〈Research Peper〉

Journal of the Korean
Statistical Society
Vol. 16, No. 2, 1987

Symmetric D-Optimal Designs for Log Contrast Models with Mixtures

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ABSTRACT

The linear and quadratic log contrast model with mixtures on the strictly positive simplex,

$$\chi_{q-1}=\left\{(x_1,\cdots,x_q) : \Sigma x_k=1 \text{ and } \delta\leq\frac{x_i}{x_j}\leq\frac{1}{\delta} \text{ for all } i,j\right\},$$

are considered. Using the invariance arguments, symmetric D-optimal designs are investigated. The class of symmetric D-optimal designs for the linear log contrasts model is given. Any D-optimal design for the quadratic log contrast model is shown to be supported by a subset of all the extreme points and the center point in χ_{q-1}. Symmetric D-optimal designs for $q=3$ and 4 cases are given.

1. Introduction

In experiments with mixtures, the response depends only on the proportions of the q components present in the mixture and not on the total amount of mixtures. The q components are all represented by a proportion, x_i, of the total mixture. Thus

$$\sum_{i=1}^{q} x_i=1 \text{ and } 0\leq a_i\leq x_i\leq b_i\leq 1,$$

where $i=1,\cdots,q$ and the a_i and b_i are constraints on the x_i imposed by the experimenter.

There are situations where only mixtures consisting of all components simultaneously are meaningful. The designs then consist only of the interior points of the simplex. Examples are the formulation of a certain bleach for the removal of ink dyes and manufacture of one particular type of flare. Recently, Aitchison and Bacon-Shone(1984)

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introduced the linear and quadratic log contrast model,

$$\eta_1(x)=\beta_0+\sum_{i=1}^{q-1}\beta_i \log(x_i/x_q) \tag{1.1}$$

and

$$\eta_2(x)=\beta_0+\sum_{i=1}^{q-1}\beta_i \log(x_i/x_q)+\sum_{i\leq j}^{q-1}\beta_{ij} \log(x_i/x_q) \log(x_j/x_q) \tag{1.2}$$

on the strictly positive simplex, i.e. $0<a_i\leq x_i\leq b_i<1$, $i=1,\cdots,q$. The log contrasts models, (1.1) and (1.2), allow consideration of the hypothesis of inactivity of any components and complete additivity of every possible partition of the q components. For further details, see Aitchison and Bacon-Shone(1984).

In this paper, we restrict consideration to the approximate design theory. The present interest is to find a symmetric D-optimal design for the linear and quadratic log contrast model on

$$\chi_{q-1}=\left\{(x_1,\cdots,x_q) : \sum x_i=1 \text{ and } \delta\leq\frac{x_i}{x_j}\leq\frac{1}{\delta} \text{ for all } i,j\right\}, \tag{1.3}$$

where the fixed constant δ is in(0,1).

Section 2 is devoted to the formulation of general design problem and the invariance theorem [Kiefer(1959), (1961)]. In section 3, the invariance theorem is applied to the log contrast models. Chan(1986) found a D-optimal design for linear log contrast model on χ_{q-1} by brutal methods. Using the invariance theorem, we then simplify arguments to find symmetric D-optimal designs for the linear log contrast model in section 4. Section 5 deals with the quadratic log contrast model. It is shown that the support of any D-optimum design is a subset of extreme points and the center point in χ_{q-1}. Symmetric D-optimal designs are shown for $q=3$ and $q=4$ cases. Similar arguments may hold for general q, but the computation will be very complicated.

2. Preliminaries

Let $x'=(x_1,\cdots,x_q)$. It is assumed that for each x in χ_{q-1}, a random variable or response $Y(x)$ can be observed. The response $Y(x)$ has expected value

$$EY(x)=\sum\theta_i f_i=\theta' f(x)$$

and

$$\text{Var } Y(x)=\sigma^2,$$

where $f(x)$ is a $p\times 1$ column vector of known functions $f_i(x)$, $i=1,\cdots,p$ and θ is a $p\times 1$

vector of unknown parameters.

A design ξ is an arbitrary probability measure on χ_{q-1} and the information matrix of a design ξ is

$$M(\xi)=\int_{\chi_{q-1}} f(x)f(x)'d\xi(x).$$

ξ^* is a D-optimal design iff $|M(\xi^*)|=\max_{\xi}|M(\xi)|$.

The D-optimality criterion is known, by the celebrated Kiefer-Wolfowitz theorem, to be equivalent to the G-optimality criterion.

Theorem 2.1. [Kiefer and Wolfowitz(1960)]. The following assertions:

(1) the design ξ^* maximizes $|M(\xi)|$

(2) the design ξ^* minimizes $\max_x d(x,\xi)$, where $d(x,\xi)=f(x)'M^{-1}(\xi)f(x)$

(3) $\max_x d(x,\xi^*)=p$

are equivalent.

In many regression problems, the regression functions $f(x)$ are appropriately symmetric with respect to a group of one-to-one transformations G of χ_{q-1} onto χ_{q-1}. The following invariance theorem [Kiefer (1959), (1961)] concludes that there exists a symmetric D-optimal design for those models.

Theorem 2.2. Suppose G is a group of transformation on χ_{q-1} such that for each g in G, there exists a $p\times p$ matrix A_g of determinant 1 or -1 such that

$$f(gx)=A_g f(x), \text{ for any } x\in\chi_{q-1}.$$

Then there exists an invariant(or symmetric) D-optimal design under G. If ξ^* is D-optimal and G is finite, then $\xi^*=\frac{1}{L}\sum_{g\in G}\xi_g{}^*$ is an invariant D-optimal design, where $\xi_g(B)=\xi(g^{-1}B)$ and L is the number of elements in G.

3. Invariance

For the convenience of notation, we sometimes represent x in χ_{q-1} by r in the sense that $r'=(r_1,\cdots,r_q)$, $r_i\geq 0$, is equivalent to $x'=(x_1,\cdots,x_q)$ with $x_i=r_i/\sum_1^q r_j$, $i=1,\cdots,q$. Let E_i, $0\leq i\leq q-1$ be the set of $\binom{q}{i}$ points in χ_{q-1} with exactly i components of r equal to 1 and $q-i$ components equal to δ. From (1.3), it can be easily checked that χ_{q-1} is a convex set which is symmetric with respect to permutations of the components of each point. Moreover, $\bigcup_{i=1}^{q-1} E_i$ is the set of all extreme points of χ_{q-1}.

Note that $(\log(x_1/x_q), \cdots, \log(x_{q-1}/x_q))' = A(\log x_1, \cdots, \log x_q)'$,

$$A=\begin{bmatrix} 1 & 0 & 0 & \cdot & \cdot & 0 & -1 \\ & 1 & 0 & \cdot & \cdot & 0 & -1 \\ & & \cdot & & \cdot & \cdot & \cdot \\ & & & \cdot & & \cdot & \cdot \\ & & & & \cdot & \cdot & \cdot \\ & & & & & 1 & -1 \end{bmatrix}$$

Thus the row space of A has rank $q-1$ and is orthogonal to $1'=(1, \cdots, 1)$. For any permutation $(x_{(1)}, \cdots, x_{(q)})$ of $(x_1, \cdots, x_q)$, there exists a $(q-1)\times(q-1)$ matrix C with $|C|=1$ or -1 such that $A^*=CA$ and $[\log(x_{(1)}/x_{(q)}), \cdots, \log(x_{(q-1)}/x_{(q)})]=A^*(\log x_1, \cdots, \log x_q)$. Since the model (1.1) and (1.2) are linear and quadratic polynomial of $(\log(x_1/x_q), \cdots, \log(x_{q-1}/x_q))$, they are invariant under permutations of the components of each point in χ_{q-1}. Thus the direct application of the invariance theorem yields that there exists a symmetric D-optimal design on χ_{q-1}.

Define

$$z_i=\log(x_i/x_q), \quad i=1, \cdots, q-1 \tag{3.1}$$

and consider a mapping $h:(x_1, \cdots, x_q)\to(z_1, \cdots, z_{q-1})$ on χ_{q-1}. It can be easily checked that h is one-to-one. Let Z_{q-1} be the image of χ_{q-1}.

Lemma 3.1. Z_{q-1} is the convex hull of those points corresponding to the extreme points in χ_{q-1}. Also Z_{q-1} is symmetric with respect to (i) permutations of the components of each point z, (ii) sign changes of z and (iii) $g(z)=(z_1-z_{q-1}, \cdots, z_{q-2}-z_{q-1}, -z_{q-1})$.

Proof. For any z and z^* in Z_{q-1}, let $x=h^{-1}(z)$ and $x^*=h^{-1}(z^*)$.

Then

$$\begin{aligned}\alpha z+(1-\alpha)z^* &= \alpha(\log(x_1/x_q), \cdots, \log(x_{q-1}/x_q)) \\ &\quad +(1-\alpha)(\log(x_1^*/x_q^*), \cdots, \log(x_{q-1}^*/x_q^*)) \\ &= \alpha(\log(x_1/x_q)+(1-\alpha)\log(x_1^*/x_q^*), \cdots, \alpha\log(x_{q-1}/x_q) \\ &\quad +(1-\alpha)\log(x_{q-1}^*/x_q^*)) \\ &= \left[\log\left(\frac{x_1}{x_1^*}\right)^\alpha\left(x_1^*/\left(\frac{x_q}{x_q^*}\right)^\alpha\right) x_q^*, \cdots, \log\left(\frac{x_{q-1}}{x_{q-1}^*}\right)^\alpha\left(x_{q-1}/\left(\frac{x_q}{x_q^*}\right)^\alpha\right) x_q^*\right] \\ &\in Z_{q-1}\end{aligned}$$

since $\left(\frac{x_i}{x_i^*}\right)^\alpha x_i^*>0$, $i=1, \cdots, q$. Thus Z_{q-1} is convex.

For the symmetry of Z_{q-1}, it suffices to show that the set of extreme points is symmetric since Z_{q-1} is convex. Recall that the mapping h is one-to-one. So, the set of extreme points of Z_{q-1} is $h\left(\bigcup_{i=1}^{q-1} E_i\right)$, which consists of $2(q-1)$ points,

$$\pm(\log\delta, 0, \cdots, 0)$$
$$\vdots \tag{3.2}$$
$$\pm(\log\delta, \log\delta, \cdots, \log\delta)$$

and all the permutations of components of each point. It can be easily checked that $(z_1-z_{q-1}, \cdots, z_{q-2}-z_{q-1}, -z_{q-1})$ is one of extreme points of Z_{q-1} for each point z in(3.2). Figure 3.1 provides a sketch of χ_{q-1} and Z_{q-1} when $q=3$

Let ξ be a symmetric design on χ_{q-1}. Then, by Lemma 3.1, the reduced design is symmetric on Z_{q-1}. Throughout the paper, we shall use the same notation ξ for a symmetric design on χ_{q-1} as well as the reduced design on Z_{q-1}.

4. Linear log contrast model

Consider the linear log contrast model

$$\eta_1(x)=\beta_0+\sum_{i=1}^{q-1}\beta_i \log(x_i/x_q)$$

on χ_{q-1}. Chan(1986) found a D-optimal design for this model by using the equivalence theorem. Using the invariance theorem, we simplify arguments to find a symmetric D-optimal design for the linear log contrast model in the following.

Let ξ^* be a symmetric D-optimal design on χ_{q-1}. Note that $d(\xi^*, z)=f(z)'M^{-1}(\xi^*)f(z)$, $f'(z)=(1, z_1, \cdots, z_{q-1})$, is a quadratic function of z_i. The equivalence theorem (1.1) implies that only extreme points in Z_{q-1} could be in the support of the reduced design ξ^*. By Lemma 3.1, we can restrict ξ being a symmetric design on $\bigcup_{i=1}^{q-1} E_i$.

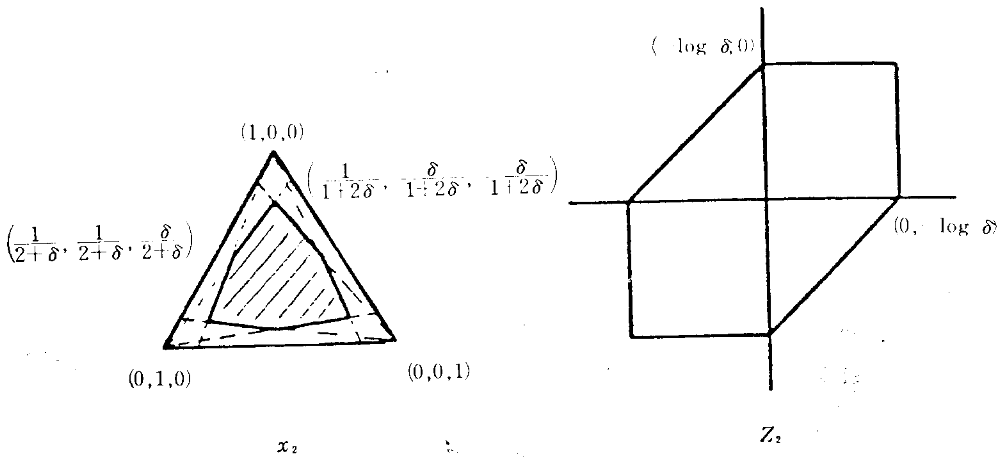

Figure 3.1. A sketch of χ_{q-1} and Z_{q-1} when $q=3$

Let ξ be a symmetric design such that

$$p_i=\xi(E_i),\ i=1,\cdots,q-1, \tag{4.1}$$

which is, ξ puts uniform mass $p_i/\binom{q}{i}$ at each point x in E_i. Now, the problem reduces to finding p_i which maximizes $|M(\xi)|$.

From the symmetry of the reduced design ξ on Z_{q-1}, $E^{\xi}z_1z_2=E^{\xi}(z_1-z_2)(-z_2)$ and $E^{\xi}z_2=E^{\xi}(-z_2)$. So

$$E^{\xi}z_1z_2=\frac{1}{2}E^{\xi}z_2^2 \text{ and } E^{\xi}z_2=0. \tag{4.2}$$

Letting $m_2=E^{\xi}z_1^2$,

$$M(\xi)=\begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2}m_2(I_{q-1}+J) \end{bmatrix} \tag{4.3}$$

Thus $\max_{\xi}|M(\xi)|$ is equivalent to $\max_{\xi}E^{\xi}z_1^2$.

By conditioning on x_q,

$$E^{\xi}z_1^2=\sum_{i=1}^{q-1}p_i\left[\frac{q-i}{q-1}\frac{\binom{q-1}{i-1}}{\binom{q}{i}}+\frac{i}{q-1}\frac{\binom{q-1}{i}}{\binom{q}{i}}\right](\log\delta)^2$$

$$=\sum_{i=1}^{q-1}p_i\cdot\frac{2i(q-i)}{q(q-1)}\cdot(\log\delta)^2.$$

Noting $i(q-i)$, $1\leq i\leq q-1$, is maximized at the nearest integer to $q/2$, we have the following theorem:

Theorem 4.1. Any symmetric D-optimal design ξ^* for the linear log contrast model on χ_{q-1} is given as follows:

$$\xi^*(E_{q/2})=1 \qquad \text{if } q \text{ is even}$$

and $\xi^*(E_{(q-1)/2})+\xi^*(E_{(q+1)/2})=1 \qquad$ if q is odd.

5. Quadratic log contrast model

Consider the quadratic log contrasts model

$$\eta_2(x)=\beta_0+\sum_{i=1}^{q-1}\beta_i\ \log(x_i/x_q)+\sum_{i\leq j}^{q-1}\beta_{ij}\ \log(x_i/x_q)\ \log(x_j/x_q)$$

on χ_{q-1}. It is well known (e.g. Scheffe(1958)) that the number of regression functions in the model is $\binom{q+1}{2}$.

Lemma 5.1. Every D-optimum design ξ^* on χ_{q-1} is supported by a subset of $E=\bigcup_{i=1}^{q-1}E_i$, which is the set of all extreme points and the center point of χ_{q-1}.

Proof. By Lemma 3.1, it is equivalent to showing that only extreme points and the center point $(0, \cdots, 0)$ of Z_{q-1} could be the support points of the reduced optimal design ξ^*. Invariance arguments yield that $d(z, \xi^*)$ for any optimum ξ^* is symmetric under the group of the symmetries of Z_{q-1}. Note $d(z, \xi^*)$ is a quadratic function in z_i. Thus $d(z, \xi^*)$ has at most only one local maximum on any ray.

Let B be the subset of Z_{q-1}, where $d(z, \xi^*)=\binom{q+1}{2}$. The equivalence theorem implies that the support of the D-optimal design ξ^* is contained in B and the function d has the maximum at each point in B. We shall show that the existence of points in $B-J$, where J is the set of all extreme points and the center point of Z_{q-1}, leads to a contradiction.

Suppose z in $B-J$ is in the interior of Z_{q-1}. By the symmetry of B, there is another point z^* in $B-J$ on the same ray. Thus the function d has two local maximums at z and z^*, which is a contradiction.

Suppose z in $B-J$ is on the boundary of Z_{q-1}. By the similar arguments, it suffices to consider that z is the linear combination of the two extreme points, say, $\log \delta(1, \cdots, 1, 1)$ and $\log \delta(1, \cdots, 1, 0)$. The symmetry of $d(z, \xi^*)$ yields that z is the middle point of those two extreme points, which is $\log \delta(1, \cdots, 1, 1/2)$. Now, set

$$z_1=z_2=\cdots=z_{q-2}=2z_{q-1}.$$

Then,

$$\begin{aligned} d((2z_{q-1}, \cdots, 2z_{q-1}, z_{q-1}), \xi^*) &= d((2z_{q-1}-z_{q-1}, \cdots, 2z_{q-1}-z_{q-1}, -z_{q-1}), \xi^*) \\ &= d((z_{q-1}, \cdots, z_{q-1}, -z_{q-1}), \xi^*). \end{aligned}$$

So $d(\log \delta(1/2, \cdots, 1/2, -1/2), \xi^*)=d(\log \delta(1, \cdots, 1, 1/2), \xi^*)=\binom{q+1}{2}$ and then, $\log \delta(1/2, \cdots, 1/2, -1/2)$ is in B. By the symmetry of B, so is $\log \delta(-1/2, \cdots, -1/2, 1/2)$. But those two points are on the same ray and interior points of Z_{q-1}, which is a contradiction. ▨

By Lemma 5.1, we restrict ξ be a symmetric design on E and let $p_i=\xi(E_i)$, $i=0, \cdots, q-1$.

We consider the $\log \delta=1$ case since the D-optimality criterion is invariant under the scale changes of independent variables for the polynomial regression. Then, from the symmetry of ξ, we get

$$\begin{aligned} &E^{\xi}z_1=E^{\xi}z_1^3=E^{\xi}z_1^2z_2=E^{\xi}z_1z_2z_3=0 \\ &E^{\xi}z_1z_2=E^{\xi}z_1^3z_2=E^{\xi}z_1^2z_2^2=(1/2)E^{\xi}z_1^2=(1/2)E^{\xi}z_1^4 \qquad (5.1) \\ &3E^{\xi}z_1^2z_2z_3-2E^{\xi}z_1z_2z_3z_4=(1/2)E^{\xi}z_1^4. \end{aligned}$$

The last equality follows from

$$E^{\xi}(z_1-z_4)(z_2-z_4)(z_3-z_4)(-z_4)=E^{\xi}z_1z_2z_3z_4.$$

For the purpose of partitioning the information matrix $M(\xi)$, it will be convenient to write $f(z)$ in the linear terms, 1 and the quadratic terms.

For $q=3$,

$$M(\xi)=\begin{bmatrix} (1/2)m_2I_2+(1/2)m_2J & 0 & 0 & 0 \\ & 1 & m_2 1_2' & (1/2)m_2 \\ & & (1/2)m_2I_2+(1/2)m_2J & (1/2)m_2 1_2 \\ & & & (1/2)m_2 \end{bmatrix}, \qquad (5.2)$$

and then,

$$|M(\xi)|=\frac{3}{64}m_2^5(2-3m_2). \qquad (5.3)$$

$|M(\xi)|$ is maximized at $m_2^*=5/9$. But

$$m_2=E^{\xi}z_1^2=\frac{2}{3}(p_1+p_2).$$

So, $p_1+p_2=5/6$ and $p_0=1/6$. Thus, any symmetric design with $\xi^*(E_0)=1/6$ and $\xi^*(E_1)=5/6-\xi^*(E_2)$ is a D-optimal design.

For $q=4$, letting $m_{211}=E^{\xi}z_1^2z_2z_3$,

$$M(\xi)=\begin{bmatrix} (1/2)m_2I_3+(1/2)m_2J & 0 & 0 & 0 \\ & 1 & (1/2)m_2 1'_3 & m_2 1'_3 \\ & & ((1/2)m_2-m_{211})I_3+m_{211}J & (m_{211}-(1/2)m_2)I_3+(1/2)m_2J \\ & & & (1/2)m_2I_3+(1/2)m_2J \end{bmatrix}. \qquad (5.4)$$

Using some formula for the determinant of the partitioned matrix and then, noting that $(a_1I+b_1J)(a_2I+b_2J)=(a_2I+b_2J)(a_1I+b_1J)$, we get

$$|M(\xi)|=\frac{1}{8}m_2^3m_{211}^3(m_2-2m_{211})^2\ (2m_2-m_{211}-3m_2^2). \qquad (5.5)$$

It can be checked that (5.5) is maximized at

$$m_2^*=\frac{87+\sqrt{87^2-7200}}{200}$$

and

$$m_{211}^*=\frac{6-9m_2}{10}.$$

But

$$m_2=E^{\xi}z_1^2=(1/2)(p_1+p_3)+(2/3)p_2$$

and

$$m_{211}=E^{\xi}z_1^2z_2z_3=(1/4)(p_1+p_3).$$

So $p_0 = .0814$, $p_2 = .4304$ and $p_1 + p_3 = .4882$. Thus a symmetric D-optimal design is given by

$$\xi^*(E_0) = .0814,\ \xi^*(E_1) = .4882 - \xi^*(E_3) \text{ and } \xi^*(E_2) = .4304.$$

Figure 5.1 provides the moments space (m_2, m_{211}).

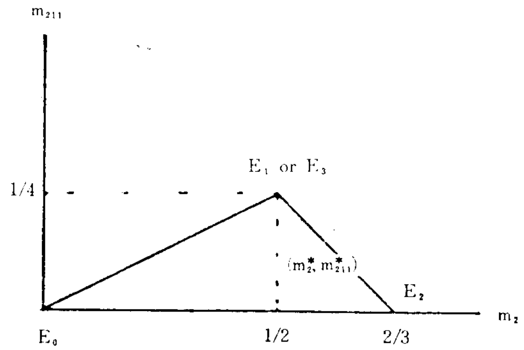

Figure 5.1. Moments space (m_2, m_{211}) when $q=4$

For $q \geq 5$, similar arguments may hold but the computation of $|M(\xi)|$ will be very complicated.

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