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D-optimal Designs for an Additive Quadratic Mixture Model with Random Regression Coefficients

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SUMMARY

In a mixture experiment, the mean response is assumed to depend only on the relative proportion of ingredients or components present in the mixture. Scheffé (1958, 1963) first systematically considered this problem and introduced different models and designs suitable in such situations. The problem of estimating parameters in a mixture model has been considered by many authors. However, in their studies, they assumed fixed regression coefficient models. In this paper, we consider an additive quadratic mixture model with random regression coefficients and find the optimum design for the estimation of mean regression coefficients using D- optimality criterion.

Keywords: Mixture experiments, Additive quadratic model, Random regression coefficients, Barycentres, D-optimality criterion.

1. INTRODUCTION

In a mixture experiment with q components, the response function η_x depends on the relative proportions $x_1, x_2, ..., x_q$ of the components. The experimental region and the response function in such an experiment differs from the ordinary response surface problem in view of the constraint $\sum_{i=l}^{q} x_i = 1$. Scheffé (1958) first introduced models in canonical forms of different degrees to represent the response function in a mixture experiment.

The commonly used mixture model is the full quadratic model of Scheffé (1958):

$$y = \sum_{i=l}^{q} \theta_i x_i + \sum_{i<j=l}^{q} \theta_{ij} x_i x_j + \varepsilon \qquad (1.1)$$

where ε is the random error with mean 0 and variance σ_ε^2.

An additive quadratic mixture model was introduced by Darroch and Waller (1985) for the case of $q = 3$ as

$$y = \sum_{i=1}^{q} \beta_i^* x_i + \sum_{i=1}^{q} \beta_{ii}^* x_i (1 - x_i) + \varepsilon, \qquad (1.2)$$

where ε has the same distribution as before.

For $q = 3$, the models (1.1) and (1.2) are equivalent, but for $q = 2$ the parameters of the model (1.2) are not uniquely determined. For $q \geq 4$, (1.2) is a special case of (1.1), with the coefficients of (1.1) being governed by a system of linear constraints. The model (1.2) is additive in $x_1, x_2, ..., x_q$, and has fewer parameters than (1.1) when $q \geq 4$. It is also often found to fit data well (see Chan 2000).

Most of the literature on mixture experiments is concerned with finding optimum designs for estimation of model parameters, see, for example, Kiefer (1961), Atwood (1969), Galil and Kiefer (1977), Chan *et al.* (1998), Draper and Pukelsheim (1999). The problem of determining optimum designs for the estimation of some non-linear functions of the regression parameters

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have been studied by Pal and Mandal (2006, 2007, 2008), Mandal and Pal (2008), Mandal *et al.* (2008a, 2008b). However, in all these studies, the authors assumed the regression coefficients to be fixed. Pal *et al.* (2010) studied Scheffé's quadratic mixture model with random regression coefficients and obtained D-optimal designs for the estimation of mean regression coefficients.

In this paper, we consider the problem of determining D-optimal design for the estimation of expected regression coefficients in the additive mixture model due to Darroch and Waller (1985), assuming random regression coefficients. The paper is organized as follows. In Section 2 we formulate and investigate the problem. In Section 3, we determine the optimum designs under the D-optimality criterion. We conclude with some remarks in Section 4.

2. THE PROBLEM AND ITS PERSPECTIVES

Consider a q-component mixture experiment with response function approximated by (1.2), and the factor space

$$\Xi = \{\boldsymbol{x} = (x_1, x_2, ..., x_q) : x_i \geq 0,\ i = 1, 2, ..., q,\ \sum_{i=1}^{q} x_i = 1\} \tag{2.1}$$

In (1.2), we assume that $\beta_i^* = \beta_i + b_i$, $\beta_{ii}^* = \beta_{ii} + b_{ii}$, $i = 1(1)\,q$, where β_i s and β_{ii} s are fixed and b_is and b_{ii}s are independent random, with $E(b_i) = 0$, $E(b_{ii}) = 0$ and $\text{Var}(b_i) = \sigma_i^2$, $\text{Var}(b_{ii}) = \sigma_{ii}^2$. Also, we assume that b_is and b_{ij}s are independent of ε.

Then we can write (1.2) as

$$y = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \beta_{ii} x_i (1 - x_i) + \varepsilon^*, \tag{2.2}$$

where

$$\varepsilon^* = \sum_{i=1}^{q} b_i x_i + \sum_{i=1}^{q} b_{ii} x_i (1 - x_i) + \varepsilon .$$

Then, given an n point design D_n, the observational equations for the modified model can be written as

$$E(\boldsymbol{Y}) = \mathbf{X}\beta, \tag{2.3}$$

where $\boldsymbol{Y}$ is the response vector, $\boldsymbol{X}$ the coefficient matrix and β the vector of fixed regression coefficients.

Hence,

$$\Sigma = \text{Disp}(\boldsymbol{Y}) = \boldsymbol{X} \Lambda \boldsymbol{X}' + \sigma_\varepsilon^2 \boldsymbol{I}_n, \tag{2.4}$$

with

$$\Lambda = \text{Diag}\,(\sigma_1^2, \sigma_2^2, ..., \sigma_q^2, \sigma_{11}^2, \sigma_{22}^2, ..., \sigma_{qq}^2).$$

We shall assume that $\boldsymbol{X'X}$ is non-singular. Then, making use of the fact that under the form (2.4) of Σ, ordinary least squares estimator (OLSE) and the generalized least squares estimator (GLSE) of β are identical (cf. Rao, 1967), we can write

$$\text{Disp}(\hat{\beta}) = \sigma_\varepsilon^2 [\boldsymbol{\Lambda}^* + (\boldsymbol{X'X})^{-1}] \tag{2.5}$$

where $\boldsymbol{\Lambda}^* = (\sigma_\varepsilon^2)^{-1} \boldsymbol{\Lambda}$.

3. DESIGNS AND BARYCENTRES

We shall work with the set up of a continuous design ξ given by:

$$\xi = \begin{Bmatrix} \boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n \\ w_1, w_2, ..., w_n \end{Bmatrix},$$

where $\boldsymbol{x}_i$s denote the support points with corresponding weights w_is.

Then, the moment matrix is given by

$$\boldsymbol{X'X} = \sum_{u=1}^{n} w_u f(\boldsymbol{x}_u) f'(\boldsymbol{x}_u) \tag{3.1}$$

where $f'(\boldsymbol{x}_u) = (x_{u1}, x_{u2}, ..., x_{uq}, x_{u1}(1 - x_{u1}), x_{u2}(1 - x_{u2}), ..., x_{uq}(1 - x_{uq}))$, $u = 1, 2, ..., n$.

We shall consider the D-optimality criterion for selection of optimal design. A design ξ is said to be D-optimal if it minimizes det. [Disp($\hat{\beta}$)], or equivalently, det. $[\Lambda^* + (\mathbf{X'X})^{-1}]$.

A point $\boldsymbol{x} \in \Xi$ is called a barycentre of depth j $(0 \leq j \leq q - 1)$ if $j + 1$ of its q coordinates are equal to $1/(j + 1)$ and the remaining are equal to zero (Galil and Kiefer 1977). The collection of all barycentres of depth j is denoted by J_j. We define $J = \bigcup_{j=0}^{q-1} j_j$. A design which assigns a weight α_{j+1} to each point in J_j $(0 \le j \le q-1)$ is called a weighted centroid design (cf. Draper and Pukelsheim 1999). By the definition of α_j (j = 1, ..., q), it follows that $C(q, 1)\ \alpha_1$ + ... + $C(q, j)\ \alpha_j$ + ... + $C(q, q)\ \alpha_q = 1$, where $C(q, j)$ denotes the binomial coefficient $\dfrac{q!}{j!(q-j)!}$.

4. D-OPTIMAL DESIGNS

In order to find the D-optimal design for estimation of β, we shall assume that $\sigma_i^2 = \lambda_1$ and $\sigma_{ii}^2 = \lambda_2$, for all i. The assumption implies that the problem is invariant with respect to the components x_is. Hence we can find the optimum design within the class of invariant designs.

For the second-degree Scheffé model, Draper *et al*. (2000) established that given any arbitrary symmetric design ξ, there exists a weighted centroid design (WCD) which dominates ξ in the Loewner order sense. Since model (1.2) can be written as a special case of Scheffé's quadratic model (1.1) with $\theta_i = \beta_i$ and $\theta_{ij} = \beta_{ii} + \beta_{jj}$, for all i, j = 1, 2, …, q, $i < j$, Loewner order of the information matrices for the Scheffé model also holds for those of the model (1.2). Hence, using the result of Draper *et al.* (2000), we may restrict our search for the optimal design within the class of WCDs.

Remark 1: From the above argument, it follows that the search for optimal design may be restricted to the class of WCDs for all optimality criteria, which are functions of the information matrix and convex with respect to it, and are invariant with respect to its components.

Remark 2: From (2.5), it is clear that the A-optimal design will be same as that for the corresponding fixed effects model.

For a q-component mixture model, it can be easily checked that the moment matrix of a WCD is obtained in the form

$$\boldsymbol{X'X} = \begin{bmatrix} a_1 I_q + a_2 J_q & b_1 I_q + b_2 J_q \\ b_1 I_q + b_2 J_q & c_1 I_q + c_2 J_q \end{bmatrix},$$

where a_is, b_is and c_is are linear functions of the weights α_js.

We, therefore, obtain $(\boldsymbol{X'X})^{-1}$ in the form

$$(\boldsymbol{X'X})^{-1} = \begin{bmatrix} e_1 I_q + e_2 J_q & d_1 I_q + d_2 J_q \\ d_1 I_q + d_2 J_q & g_1 I_q + g_2 J_q \end{bmatrix},$$

where e_is, f_is and d_is are non-linear functions of α_js.

We have numerically computed α_js for several combinations of (λ_1, λ_2) and for q = 3, 4, …, 10. The following observations have been made from the study

1. For all $3 \le q \le 10$, barycentres of depth atmost 2 form the support points of the D-optimal design. Among these, the barycentres of depth 0 are necessarily the support points of the optimal design.
2. For q = 3, 4, the optimal design assigns positive weights to barycentres of depths 0 and 1 only. Thus, for q = 3, the D-optimal design is saturated.
3. For $5 \le q \le 7$, the optimal design can assign positive weights to barycentres of depths 0, 1and 2 only. However, for given λ_1 as λ_2 increases, the weight at barycentres of depth 2 decreases and tends towards zero while for given λ_2, as λ_1 increases, the weight at barycentres of depth 1 tends towards zero.
4. For $8 \le q \le 10$, the optimal design assigns positive weights to barycentres of depths 0 and 2 only.

Table 4.1 gives the D-optimal designs for q = 3, 4, …, 10 for some combinations of (λ_1, λ_2).

Table 4.1: Showing D-optimal designs for some combinations of (λ_1, λ_2)

q	λ_1	λ_2	$C(q, 1)\alpha_1$	$C(q, 2)\alpha_2$	$C(q, 3)\alpha_3$
3	0	0	0.5000	0.5000	0.0000
	1	1	0.4848	0.5152	0.0000
	1	5	0.4994	0.5006	0.0000
	1	10	0.5149	0.4851	0.0000
	5	1	0.4449	0.5551	0.0000
	5	5	0.4535	0.5465	0.0000
	5	10	0.4633	0.5367	0.0000
4	0	0	0.5000	0.5000	0.0000
	1	1	0.4890	0.5110	0.0000
	1	5	0.5254	0.4746	0.0000

	1	10	0.5590	0.4410	0.0000
	5	1	0.4605	0.5395	0.0000
	5	5	0.4749	0.5251	0.0000
	5	10	0.4911	0.5089	0.0000
5	0	0	0.4946	0.4077	0.0977
	1	1	0.4882	0.4265	0.0853
	1	5	0.4994	0.4368	0.0638
	1	10	0.5117	0.4440	0.0443
	5	1	0.4524	0.3343	0.2133
	5	5	0.4613	0.3524	0.1863
	5	10	0.4712	0.3688	0.1600
	5	200	0.6302	0.3698	0.0000
	50	10	0.3647	0.0000	0.6353
6	0	0	0.4959	0.2753	0.2288
	1	1	0.4869	0.2350	0.2781
	1	5	0.4967	0.2554	0.2479
	1	10	0.5076	0.2731	0.2193
	5	1	0.4538	0.0837	0.4625
	5	5	0.4616	0.1094	0.4290
	5	10	0.4705	0.1343	0.3952
	50	10	0.3764	0.0000	0.6236
7	0	0	0.4897	0.0877	0.4146
	1	1	0.4903	0.0397	0.4700
	1	5	0.4987	0.0640	0.4373
	1	10	0.5082	0.0868	0.4050
	5	1	0.4593	0.0000	0.5407
	5	5	0.4666	0.0000	0.5334
	5	10	0.4748	0.0000	0.5252
8	0	0	0.0500	0.0000	0.5000
	1	1	0.4923	0.0000	0.5077
	1	5	0.5004	0.0000	0.4996
	1	10	0.5096	0.0000	0.4904
	5	1	0.4634	0.0000	0.5366
	5	5	0.4703	0.0000	0.5297
	5	10	0.4778	0.0000	0.5222
9	0	0	0.5000	0.0000	0.5000
	1	1	0.4932	0.0000	0.5068
	1	5	0.5005	0.0000	0.4995
	1	10	0.5089	0.0000	0.4911
	5	1	0.4667	0.0000	0.5333
	5	5	0.4728	0.0000	0.5272
	5	10	0.4801	0.0000	0.5199
10	0	0	0.5000	0.0000	0.5000
	1	1	0.4938	0.0000	0.5062
	1	5	0.5005	0.0000	0.4995
	1	10	0.5083	0.0000	0.4917
	5	1	0.4694	0.0000	0.5406
	5	5	0.4751	0.0000	0.5249
	5	10	0.4819	0.0000	0.5181

5. COMPARISON WITH SATURATED DESIGNS

From Table 4.1 we note that for $4 \le q \le 10$, the D-optimal designs are not saturated. It would, therefore, be interesting to compare the performance of optimum saturated designs as against the optimum designs in the entire class of competing designs. Here we consider a simple sub-class of saturated designs $\mathcal{D}_s$ based on barycentres of depths 0 and (q–2), for a q-component mixture experiment.

In Table 5.1 we give the efficiency factor of the D-optimum design in $\mathcal{D}_s$ with respect to the optimum design given in Table 4.1, for $4 \le q \le 6$.

Table 5.1: Showing the D-optimum design in $\mathcal{D}_s$ for some combinations of (λ_1, λ_2) and its efficiency for $4 \le q \le 6$

q	λ_1	λ_2	$C(q, 1)\alpha_1$	$C(q, q-2)\alpha_{q-2}$	Efficiency
4	0	0	0.5000	0.5000	7.40×10^{-2}
	1	1	0.4854	0.5146	3.95×10^{-1}
	1	5	0.4983	0.5017	3.87×10^{-1}
	1	10	0.5111	0.4889	3.90×10^{-1}
	5	1	0.4392	0.5608	4.80×10^{-1}
	5	5	0.4474	0.5526	4.68×10^{-1}
	5	10	0.4564	0.5436	4.60×10^{-1}
5	0	0	0.5000	0.5000	3.63×10^{-3}
	1	1	0.4798	0.5202	4.54×10^{-3}
	1	5	0.4838	0.5166	5.33×10^{-3}
	1	10	0.4877	0.5123	6.41×10^{-3}
	5	1	0.4229	0.5771	7.65×10^{-3}
	5	5	0.4262	0.5738	8.69×10^{-3}
	5	10	0.4303	0.5697	1.01×10^{-2}
	5	200	0.5304	0.4696	1.12×10^{-1}
	50	10	0.2843	0.7157	3.91×10^{-2}
6	0	0	0.5000	0.5000	7.99×10^{-5}
	1	1	0.4822	0.5178	1.03×10^{-4}
	1	5	0.4843	0.5157	1.26×10^{-4}
	1	10	0.4870	0.5130	1.58×10^{-4}
	5	1	0.4295	0.5705	1.80×10^{-4}
	5	5	0.4316	0.5684	2.20×10^{-4}
	5	10	0.4341	0.5659	2.75×10^{-4}
	50	10	0.2785	0.7215	1.40×10^{-3}

Remark 5.1: The above table shows that the optimum design in the entire class of competing designs is highly efficient in comparison to the optimum design in the saturated class $\mathcal{D}_s$.

One can also consider another subclass of saturated designs by making use of a subset of barycentres of depth 1, and check the relative performance of the D-optimal design in it as against the D-optimal design in the whole class of competing designs.

Let us consider $q = 4$. In this case, a reasonable choice of a subset of 4 barycentres of depth 1 can be made by deleting two points which have either no or only one component in common. Let $\mathcal{D}_{s1}$ and $\mathcal{D}_{s2}$ denote respectively the two sub-classes of designs thus obtained. In the former situation, the information matrix is singular. In the second case, the efficiency of the best design in $\mathcal{D}_{s2}$ relative to the optimum design in the entire class is found to be sufficiently small. The efficiency for some combinations of (λ_1, λ_2) is shown in Table 5.2.

Table 5.2: Showing the D-optimal design in $\mathcal{D}_{s2}$ and its efficiency for some combinations of (λ_1, λ_2) when $q = 4$

λ_1	λ_2	$C(q, 1)\alpha_1$	$C(q, 1)\alpha_2$	Efficiency
0	0	0.5928	0.4072	1.54×10^{-1}
1	1	0.5742	0.4258	1.75×10^{-1}
1	5	0.5784	0.4216	1.91×10^{-1}
1	10	0.5834	0.4166	2.13×10^{-1}
5	1	0.5255	0.4745	2.26×10^{-1}
5	5	0.5287	0.4713	2.39×10^{-1}
5	10	0.5325	0.4675	2.55×10^{-1}

Remark 5.2: Comparing the efficiency factors obtained in Table 5.2 and in Table 5.1 for $q = 4$, it is evident that the D-optimal design in $\mathcal{D}_{s2}$ performs better than that in $\mathcal{D}_s$.

6. CONCLUSIONS

The paper considers an additive quadratic mixture model with random regression coefficients and attempts to find the D-optimal design for the estimation of mean regression coefficients, under equality of the variances of the coefficients corresponding to the linear terms and the quadratic terms respectively. It has been shown that the search for the optimum design may be confined to the sub-class of weighted centroid designs. Numerical computation with the number of mixing components $3 \leq q \leq 10$ revealed that barycentres of depth 0 are necessarily support points of the optimal designs, and the other support points remain confined to barycentres of depth atmost 2. Since the optimum designs are not saturated for $q \geq 4$, their performance has been compared with that of the optimum designs in some simple sub-classes of saturated designs, which showed that the optimum designs obtained in the whole class are highly efficient.

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REFERENCES

Atwood, C.L. (1969). Optimal and efficient designs of experiments. *Ann. Math. Statist.*, **40**, 1570-1602.

Chan, L.Y. (2000). Optimal designs for experiments with mixtures: A survey. *Comm. Statist. -Theory Methods* (Special Issue), **29(9&10)**, 2281-2312.

Chan, Ling-Yau, Guan, Ying-Nan and Zhang, Chong-Qi (1998). A-optimal design for an additive quadratic mixture model. *Statistica Sinica*, **8**, 979-990.

Darroch, J.N. and Waller, J. (1985). Additivity and interaction in three-component experiments with mixture. *Biometrika,* **72**, 153-163.

Draper, N.R. and Pukelsheim, F. (1999). Kiefer ordering of simplex designs for first and second degree mixture models. *J. Statist. Plann. Inf.*, **79**, 325-348.

Draper, N.R., Heiligers, B. and Pukelsheim, F. (2000). Kiefer ordering of simplex designs for second-degree mixture models with four or more ingredients. *Ann. Statist.*, **28(2)**, 578-590.

Galil, Z. and Kiefer, J. (1977). Comparison of simplex designs for quadratic mixture models. *Technometrics*, **19**, 445-453.

Kiefer, J. (1961). Optimum designs in regression problems II. *Ann. Math. Statist.*, **32**, 298-325.

Mandal, N.K. and Pal, M. (2008). Optimum mixture design using deficiency criterion. *Comm. Statist. -Theory Methods*, **37(10)**, 565-575.

Mandal, N.K., Pal, M., Sinha, B.K. and Das, P.(2008a). Optimum mixture designs : A pseudo-Bayesian approach. *J. Ind. Soc. Agril. Statist*., **62(2)**, 174-182.

Mandal, N.K., Pal, M., Sinha, B.K. and Das, P.(2008b). Optimum mixture designs under constraints on mixing components. *Statist. Appl.*, **6(1 & 2)** (New Series), 189-205.

Pal, M. and Mandal, N.K. (2006). Optimum designs for optimum mixtures. *Statist. Probab. Lett*., **76**, 1369-1379.

Pal, M. and Mandal, N.K. (2007). Optimum mixture design via equivalence theorem. *J. Comb. Inf. Syst. Sci.* (*JCISS*), **32(2)**, 107-126.

Pal, M. and Mandal, N.K. (2008). Minimax designs for optimum mixtures. *Statist. Probab. Lett*., **78(6)**, 608-615.

Pal, M., Mandal, N.K., Sinha, B.K. and Das P. (2010). Optimum mixture designs under random regression coefficients. *Jour. Appl. Prob. Statist.*, **5(1)**, 15-29.

Rao, C.R. (1967). Least squares theory using an estimated dispersion matrix and its applications to measurement of signals. Proceedings *of Fifth Berkeley Symposium on Mathematics and Probability*, **1**, 355-372.

Scheffé, H. (1958). Experiments with mixtures. *J. Roy. Statist. Soc.*, **B20**, 344-360.

Scheffé, H. (1963). Simplex – centroid design for experiments with mixtures. *J. Roy. Statist. Soc.,* **B25**, 235-263.