K-model based Mixture Design using D-optimal and A-optimal with Qualitative Factors

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Abstract

Objectives: To obtain a reliable approximation for the K-model in mixture experiments and design. Methods/Statistical Analysis: Here, the problem of mixture experiments, according to qualitative factors and finding A-optimal and D-optimal design for K-model is taken into account. Also, an improvement of Lee method is used to aim of this goal. In addition, a new procedure of Lee method for approximation of K-model is proposed. Moreover, illustrated examples are simulated in R software. Findings: It is demonstrated that the qualitative factor has a directly relation with A-optimal and D-optimal design. Such that, firstly, if the qualitative factor, on the region of factors, be a uniform design, then for A-optimal design, the trace of the inverse of the information matrix should be minimized. Secondly, for D-optimal design, maximization of the determinant of information matrix is necessary. Moreover, in a product function, the dispersion function can be detached into 3 sections corresponding to the 2 marginal design. Application/Improvements: This research is using of an amount of convenient mixture design in engineering and manufacturing can be detached into 3 sections corresponding to the 2 marginal design.

Keywords: Information Matrix, K-model, Mixture Experiment, Optimality, Qualitative Factors

1. Introduction

Recently, Mixture experiments have found a special importance in science and application. For instance, in food science, green manure, Agriculture and so on, one can see the role of mixture experiments ¹². For a better understanding, almost all of the cakes, are combined by a lot of materials such as, flour, water, eggs, oil and etc. The amount of this material is very important to set the best product sometimes due to increase or decrease of the materials. In most cases, the result is not desired the cakes taste, flavor and amount of puffing up depend on ingredients.

The reason of delicacy of this product can be divided to two main sectors. The first sector is using the best material and the second one is this question that how long the material should be mix together ¹². We have suggested a general model for the linear combination of variables. The model is presented as follows:

\[ E[y(j, \tau)] = f_1^T(\tau)\beta_j + f_2^T(\tau)\gamma, \quad \tau \in \chi \]  

(1)

Where, it shows the j-th level of a r-level qualitative factor and and \( f_1(x) \) is the part of the regression function having disruption with the qualitative property, and
The model-based mixture design using D-optimal and A-optimal with qualitative factors can be considered as the sector of the level effect, but $f_1$ is the part which is invariant at each qualitative level and $f_2(x)r$ can be considered at the part of the common effect. Also, $B=(B_1,B_2,...,B_q,B_1,2,...,B_{q+q})^T$ and $r=(r_1,r_2,...,r_m)^T$ are vectors of unknown parameters vector, respectively.

Now, the q-components mixture system can be expressed for the experimental region of quantitative factors as:

$$X = \left\{ (x_1, x_2, ..., x_q) : \sum_{i=1}^{q} x_i = 1, x_i \geq 0, i = 1, 2, ..., q, C's \right\},$$

(2)

Where the $C's$ is additional constraints condition as in defined. If the model without constraints $C's$, symbol the $x$ as $S^{p-1}$ the two part of regression function $f_1(z)$ and $f_2(z)$ are $p_1$ and $p_2$ dimension vectors containing the qualitative effects, respectively. Clearly, model (1) has more effect to feed and represent the relationship during variables. Recently, some research studies have been reported in the literature. For example the theoretical verification of D-optimal designs has addressed in. In5 have extended this model to multiresponse cases, as well as the construction model. But, almost all of the previous works in the literature have mixtivsely focused on D-optimal which it couldn't be applied for mixture experiments. In this study, based on the result of5 some concepts of A-optimal and D-optimal design is extended. The rest of the paper is as follows. In section 2 some preliminaries and some essential concepts to drive the tree of the information matrix of model (1) is presented. The main and analytical results are mentioned in section 3 such that according to the different condition of model (1), the A-optimal design for the mixture K-Model is found. Finally conclusion and discussions are provided in section 4.

2. Preliminaries

Here, the general linear model is introduced by:

$$E(y(x)) = f^T(x)\theta,$$

(3)

Where $y(x)$ is the response variable, $\theta$ is a vector of unknown parameters, $f(x)$ is a given vector of the regression function of $x \in \Omega$. An approximate design is probability distribution with finite support on the factor space $\Omega$ and is represented by $\zeta = (z_1, z_2, ..., z_n; w_1, w_2, ..., w_n)$, which assigns, respectively masses $w_1, w_2, ..., w_n; w_i > 0, \sum w_i = 1$ to the the distinct support point $x_1, x_2, ..., x_n$ of the design $\zeta$ in the experimental area.

And the design is measured by its information matrix worthy, which is demonstrated by:

$$M(\zeta) = \int_{\Omega} g(z)g^T(z)\zeta(dz).$$

(4)

2.1 A-optimal

A design is stated to be $A$-optimal if it minimizes the trance of the inverse of the information matrix. Works4 have extended this model to multiresponse cases, as well as the construction model. But, almost all of the previous works in the literature have mixtivsely focused on D-optimal which it couldn't be applied for mixture experiments. In this study, based on the result of5 some concepts of A-optimal and D-optimal design is extended. The rest of the paper is as follows. In section 2 some preliminaries and some essential concepts to drive the tree of the information matrix of model (1) is presented. The main and analytical results are mentioned in section 3 such that according to the different condition of model (1), the A-optimal design for the mixture K-Model is found. Finally conclusion and discussions are provided in section 4.
define the Kronecker result of two matrices. Let \( x_\alpha = \{1,2,\ldots,s\} \) be the index set of the qualitative levels and \( \Omega = x_\alpha \times x_\alpha \) be the experimental region.

Supposes that, the information matrix of the design \( \xi \) is:

\[
M_f(\xi) = \begin{bmatrix}
M_{11}(\xi) & M_{12}(\xi) \\
M_{21}(\xi) & M_{22}(\xi)
\end{bmatrix}
\]

(6)

where associated with the model

\[
E[y(\tau)]=[f_1^T(\tau), f_2^T(\tau)]\beta^T, \gamma^T]
\]

and arbitrary design \( \zeta \) on \( \Omega \) can be stated as:

\[
\zeta(j, \tau) = \eta(j)\xi_j(\tau)
\]

where \( \eta \) and \( \xi_j \) are the marginal and the conditionally designed on \( X_\alpha \) and \( X \), respectively.

If \( \zeta \) is considered as a product design and defined by \( \zeta = \eta \times \xi \), which shows that \( \xi_j = \xi \) for all \( j \).

Due to the result of\(^5\), the information matrix of \( \zeta \) is presented as:

\[
M_g(\zeta) = \begin{bmatrix}
D \otimes M_{11}(\xi) & \eta \otimes M_{21}(\xi) \\
\eta^T \otimes M_{11}(\xi) & M_{22}(\xi)
\end{bmatrix}
\]

where

\[
M_u(\xi) = \int_{x_\alpha} f_u(\tau)f_v^T(\tau)\xi(\tau)d\tau, \quad u, v \in \{1,2\}
\]

and

\[
D = \text{diag}(\eta(1), \eta(2), \ldots, \eta(s)), \quad \eta = (\eta(1), \eta(2), \ldots, \eta(s))^T
\]

Calculating the inverse matrix of \( M_g(\zeta) \) then we can get the Lemma 1.

**Lemma 1.** Let we have an arbitrary design \( \zeta(j, \tau) = \eta(j)\times \xi(\tau) \) which \( \eta \) and \( \xi \) are the marginally and the conditionally designed on \( X_\alpha \) and \( X \), respectively. Then the model (1) implies following equation of trace:

\[
\text{tr}[M_g^{-1}(\xi)] = \text{tr}(M_{11}^{-1}(\xi))\sum_{j=1}^{s} \frac{1}{\eta(j)} + s \text{tr}(K_0) + \text{tr}(D_{22}(\xi))
\]

In which:

\[
D_{22}(\xi) = [M_{22}(\xi) - M_{21}(\xi)M_{11}^{-1}(\xi)M_{12}(\xi)]^{-1}
\]

\[
K_0 = M_{11}^{-1}(\xi)M_{12}(\xi)D_{22}(\xi)M_{21}(\xi)M_{11}^{-1}(\xi)
\]

**Proof.**

According to computation of the inverse matrices of \( M_f(\xi) \) and \( M_g(\zeta) \), we get:

\[
M_f^{-1}(\xi) = \begin{bmatrix}
M_{11}^{-1}(\xi) + K_0 & -M_{11}^{-1}(\xi)M_{12}(\xi)D_{22}(\xi) \\
-D_{22}(\xi)M_{21}(\xi)M_{11}^{-1}(\xi) & M_{22}(\xi)
\end{bmatrix}
\]

\[
M_g^{-1}(\zeta) = \begin{bmatrix}
D_{11}(\xi) & D_{12}(\xi) \\
D_{21}(\xi) & D_{22}(\xi)
\end{bmatrix}
\]

In which \( 1_s \) is \( s \times 1 \) vector of all ones.

\[
D_{11}(\zeta) = D^{-1} \otimes M_{11}(\zeta) + J_s \otimes K_0,
\]

\[
D_{12}(\zeta) = -1_s \otimes [M_{11}^{-1}(\xi)M_{12}(\xi)D_{22}(\zeta)] = D_{21}(\zeta),
\]

\[
D_{22}(\zeta) = [M_{22}(\zeta) - M_{21}(\zeta)M_{11}^{-1}(\xi)M_{12}(\zeta)]^{-1} = D_{22}(\zeta),
\]

and

\[
K_0 = M_{11}^{-1}(\xi)M_{12}(\xi)D_{22}M_{21}(\xi)M_{11}^{-1}(\xi).
\]

So one has
\[ tr\left[M^{-1}_g(\xi)\right] = tr\left[D^{-1} \otimes M^{-1}_1(\xi)\right] + tr\left[J_s \otimes K(0)\right] + tr\left[D_{22}(\xi)\right] \]

\[ = tr\left(M^{-1}_1(\xi)\right) \sum_{j=1}^s \frac{1}{\eta(j)} + s \cdot tr\left(K(0)\right) + tr\left(D_{22}(\xi)\right) \]

Therefore, the proof is completed.

In practice, while the design \( \eta(j) \) is a uniform design on \( x_1 \), i.e.
\( \eta(j) = \frac{1}{s} \), \( j = 1, 2, \ldots, s \), thus one gets

\[ tr\left[M^{-1}_g(\xi)\right] = s^2 \cdot tr\left(M^{-1}_1(\xi)\right) + s \cdot tr\left(K(0)\right) + tr\left(D_{22}(\xi)\right) \]

\[ = s^2 \cdot (M^{-1}_1(\xi)) + (s^2 - s) \cdot tr\left(M^{-1}_1(\xi)\right) + (1 - s) \cdot tr\left(D_{22}(\xi)\right) \]

Moreover, it also follows that, for \( \xi \) to be \( A \)-optimal, all the elements of \( \eta \) must be equal, i.e.
\( \eta(j) = \frac{1}{s}, \quad j = 1, 2, \ldots, s \). In next section, we want to find the \( A \)-optimal designs for the K-model when the condition \( \eta(j) = \frac{1}{s}, \quad j = 1, 2, \ldots, s \).

\section{3. K-model Approximation based on A-optimal Designs}

\textbf{Theorem 1.} Let the same assumptions of Lemma 1 is true and suppose that \( \eta(j) = \frac{1}{s}, \quad j = 1, 2, \ldots, s \). Then:

\[ \psi_g(j, \tau; \xi) = s \psi_j(\tau; \xi) + (1 - s) \left\| z(\tau; \xi) \right\|^2 + (s^2 - s) \psi_j(\tau; \xi), \]

where

\[ \psi_j(\tau; \xi) = f'^T(\tau) M^{-1}_1(\xi) f_j(\tau) \]

and

\[ z(\tau, \xi) = \left[ D_2(\xi) f_j(\tau) M^{-1}_1(\xi) D_2(\xi) f'_j(\tau) \right] f(\tau) \]

\[ = f'^T(\tau) M^{-1}_1(\xi) f(\tau) \]

\textbf{Proof.} It is better that for simplification, Equation (6) can be rewritten as \( M_j(\xi) = \{ M_j \}_{j=1}^4 \), thus the following relations can be released.

\[ \psi_{j}(\tau, \xi) = \frac{1}{\eta(j)} \psi_{j}(\tau, \xi) + \left( \frac{1}{\eta(j)} \right) \sum_{i=1}^4 A_i(\tau, \xi) + \left( 1 - \frac{1}{\eta(j)} \right) \sum_{i=1}^4 B_i(\tau, \xi) \]

\[ + \left( \frac{1}{\eta^2(j)} - \frac{1}{\eta(j)} \right) \psi_{j}(\tau, \xi) \]

In which:

\[ A_1(\tau, \xi) = f'^T(\tau) f_j(\tau), \quad A_2(\tau, \xi) = f'^T(\tau) K_0 f_j(\tau), \quad A_3(\tau, \xi) = f'^T(\tau) D_2 M_1 f_j(\tau), \]

\[ A_4(\tau, \xi) = f'^T(\tau) D_2 M_1 f_j(\tau), \]

\[ B_1(\tau, \xi) = f'^T(\tau) f_j(\tau), \quad B_2(\tau, \xi) = f'^T(\tau) M^{-1}_1 f_j(\tau), \]

\[ B_3(\tau, \xi) = f'^T(\tau) D_2 M_1 f_j(\tau), \]

\[ B_4(\tau, \xi) = f'^T(\tau) D_2 M_1 f_j(\tau), \]

and \( K_0 = M^{-1}_1 f_j(\tau) \). Since

\[ \sum_{i=1}^4 B_i(\tau, \xi) = \left\| z(\tau; \xi) \right\|^2 = \left[ f'^T(\tau) M^{-1}_1(\xi) f(\tau) \right]^2 \]

Clearly, the theorem is satisfied when

\[ \eta(j) = 1/s, \quad j = 1, 2, \ldots, s \]. So the proof is finished.
We suppose that the $q$ components mixture K-model symbol is demonstrated as:

$$E[y(\tau)] = \sum_{k=1}^{q} f^{T}_L(\tau)\beta_k, \quad \tau \in \mathcal{S}^{q-1}$$  \hspace{1cm} (8)

Where:

$$f^{T}_{L_1}(\tau) = (x_1, x_2, \ldots, x_q)^T$$

$$f^{T}_{L_2}(\tau) = (x_1, x_2, x_3, \ldots, x_{q-1}, x_q)^T$$

$$f^{T}_{L_3}(\tau) = (x_1x_2, x_2x_3, \ldots, x_{q-2}x_{q-1}, x_q)^T, \ldots, f^{T}_{L_q}(\tau) = x_1x_2\ldots x_q$$

To fix ideas, we concentrate on the model which is given on $S^{q-1}$ by:

$$E[y(\tau)] = f^{T}_{L_1}(\tau)\beta_1 + f^{T}_{L_2}(\tau)\beta_2.$$  \hspace{1cm} (9)

We mostly consider three kinds of model which form as (1) given.

For the general multi-response model:

$$E[y(j, \tau)] = \left(f^{T}_{L_1}(\tau), f^{T}_{L_2}(\tau)\right)\beta_j, \quad j=1,2,\ldots,s$$  \hspace{1cm} (9)

which have different function on the different levels and it is without qualitative factors.

If we consider the $f^{T}_{L_2}(\tau)$ as qualitative factors and suppose $f^{T}_{L_3}(\tau)$ having interaction with the qualitative factor, the model can be shown as:

$$E[y(j, \tau)] = f^{T}_{L_1}(\tau)\beta\beta^{L_1}_j + f^{T}_{L_2}(\tau)\gamma^{L_2}$$  \hspace{1cm} (10)

Likewise, we can change the two part of regression function as quantitative and qualitative factor, the model set as:

$$E[y(j, \tau)] = f^{T}_{L_1}(\tau)\beta^{L_1}_j + f^{T}_{L_2}(\tau)\gamma^{L_2}$$  \hspace{1cm} (11)

However, there is no difference between fitting model (9) to model (11). In this work, qualitative and quantitative factors considered simultaneously, the design problems for estimation of the unknown parameters will be considered where it is assumed to have one qualitative factor with $s$ levels.

The K-model stated that for model (9), (10) and (11), $\Psi_g(j, \tau; \xi)$ attains its maximum only at the barycentres of $S^{q-1}$. Hence only the barycentres are viable support points for $A$-optimal designs. At first, we define $M_i$ is a $C(q,i) \times q$ matrix, such that the first $i$ elements in the first row of $M_i$ are 1 and the remaining elements in the first row are 0, and the remaining $C(q,i) - 1$ rows of $M_i$ are the different permutations of the first row due to lexicographical order.

(For example, when $i = 2$ and $q = 4$, $M_i$ is a $6 \times 4$ matrix, and its 1st, 2nd, ..., 6th rows are (1,1,0,0) (1,0,1,0) (1,0,0,1) (0,1,1,0) (0,1,0,1) (0,0,1,1) , respectively.)

Let $T_i$ is the points set which elements are each rows of $i^{-1}M_i$, $i = 1, 2, \ldots, q$. The $T_i$ is the set of all vertexes of $S^{q-1}$, $T_2$ is the set of barycenter on the $q$-2 dimension boundary. So we can state the design $\xi$ according to the model (9), (10) and (11) as follows:

$$\xi = \left(T_1, T_2; w_1, w_2\right)$$  \hspace{1cm} (12)

where the weight $w_1$ and $w_2$ satisfy

$$qw_1 + C(q,2)w_2 = 1.$$  

Hence, the information matrix $M_f(\xi)$ associate with model (9) can be expressed as:
where $Q = q(q - 1) / 2$, and $I_q$ is the $q \times q$ identity matrix. We can express following lemma based on previous symbols.

**Lemma 2.** Let we have a design $\xi$ as defined in (12), then the function $\psi_{\beta}(j; \tau; \xi)$ with $f^T(\tau) = [f_1^T(\tau) + f_2^T(\tau)]$ in one of the (10) and (11) models can be presented as:

$$
\psi_{\beta}(\tau; \xi) = a_0 + \sum_{i=1}^{q} [a_1 x_i^2 + a_2 x_i^3 (1 - x_i) + a_3 x_i^3 (1 - x_i)^2]
+ \sum_{i<j} [a_4 x_i x_j + a_5 x_i^2 x_j^2 + a_6 \left( \sum_{i<j} x_i x_j \right)^2]$$

Which:

$$
a_0 = \frac{4}{w_1}, a_1 = \frac{4q - 7}{w_1^2}, a_2 = -\frac{32}{w_1^2}, a_3 = \frac{64 w_1 + 4(4q - 7) w_2}{w_1^2 w_2},
a_4 = \frac{56}{w_2}, a_5 = \frac{64}{w_2^2}, a_6 = \frac{128 w_1 + 4(4q - 7) w_2}{w_1^2 w_2}
$$

**Proof.**

With calculating of the inverse matrix of $M_j(\xi)$, one gets:

$$
M_j^{-1}(\xi) = \begin{bmatrix}
\frac{1}{w_1} I_q & -\frac{2}{w_2} M_2^T \\
-\frac{2}{w_1} M_2 & \frac{4}{w_1} M_2 M_2^T + \frac{16}{w_2} I_q
\end{bmatrix}
$$

Since $J(k, l) = I^T_k I^T_l$, $J_1 = I^T_1 I^T_1$ and the matrix

$$
M_j^{-2}(\xi) = \left\{ A_j \right\}_{i,j=1}^2,
$$

where:

$$
A_{11} = \frac{4q - 7}{w_1^2} I_q + \frac{4}{w_1^2} J_q, A_{12} = -\frac{16}{w_1^2} J(q, Q) - \frac{32 w_1 + 4(4q - 7) w_2}{w_1^2 w_2} M_2^T = A_{21},
A_{22} = \frac{256}{w_2^2} I_q + \frac{64}{w_1^2} J_q + \frac{128 w_1 + 4(4q - 7) w_2}{w_1^2 w_2} M_2 M_2^T.
$$

In the model (10), the organization of information matrix is same as (13), then we obtain:

$$
M_{11}^{-1}(\xi) = -\frac{4q}{4 - q^2} I_q + \frac{q^2 w_2}{4 - q^2} J_q,
M_{12}^{-1}(\xi) = \frac{16 q^2}{(q^2 w_2 - 4)^2} I_q + \frac{-q^3 w_2 + q^2 w_2^2}{(q^2 w_2 - 4)^2} J_q,
M_{11}^{-1}(\xi) M_{12}^{-1}(\xi) = c M_2^T
$$

where $c = \frac{4q}{2 + q w_2 - q^2 w_2}$.

In the model (11), note $M_{11}^{-1}(\xi) = \{\overline{D}_j(\xi)\}_{i,j=1}^2$, the organization of information matrix is:

$$
\overline{M}_j(\xi) = \{\overline{M}_j(\xi)\}_{i,j=1}^2 = \left[ \begin{array}{cc}
M_2(\xi) & M_1(\xi)
\end{array} \right],
$$

$$
\overline{M}_{11}^{-1}(\xi) = \frac{256}{w_2^2} I_q, \overline{D}_{22}(\xi) = \frac{1}{w_2} I_q, \overline{M}_{11}^{-1}(\xi) \overline{M}_{12}(\xi) \overline{D}_{22}(\xi) = -\frac{1}{w_2} M_2
$$

So we can obtain the result of $\psi_{\beta}(\tau; \xi)$ by calculating

$$
f^T(x) M_j^{-2}(\xi) f(x) = f_1^T(x) M_1^{-2}(\xi) f_1(x)
$$

and $\pi(\tau; \xi)$ by calculating

$$
f^T(x) M_j^{-2}(\xi) f(x) = f_1^T(x) M_1^{-2}(\xi) f_1(x)
$$
and \(|D_{22} M_{21} M_{11}^{-1} D_{22}| f(x)\), respectively. Therefore the proof is done.

In the model (10),

\[
\psi_{\delta} (\tau; \xi) = \frac{16q^2}{(q^2 - w_1)} \sum_{i,m} x_i^2 + \frac{8q^2 w_2}{(q^2 - 4)} w_1, \quad \| \psi_{\delta} (\tau; \xi) \|^2 = \sum_{i,j} \delta_{ij}^2 (\tau),
\]

\[
\delta_{ij}^2 (\tau) = \left( \frac{4}{w_1} - c \right) (x_i + x_j) - \frac{4}{w_1} (x_i^2 + x_j^2), \quad 1 \leq j \leq q,
\]

where and

\[
c = \frac{4q}{2 + q w_2 - q^2 w_2}.
\]

In the model (11),

\[
\psi_{\delta} (\tau; \xi) = \frac{256}{w_2^2} \sum_{i,j} x_i^2 x_j^2, \quad \| \psi_{\delta} (\tau; \xi) \|^2 = \sum_{i,j} \delta_{ij}^2 (\tau)
\]

where \(\delta_{ij} (\tau) = -\frac{2}{w_1} (2x_i^2 - x_j), i = 1, 2, \ldots, q\).

We can explain the function (7) due to Theorem 1, Lemma 2 here, the condition is: \(w_1 = 1 / q - w_2 (q - 1) / 2\) and we have \(\tau_i \in T_i, i = 1, 2\), the function (7) can be expressed as

\[
h_i (w_2) = \psi_{\delta} (j; \tau; \xi) = sh_i (w_2) + (s^2 - s) h_{22} (w_2) + (1 - s) h_1 (w_2).
\]

In the model (10), we have

\[
h_i (w_2) = a_0 + a_i, h_i (w_2) = \frac{16q^2 - 8q^2 w_1 + 5q^2 w_2}{(q^2 w_2 - 4)^2}, h_1 (w_2) = (q - 1) c;
\]

\[
h_2 (w_2) = a_0 + \frac{a_2 + a_3 + a_4}{4} + \frac{a_4 + a_5 + a_6}{16} + \frac{a_6}{8}, h_{22} (w_2) = \frac{8q^2 - 8q^2 w_1 + 5q^2 w_2}{(q^2 w_2 - 4)^2},
\]

\[
h_{21} (w_2) = \left( \frac{4}{w_1} - \frac{4}{w_2} - c \right) + (2q - 4) \left( \frac{4}{w_1} - \frac{c}{2} \right).
\]

In the model (11), \(h_{11} (w_2)\) and \(h_{22} (w_2)\) are same as model (10), then we have:

\[
h_1 (w_2) = 0, h_1 (w_2) = 1 / w_1^2, h_{22} (w_2) = 16 / w_2^2, h_{23} (w_2) = 0.
\]

Now, we should solve following equation to find the \(A\)–

Figure 1. The portrait for A–optimality design in model (10) and model (11).
optimal design $\zeta^*$ for the models (10) and (11),
\[
\psi_g(j, \tau_1; \zeta^*) = \psi_g(j, \tau_2; \zeta^*).
\]
(14)

Beside, the solution of equation $w_i = u_i(q_i, s_i)$ $i = 1, 2$ is too complex, so one can gets the approximate optimal design by calculating the result of Lemma 2. For instance, let $q = 30, s = 20$, we can find the $A-$optimal design $\zeta^* = \eta^* \times \xi^*$ on the region $X_s \times S^{q-1}$, where $\eta^*$ is a uniform design on $X_s$, and we can find the optimal design $\xi^*$ on $S^{q-1}$ by calculate $\log h_1(w_2) \log h_2(w_2)$ and $\log r(M_g^{-1}(\zeta))$ in $w_2 \in (0, 1/4)$.

For the model (10), we find that $\min_{w_2 \in (0, 1/4)} \left\{ \log tr(M_g^{-1}(\zeta)) \right\} = 21.37664$ when $w_2^* = 0.2911$, so the design
\[
\zeta^* = (T_1, T_2; 0.0411, 0.2911).
\]

For the model (11), we have
\[
\min_{w_2 \in (0, 1/4)} \left\{ \log tr(M_g^{-1}(\zeta)) \right\} = 26.12341
\]
when $w_2^* = 0.0768$, so the design:
\[
\zeta^* = (T_1, T_2; 0.0077, 0.2577).
\]

As we expressed above satisfy equivalence condition (14), we can confirm the design $\zeta^*$, because the three curves $\log h_1(w_2) \log h_2(w_2)$ and $\log r(M_g^{-1}(\zeta))$ intersect at the same point as Figures 1 and 2 shown.

We also lists the optimal weights for model (9), (10) and (11) with $q \in \{3, 4, \ldots, 6\}$ and $s \in \{2, 3, \ldots, 6\}$ as the Table 1 shown.

The performance of designs comparing to the $A-$optimal design for model $g(\tau)$ defined as below, which are measured by the $A-$efficiency.
\[
A_{eff}(\xi) = \frac{tr[M_g^{-1}(\xi^*)]}{tr[M_g^{-1}(\xi)]}
\]
Table 1. The weights of $D$-optimal design for $3 \leq q \leq 6$ and $2 \leq s \leq 6$

| $q$ | $s$ | $w_1^*$ | $w_2^*$ | $w_1^*$ | $w_2^*$ |
|-----|-----|----------|----------|----------|----------|
| 3   | 2   | 0.21540  | 0.54870  |          |          |
| 4   | 2   | 0.13643  | 0.25760  | 0.1246   | 0.2531   |
| 5   | 2   | 0.09364  | 0.14680  |          |          |
| 6   | 2   | 0.06869  | 0.09410  |          |          |
| 3   | 3   | 0.24390  | 0.57720  |          |          |
| 4   | 3   | 0.15854  | 0.27240  | 0.1366   | 0.2577   |
| 5   | 3   | 0.11321  | 0.15660  |          |          |
| 6   | 3   | 0.08388  | 0.10020  |          |          |
| 3   | 4   | 0.26103  | 0.59440  |          |          |
| 4   | 4   | 0.17462  | 0.28310  | 0.1426   | 0.2617   |
| 5   | 4   | 0.12675  | 0.16340  |          |          |
| 6   | 4   | 0.09673  | 0.10540  |          |          |
| 3   | 5   | 0.27240  | 0.60570  |          |          |
| 4   | 5   | 0.18668  | 0.29110  | 0.1473   | 0.2649   |
| 5   | 5   | 0.13729  | 0.16860  |          |          |
| 6   | 5   | 0.10491  | 0.10860  |          |          |
| 3   | 6   | 0.28100  | 0.61430  |          |          |
| 4   | 6   | 0.19472  | 0.29650  | 0.1500   | 0.2667   |
| 5   | 6   | 0.14481  | 0.17240  |          |          |
| 6   | 6   | 0.11192  | 0.11140  |          |          |

Note: $\xi_j^* = \eta_j^* \times \xi_j^*, j = 1, 2, 3$ are $A$-optimal design for model (9), (10) and (11), respectively. For $q \in \{3, 4, \ldots, 6\}$ and $s \in \{2, 3, \ldots, 6\}$, these designs should be compared mutually with each other and the $A$-efficiencies are presented in Table 2.
**Table 2.** Comparisons of $A$-Optimal for $3 \leq q \leq 6$ and $2 \leq s \leq 6$

| $q$ | $s$ | $\xi_1^*$ | $\xi_2^*$ |
|----|----|----------|----------|
| 3  | 2  | 0.2154   | 0.5487   | 0.2230   | 0.5563   |
| 4  | 2  | 0.1364   | 0.2576   | 0.1250   | 0.2500   |
| 5  | 2  | 0.0936   | 0.1468   | 0.0799   | 0.1399   |
| 6  | 2  | 0.0686   | 0.0941   | 0.0555   | 0.0889   |
| 3  | 3  | 0.2439   | 0.5772   | 0.2496   | 0.5829   |
| 4  | 3  | 0.1585   | 0.2723   | 0.1364   | 0.2576   |
| 5  | 3  | 0.1132   | 0.1566   | 0.0858   | 0.1429   |
| 6  | 3  | 0.0838   | 0.1002   | 0.0589   | 0.0902   |
| 3  | 4  | 0.2610   | 0.5943   | 0.2673   | 0.6006   |
| 4  | 4  | 0.1746   | 0.2831   | 0.1428   | 0.2619   |
| 5  | 4  | 0.1267   | 0.1634   | 0.0888   | 0.1444   |
| 6  | 4  | 0.0967   | 0.1053   | 0.0604   | 0.0908   |
| 3  | 5  | 0.2724   | 0.6057   | 0.2791   | 0.6124   |
| 4  | 5  | 0.1866   | 0.2911   | 0.1466   | 0.2644   |
| 5  | 5  | 0.1372   | 0.1686   | 0.0906   | 0.1453   |
| 6  | 5  | 0.1049   | 0.1086   | 0.0617   | 0.0913   |
| 3  | 6  | 0.2810   | 0.6143   | 0.2850   | 0.6183   |
| 4  | 6  | 0.1947   | 0.2965   | 0.1504   | 0.2669   |
| 5  | 6  | 0.1448   | 0.1724   | 0.0924   | 0.1462   |
| 6  | 6  | 0.1119   | 0.1114   | 0.0625   | 0.0917   |
4. D-optimal Designs for the K-model

Atkinson and Donev (1989) stated the BLKL-exchange algorithm due to the D-criterion for searching exact optimal designs with special block sizes.

We can get lemma 3 easily because we have the information matrix in preliminaries.

**Lemma 3.** Suppose that $\tau$ be a product design with the marginal designs $\eta$ and $\xi$ on $X_s$ and $X$, respectively.

Then, the following equation of determinants is expressed for models (3) and (10):

$$ \det(M_g(\xi)) = \left( \prod_{s=1}^{S} \eta(s) \right) [\det(M_1(\xi))]^{s-1} \det(M_f(\xi)) $$

(15)

where $\rho_1$ shows the dimension of $M_{11}$.

The above lemma indicates the marginal design $\rho$ is defined as an unique design on $\chi_j$, according to D-criterion as defined $\eta(j) = \frac{1}{j}$ for all $j$, where the maximization of $\det(M_g(\tau))$ can be divided in two parts due to the marginal designs.

Since the D-optimality should be prove by the equivalence theorem in next section. This function is proportional to the variance of the predicted response and defined by:

$$ d_h(z; \tau) := h^T(z)M_h^{-1}(\tau)h(z) \quad \text{for } z \in Q $$

(16)

In the following, a connection of dispersion functions between the model (11) and (10) is derived for product designs. The determinant and inverse of a partitioned matrix can be obtained according to the formulas in Khuri (2003, pp. 35–6).

**Lemma 4.** Let we have the same assumptions of Lemma 1, then:

$$ d_g(j, x^T; \tau) = d_f(x, \xi) + \frac{1}{\eta(s)} \Delta_g(x, \xi) \quad \text{for } (j, x) \in X_j \times X, $$

(17) which $d_g(j, x^T; \tau)$ and $d_f(x; \xi)$ demonstrate the associated dispersion functions with the models (11) and (10), respectively and,

$$ \Delta_g(x, \xi) = f_i^T(x)M_1^{-1}(\xi)f_i(x) $$

(18)

5. Conclusions

The problem of mixture design and approximation of the A-optimal and D-optimal design for the K-model with qualitatives factors are investigated. Based on a modification of Lee method in designing of mixture, the results are reached. Also, it is demonstrated that the qualitative factor has a directly relation with A-optimal and D-optimal design. Such that, at the first step, on the region of factors, if the qualitative factors have a uniform design then the trace of the inverse of information matrix is minimize for A-optimal design. Also, in the second step, maximization of the determination of information matrix is essential for D-optimal design. In addition, for a product function, based on three sections corresponding to the two marginal design, the dispersion function can be detected.

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