 & 0\ldots0 \\ 1 & 0 & 0 & 0\ldots0 \\ \hline & 0 & & P_{q-2} \end{array}\right],$$

where P_{q-2} denotes a permutation of the matrix I_{q-2}.

Example 3.2: Suppose $s = 3$. In this case model (2) reduces to

$$E(Y \mid x) = \zeta_x^{(2)} = \sum_i \beta_i x_i + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3,$$

and the hypothesis to be tested is $H_0 : \beta_{12} = \beta_{13} = 0$. Thus, the problem is invariant with respect to x_2 and x_3, and with respect to $x_4, x_5 \ldots, x_q$, and the permutation matrix is

$$P = \left[\begin{array}{c|cc|c} 1 & 0 & 0 & 0\ldots0 \\ \hline 0 & 0 & 1 & 0\ldots0 \\ 0 & 1 & 0 & 0\ldots0 \\ \hline 0 & & 0 & P_{q-3} \end{array}\right],$$

where P_{q-3} denotes a permutation of the matrix I_{q-3}.

In fact, for any general $s, 3 \le s \le q$, the problem is invariant with respect to $x_2, x_3, \ldots, x_s$, and with respect to $x_{s+1}, x_{s+2}, \ldots, x_q$, and the permutation matrix has the form

$$P = \left[\begin{array}{c|c|c} 1 & \underline{0}' & \underline{0}' \\ \hline \underline{0} & P_{s-1} & 0 \\ \hline \underline{0} & 0 & P_{q-s} \end{array}\right],$$

Then, ξ_P is also a restricted D-optimal design since both $\mid M_{11} \mid$ and $\lambda_{\min}(M_{22,1}^{-1})$ are invariant with respect to the corresponding permutations.

Now, consider the design ξ^* defined as $\xi^* = \frac{1}{Q} \sum_{i=1}^{Q} \xi_{P_1}$, where Q denotes the number of permutations leading to invariant null hypothesis. In example 3.1, $Q = 2!.(q-2)!$, while in example 3.2, $Q = 2!(q-3)!$. In the case of general $s, 3 \le s \le q, Q = (s-1)!(q-s)!$.

Since the set of restricted D-optimal designs forms a convex subset of $\mathcal{D}(C_0), \xi^*$, which is a permutation invariant design, is also a restricted D-optimal design.

Thus, we have the following theorem:

Theorem 3.1: *There exists a permutation invariant restricted D-optimal design in* $\mathcal{D}(C_0)$.

The theorem simplifies the search for the optimal design by restricting to the class of symmetric designs that are permutation-invariant with respect to the invariant components under the null hypothesis. The search can be further reduced by the following consideration:

Lemma 3.1: Consider the model $E(Y \mid x) = \zeta_x^{(2)} = \sum_i \beta_i x_i + \sum_{1\leq i<j\leq q} \beta_{ij} x_i x_j, \boldsymbol{x} \in \Xi$, and let $(x_1, x_2, \dots x_i, \dots x_j, \dots, x_q)$ be a support point of an arbitrary design ξ. If $\beta_{ij} = 0$ for some $i < j$, it is always possible to find two support points viz. $(x_1, x_2, \dots, x_i + x_j, \dots, 0, \dots, x_q)$ and $(x_1, x_2, \dots, 0, \dots, x_i + x_j, \dots, x_q)$ with weights $x_i/(x_i + x_j)$ and $x_j/(x_i + x_j)$, respectively such that its information matrix dominates the information matrix of the single point design $(x_1, x_2, \dots, x_i, \dots x_j, \dots, x_q)$.

The proof is routine.

Hence, if an interaction effect, say β_{ij}, is absent in the model then an improved design can be obtained by including support points in which x_i and x_j are not simultaneously non-zero. In our study we have, therefore, confined our search to the class of designs $\mathcal{D}_1(C_0)(\subset \mathcal{D}(C_0))$ with support points

(i) $(1, 0, \dots, 0)$ and its permutations, and

(ii) points of the form $(a, 0, \dots, 1 - a, \dots, 0)$ (with non-zero elements in the first and j-th positions) if $\beta_{1j} \neq 0$. (7)

Remark 3.1: When $\beta_{1j} = 0, 3 \leq j \leq q$, there is invariance between x_1 and x_2, and therefore the support points of the optimum design are the extreme points of the simplex and the point $(1/2, 1/2, 0, \dots, 0)$.

Remark 3.2: When $\beta_{1j} = 0, s + 1 \leq j \leq q$, for some $s \geq 3$, there is invariance between $x_2, \dots x_s$ and between $x_{s+1}, x_{s+2}, \dots, x_q$.

4 Optimum designs in specific situations

In this section we find the optimum design within $\mathcal{D}_1(C_0)$ for various forms of the alternative model (2).

4.1 Suppose the alternative model is $\zeta_x^{(2)} = \sum_i \beta_i x_i + \beta_{12} x_1 x_2$.

Here, there is invariance between components 1 and 2, and between components $x_3, x_4, \ldots, x_q$. The optimal design for the problem (5), therefore belongs to a class that assigns mass α to the extreme points $(1, 0, \ldots, 0)$ and $(0, 1, \ldots, 0)$, mass γ to each of the remaining extreme points of the simplex and a mass β to the point $(1/2, 1/2, 0, \ldots, 0)$, where $2\alpha + (q-2)\gamma + \beta = 1$.

For any design ξ, we get

$$\phi_2(\xi) = \alpha\gamma^{q-2}[\alpha + \frac{1}{2}\beta] = \frac{\alpha\gamma^{q-2}}{2}[1-(q-2)\gamma],$$

$$\phi_1(\xi) = \frac{\alpha(1-2\alpha-(q-2)\gamma)}{8[1-(q-2)\gamma]} \leq \frac{1}{64}.$$

For a given C_0, the optimal value of α and γ can be obtained by solving the non-linear programming problem

$$\text{maximize } f(\alpha,\gamma) = \alpha\gamma^{q-2}[\alpha + \frac{1}{2}\beta] = \frac{\alpha\gamma^{q-2}}{2}[1-(q-2)\gamma],$$

$$\text{subject to } \frac{\alpha(1-2\alpha-(q-2)\gamma)}{8[1-(q-2)\gamma]} \geq C_0, \alpha+\gamma \leq 1, 0 \leq \alpha \leq \frac{1}{2}, 0 \leq \gamma \leq \frac{1}{q-2}.$$

Since $M_{22.1} \leq \frac{1}{64}, C_0$ cannot exceed $\frac{1}{64}$.

Table 4.1 gives the optimal values of α and γ for some values of $q (\geq 3)$ and C_0.

Table 4.1: Optimum designs in $\mathcal{D}_1$ for some values of C_0 in a q- component mixture

q	C_0	α	β	γ	$\mid M_{11} \mid$
3	0.002	0.3195	0.0337	0.3273	0.03517322848
	0.006	0.2885	0.1152	0.3078	0.03073559859
	0.010	0.2534	0.2338	0.2594	0.02433944299
	0.015	0.2454	0.4697	0.0395	0.004659133855
4	0.002	0.2376	0.0344	0.2452	0.003640516384
	0.006	0.2114	0.1242	0.2264	0.0029661401933
	0.010	0.2000	0.2668	0.1666	0.0018514518642
	0.015	0.2426	0.4750	0.0198	4.59289961E-5
5	0.002	0.1885	0.0350	0.1960	2.92409516E-4
	0.006	0.1681	0.1343	0.1765	2.17382987E-4
	0.010	0.1825	0.2855	0.1165	9.38669829E-5
	0.015	0.2407	0.4796	0.0130	2.53391735E-7
6	0.002	0.1551	0.0428	0.1617	1.8740489948E-5
	0.006	0.1436	0.1512	0.1404	1.2233908896E-5
	0.010	0.1753	0.2950	0.0886	3.490347345E-6
	0.015	0.2454	0.4896	0.0049	7.149964739E-11

4.2 Suppose the alternative model is $\zeta_x^{(2)} = \sum\limits_i \beta_i x_i + \sum\limits_{2 \leq j \leq q} \beta_{1j} x_1 x_j$.

In this case, there being invariance among components $2, 3, \ldots, q$, we confine to the class that assigns a mass α to the extreme point $(1, 0, \ldots, 0)$, mass γ to each of the remaining extreme points of the simplex and a mass β to each of the points of the form $(a, 1-a, 0, \ldots, 0), (a, 0, 1-a, 0, \ldots, 0), \ldots, (a, 0, \ldots, 0, 1-a)$, where $\alpha+(q-1)(\beta+\gamma) = 1$. Clearly, the design is saturated.

Then, for any design ξ,

$$\phi_2(\xi) = [\gamma + (1-a)^2\beta]^{q-2}[\alpha\{\gamma + (1-a)^2\beta\} + (q-1)a^2\beta\gamma] \tag{8}$$

$$M_{22.1} = \frac{a^2(1-a)^2\beta}{\gamma + (1-a)^2\beta}\left[\gamma \boldsymbol{I}_{q-1} - \frac{a^2\gamma^2}{(q-1)a^2\beta\gamma + (\gamma + (1-a)^2\beta)\alpha}\beta \mathbf{1}_{q-1}\mathbf{1}'_{q-1}\right].$$

The distinct eigen values of $M_{22.1}$ are $\lambda_1 = \frac{a^2(1-a)^2\beta\gamma}{\gamma+(1-a)^2\beta}$ and $\lambda_2 = a^2(1-a)^2\beta\gamma\alpha[\{\alpha + (q-1)a^2\beta\}\gamma + (1-a)^2\beta\alpha]^{-1}$. It is easy to check that λ_2 is the minimum eigen value, whatever be the unknown parameters.

So, our problem is to maximize (8) with respect to a, α, β and γ subject to $\lambda_2 \geq C_0, \alpha + (q-1)(\beta+\gamma) = 1, 0 \leq a, \alpha \leq 1, 0 \leq \beta, \gamma \leq 1/(q-1)$.

Using Cauchy-Schwartz inequality, it is easy to check that $\lambda_2 \leq 1/64(q-1) = c_0$, say. Hence, C_0 cannot exceed c_0. However, this is a very crude bound and may not be attained by λ_2.

Table 4.2 gives the optimal values of a, α, β and γ for some values of $q(\geq 3)$ and C_0.

Table 4.2: Optimum designs in $\mathcal{D}_2$ for some values of C_0 in a q-component mixture

q	C_0	α	β	γ	a	$\mid M_{11} \mid$
3	0.001	0.2382	0.0167	0.3642	0.4892	0.0123179745
	0.002	0.2270	0.0353	0.3512	0.4782	0.011401509
	0.006	0.1996	0.1433	0.2569	0.4444	0.0067704440
	0.007	0.2068	0.1868	0.2098	0.4507	0.0050268905
4	0.001	0.1844	0.0174	0.2545	0.4771	8.8529086E-4
	0.002	0.1723	0.0386	0.2373	0.4547	7.4725697E-4
	0.003	0.1666	0.0656	0.2122	0.4365	5.9183265E-4
	0.005	0.2101	0.1466	0.1167	0.4607	1.7940228E-4
5	0.0005	0.1576	0.0091	0.2015	0.4773	5.8550308E-5
	0.001	0.1496	0.0190	0.1936	0.4590	5.1783620E-5
	0.002	0.1435	0.0443	0.1698	0.4279	3.6873693E-5
	0.003	0.1600	0.0788	0.1312	0.4230	2.0033288E-5
6	0.0005	0.1462	0.0217	0.1490	0.4114	2.4108438E-6
	0.001	0.1452	0.0322	0.1388	0.4072	1.9417063E-6
	0.002	0.1716	0.0632	0.1025	0.4216	7.7929237E-7
	0.003	0.2496	0.0969	0.0531	0.4951	7.3477238E-8

4.2 Suppose the alternative model is $\zeta_x^{(2)} = \sum_i \beta_i x_i + \sum_{2\leq<j\leq s} \beta_{ij} x_i x_j, 3 \leq s \leq q-1$.

Here there is invariance among components $2, 3, \ldots, s$, and among components $s+1, s+2, \ldots, q$. So we confine to the class of designs that assign a mass α to the extreme point $(1, 0, \ldots, 0)$, mass γ to each of the $(s-1)$ extreme points $(0, 1, 0, \ldots, 0, \ldots, 0)$, $(0, 0, 1, \ldots, 0, \ldots, 0), \ldots, (0, 0, 0, \ldots, 1, \ldots, 0)$ and mass δ to each of the remaining $(q-s)$ extreme points of the simplex, and a mass β to each of the $(s-1)$ points of the form $(a, 1-a, 0, \ldots, 0), (a, 0, 1-a, 0, \ldots, 0), \ldots, (a, 0, \ldots, 1-a, \ldots, 0)$, where $\alpha + (s-1)(\beta+\gamma) + (q-s)\delta = 1$.

For any design ξ we therefore have

$$\phi_2(\xi) = \delta^{q-s}[\gamma + (1-a)^2\beta]^{s-2}[\alpha\{\gamma + (1-a)^2\beta\} + (s-1)a^2\beta\gamma] \tag{9}$$

$$M_{22.1} = \frac{a^2(1-a)^2\beta}{\gamma + (1-a)^2\beta}\left[\gamma \boldsymbol{I}_{s-1} - \frac{a^2\gamma^2}{(s-1)a^2\beta\gamma + (\gamma + (1-a)^2\beta)\alpha}\beta \mathbf{1}_{s-1}\mathbf{1}'_{s-1}\right].$$

The expression for $M_{22.1}$ is similar to that in Case 2, except that q is replaced by s. Hence, it is easy to find the minimum eigen value of $M_{22.1}$.

The optimal values of a, α, β and γ for some values of $q(\geq 3)$ and C_0 are given in Table 4.3.

Table 4.3: Optimum designs in $\mathcal{D}_3$ for some values of C_0 and $s = 3$ in a q-component mixture

q	C_0	α	β	γ	δ	a	$\mid M_{11} \mid$
4	0.002	0.1796	0.0363	0.2782	0.1915	0.4730	8.9563062E-4
	0.005	0.1679	0.1187	0.2180	0.1587	0.4444	5.4504091E-4
5	0.002	0.1483	0.0384	0.2286	0.1588	0.4672	5.6954921E-5
	0.005	0.1536	0.1290	0.1712	0.1229	0.4469	2.7636170E-5
6	0.002	0.1346	0.0591	0.1784	0.1301	0.4460	2.6087455E-6
	0.005	0.1821	0.1552	0.1297	0.0827	0.4650	6.9305479E-7

5 Conclusion

We discuss the necessary theoretical framework and computations for the study and specification of D-optimal mixture designs that permit efficient inferences to be made about the assumed mixture model while still allowing the model to be checked for adequacy. We confine our study to the cases where the competence of a first degree mixture model is examined against possible presence of some quadratic terms.

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