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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 taking 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 determination 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[1,7]. For a better understanding, almost all of the cakes, are combined by alot of materials such as, flour, water, eggs, oil and etc. The amount of this material is very important to set the best product sometime 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[5] have suggested a general model for the linear combination of variables. The model is presented as follows:

$$E[y(j,\tau)] = f_1^T(\tau)\beta_j + f_2^T(\tau)\gamma, \quad \tau \in \chi \tag{1}$$

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

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$f_1 B_j$ can be considered as the sector of the level effect, but f_z is the part which is invariant at each qualitative level and $f_z(x)\gamma$ can be considered at the part of the common effect. Also, $B=\left(B_1,B_2,\ldots,B_q,B_{1,2},\ldots B_{q-1,q}\right)^T$ and $\gamma=\left(\gamma_1,\gamma_2,\ldots,\gamma_{p_2}\right)^T$ are vectors of unknown parameters vector, respectively.

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

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

Where the $C's$ is additional constrains condition as in[6] defined. If the model without constraints $C's$, symbol the x as S^{q-1} the two part of regression function $f_1(z)$ and $f_2(z)$ are p_1- and p_2- dimension vectors containing the quantitative 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[2]. In[8] have extended this model to multiresponse cases, as well as the construction model. But, almost all of the previous works in the literature have mixtsively focused on D-optimal which it couldn't be applied for mixture experiments. In this study, based on the result of[5] 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 finded. Finally conclusion and discussions are provided in section 4.

2. Preliminaries

Here, the general linear model is introduced by:

$$E\left(y(x)\right)=f^T(x)\theta, \tag{3}$$

Where $y(x)$ is the response variable, θ 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 Ω and is represented by $\zeta=\left(z_1,z_2,\ldots,z_n;w_1,w_2,\ldots w_n\right)$, which assigns, respectively masses $w_1,w_2,\ldots,w_n;w_i>0,\ \sum w_i=1$ to the n distinct support point $x_1,x_2,\ldots,x_n$ of the design ζ in the experimental area.

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

$$M(\zeta)=\int_{\Omega}g(z)g^T(z)\zeta(dz). \tag{4}$$

2.1 A-optimal

A design is stated to be A-optimal if it minimizes the trance of the inverse of the information matrix. Works[4]Jack</author></authors></contributors><titles><title>General equivalence theory for optimum designs (approximate theory and[3] gave us an effective way to check the $A-$optimality of arbitrary design ζ, and for a design ζ which is $A-$optimal if and only if:

$$f^T(x)M^{-2}(\zeta)f(x)-tr\left[M^{-1}(\zeta)\right]\leq 0 \tag{5}$$

Let the general model (1) be written as:

$$E\left[y(j,\tau)\right]=\left[e_j^T\otimes f_1^T(x),f_2^T\right]\left(\beta_1^T,\beta_2^T,\ldots,\beta_s^T,\gamma^T\right)=g^T(j,\tau)\theta$$

where $e_j\in R^s$ is the unit vector whose $j-$th component is equal to 1 and all others are 0 and $\otimes$ is used to define the Kronecker result of two matrices. Let $x_s = \{1,2,\ldots,s\}$ be the index set of the qualitative levels and $\Omega = x_s \times x$ be the experimental region.

Supposes that, the information matrix of the design ξ is:

$$M_f(\xi) = \begin{bmatrix} M_{11}(\xi) & M_{12}(\xi) \\ M_{21}(\xi) & M_{22}(\xi) \end{bmatrix} \tag{6}$$

where associated with the model

$E[y(\tau)] = [f_1^T(\tau), f_2^T(\tau)](\beta^T, \gamma^T)^T$ and arbitrary design ζ on Ω can be stated as:

$$\zeta(j,\tau) = \eta(j)\xi_j(\tau)$$

where η and ξ_j are the marginal and the conditional designs on χ_s and χ, respectively.

If ζ 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 ζ is presented as:

$$M_g(\zeta) = \begin{bmatrix} D \otimes M_{11}(\xi) & \eta \otimes M_{12}(\xi) \\ \eta^T \otimes M_{21}(\xi) & M_{22}(\xi) \end{bmatrix}$$

where

$$M_{uv}(\xi) = \int_x f_u(\tau) f_v^T(\tau)\xi(d\tau), \quad u,v \in \{1,2\}$$

and

$$D = diag(\eta(1),\eta(2),\ldots,\eta(s)), \ \eta = (\eta(1),\eta(2),\ldots,\eta(s))^T .$$

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 η *and* ξ are the marginally and the conditionally designed on X_s and X, respectively. Then the model (1) implies following equation of trace :

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

In which:

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

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

Proof.

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

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

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

In which 1_S is $s \times 1$ vector of all ones.

$$D_{11}(\zeta) = D^{-1} \otimes M_{11}(\xi) + J_s \otimes K_{(1)},$$

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

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

and

$$K_{(1)} = M_{11}^{-1}(\xi) M_{12}(\xi) D_{22} M_{21}(\xi) M_{11}^{-1}(\xi).$$

So one has

$$tr\left[M_g^{-1}(\zeta)\right]=tr\left[D^{-1}\otimes M_{11}^{-1}(\xi)\right]+tr\left[J_s\otimes K_{(1)}\right]+tr\left[D_{22}(\xi)\right]$$

$$=tr\left(M_{11}^{-1}(\xi)\right)\sum_{j=1}^{s}\frac{1}{\eta(j)}+s.tr\left(K_{(1)}\right)+tr\left(D_{22}(\xi)\right)$$

Therefore, the proof is completed.

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

$$tr\left[M_g^{-1}(\zeta)\right]=s^2.tr\left(M_{11}^{-1}(\xi)\right)+s.tr\left(K_{(1)}\right)+tr\left(D_{22}(\xi)\right)$$

$$=s^2.\left(M_{11}^{-1}(\xi)\right)+\left(s^2-s\right).tr\left(M_{11}^{-1}(\xi)\right)+(1-s).tr\left(D_{22}(\xi)\right)$$

Moreover, it also follows that, for ζ to be $A-$optimal, all the elements of η 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 $\eta(j)=\frac{1}{s},\quad j=1,2,\ldots,s$.

3. K-model Approximation based on A-optimal Designs

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:

$$\psi_g(j,\tau;\zeta)=s.\psi_f(\tau;\xi)+(1-s)\left\|z(\tau;\xi)\right\|^2+(s^2-s)\psi_{f_1}(\tau;\xi),\tag{7}$$

where

$$\psi_{f_1}(\tau;\xi)=f_1^T(\tau)M_1^{-2}(\xi)f_1(\tau)\ \psi_f(\tau;\xi)=f^T(\tau)M_f^{-2}(\xi)f(\tau)$$

and

$$z(\tau;\xi)=\left[-D_2(\xi)M_2(\xi)M_1^{-1}(\xi),D_2(\xi)\right]f(\tau),\quad f^T(\tau)=\left[f_1^T(\tau),f_2^T(\tau)\right]$$

Proof. It is better that for simplification, Equation (6) can be rewritten as $M_f(\xi)=\left\{M_j\right\}_{i,j=1}^2$, thus the following relations can be released.

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

$$+\left(\frac{1}{\eta^2(j)}-\frac{1}{\eta(j)}\right)\psi_{f_1}(\tau;\xi)$$

In which:

$$A_1(\tau;\xi)=f_1^T(\tau)K_{(1)}^2f_1(\tau),\quad A_2(\tau;\xi)=f_1^T(\tau)K_{(1)}M_1^{-1}M_2D_2\ f_2(\tau),$$

$$A_3(\tau;\xi)=f_2^T(\tau)D_2\ M_2\ M_1^{-1}K_{(1)}\ f_1(\tau),$$

$$A_4(\tau;\xi)=f_2^T(\tau)D_2\ M_2\ M_1^{-1}M_2\ D_2\ \ f_2(\tau).$$

$$B_1(\tau;\xi)=f_1^T(\tau)K_{(2)}f_1(\tau),\quad B_2(\tau;\xi)=f_1^T(\tau)M_1^{-1}M_2\ D_2^2\ f_2(\tau),$$

$$B_3(\tau;\xi)=f_2^T(\tau)D_2^2\ M_2\ M_1^{-1}f_1(\tau),$$

$$B_4(\tau;\xi)=f_2^T(\tau)D_2^2\ \ f_2(\tau).$$

and $K_{(2)}=M_1^{-1}M_2\ D_2^2\ M_2\ M_1^{-1}$. Since

$$\sum_{i=1}^4 B_i(\tau;\xi)=\left\|z(\tau;\xi)\right\|^2=\left\|\left[-D_2(\xi)M_2(\xi)M_1^{-1}(\xi),D_2(\xi)\right]f(\tau)\right\|^2$$

Clearly, the theorem is satisfied when

$\eta(j)=1/s,\ \ j=1,2,\ldots,s$. So the proof is finished.

We suppose that the q components mixture K-model symbol is demonstrated as:

$$E[y(\tau)] = \sum_{k=1}^{q} f_{l_k}^T(\tau)\beta_k,\ \tau \in \chi \subseteq s^{q-1} \tag{8}$$

Where:

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

$$f_{L_2}(\tau) = (x_1x_2, x_1x_3, \ldots, x_{q-1}x_q)^T$$

$$f_{L_3}(\tau) = (x_1x_2x_3, x_2x_3x_4, \ldots, x_{q-2}x_{q-1}x_q)^T, \ldots, f_{L_q}(\tau) = x_1x_2x_3\ldots x_q$$

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

$$E[y(\tau)] = f_{L_1}^T(\tau)\beta_1 + f_{L_2}^T(\tau)\beta_2.$$

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

For the general multi-response model:

$$E[y(j,\tau)] = \left(f_{L_1}^T(\tau), f_{L_2}^T(\tau)\right)\beta_j,\ \ j = 1, 2, \ldots, s \tag{9}$$

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

If we consider the $f_{L_2}^T(\tau)$ as qualitative factors and suppose $f_{L_1}^T(\tau)$ having interaction with the qualitative factor, the model can be shown as:

$$E[y(j,\tau)] = f_{L_1}^T(\tau)\beta^{(L_1)}{}_j + f_{L_2}^T(\tau)\gamma^{(L_2)} \tag{10}$$

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

$$E[y(j,\tau)] = f_{L_2}^T(\tau)\beta^{(L_2)} + f_{L_1}^T(\tau)\gamma^{(L_1)} \tag{11}$$

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 6×4 matrix, and its 1st, 2nd,$\cdots$, 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 ξ according to the model (9), (10) and (11) as follows:

$$\xi = (T_1, T_2; w_1, w_2), \tag{12}$$

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:

$$M_f(\xi)=\begin{bmatrix} \frac{w_2}{4}M_2^T M_2 I_Q + w_1 I_Q & \frac{w_2}{8}M_2^T I_Q \\ \frac{w_2}{8}M_2 I_Q & \frac{w_2}{16}I_Q \end{bmatrix} \tag{13}$$

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 ξ as defined in (12), then the function $\psi_g(j,\tau;\xi)$ with $f^T(\tau)=\left[f_1^T(\tau)+f_2^T(\tau)\right]$ in one of the (10) and (11) models can be presented as:

$$\psi_f(\tau;\xi)=a_0+\sum_{i=1}^{q}\left[a_1x_i^2+a_3x_i^2(1-x_i)+a_6x_i^2(1-x_i)^2\right]$$
$$+\sum_{i<j}^{q}\left[a_2x_ix_j+a_4x_i^2x_j^2\right]+a_5\left(\sum_{i<j}^{q}x_ix_j\right)^2$$

Which:

$$a_0=\frac{4}{w_1^2},a_1=\frac{4q-7}{w_1^2},a_2=-\frac{32}{w_1^2},a_3=\frac{64w_1+4(4q-7)w_2}{w_1^2w_2},$$
$$a_4=\frac{256}{w_2^2},a_5=\frac{64}{w_2^2},a_6=\frac{128w_1+4(4q-7)w_2}{w_1^2w_2}$$

Proof.

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

$$M_f^{-1}(\xi)=\begin{bmatrix} \frac{1}{\mathrm{w}_1}I_q & -\frac{2}{\mathrm{w}_2}M_2^T \\ -\frac{2}{w_1}M_2 & \frac{4}{w_1}M_2M_2^T+\frac{16}{w_2}I_Q \end{bmatrix}$$

Since $J(k,l)=1_k1_l^T$, $J_k=1_k1_l^T$ and the matrix $M_f^{-2}(\xi)=\{A_j\}_{i,j=1}^2$, where:

$$A_{11}=\frac{4q-7}{w_1^2}I_q+\frac{4}{w_1^2}J_q, A_{12}=-\frac{16}{w_1^2}J(q,Q)-\frac{32w_1+2(4q-7)w_2}{w_1^2w_2}M_2^T=A_{21}^T,$$
$$A_{22}=\frac{256}{w_2^2}I_Q+\frac{64}{w_1^2}J_Q+\frac{128w_1+4(4q-7)w_2}{w_1^2w_2}M_2M_2^T.$$

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

$$M_{11}^{-1}(\xi)=-\frac{4q}{4-q^2w_2}I_q+\frac{q^2w_2}{4-q^2w_2}J_q,$$
$$M_{11}^{-2}(\xi)=\frac{16q^2}{(q^2w_2-4)^2}I_q+\frac{-8q^3w_2+q^5w_2^2}{(q^2w_2-4)^2}J_q,$$
$$M_{11}^{-1}(\xi)M_{12}(\xi)D_{22}(\xi)=cM_2^T,$$

where $c=\dfrac{4q}{2+qw_2-q^2w_2}$.

In the model (11), note $\overline{M}^{-1}(\xi)=\{\overline{D}_{ij}(\xi)\}_{i,j=1}^2$, the

$$f^T(x)=\left[f_1^T(x)\ f_2^T(x)\right]=\left[f_{L_2}^T(x)\ f_{L_1}^T(x)\right]$$

the organization of information matrix is:

$$\overline{M}_f(\xi)=\{\overline{M}_j(\xi)\}_{i,j=1}^2=\begin{bmatrix} M_2(\xi) & M_2(\xi) \\ M_1(\xi) & M_1(\xi) \end{bmatrix}$$

$$\overline{M}_{11}^{-2}(\xi)=\frac{256}{w_2^2}I_Q,\ \overline{D}_{22}(\xi)=\frac{1}{w_1}I_q,\ \overline{M}_{11}^{-1}(\xi)\overline{M}_{12}(\xi)\overline{D}_{22}(\xi)=-\frac{16}{w_2}M_2$$

So we can obtain the result of $\psi_f(\tau;\xi)$ $\psi_{f_1}(\tau;\xi)$ and $z(\tau;\xi)$ by calculating $f^T(x)M_f^{-2}(\xi)f(x)$ $f_1^T(x)M_1^{-2}(\xi)f_1(x)$

and $\left[D_{22}M_{21}M_{11}^{-1}, D_{22}\right]f(x)$, respectively. Therefore the proof is done.

In the model (10),

$$\psi_{f_1}(\tau;\xi)=\frac{16q^2}{(q^2w_2-4)^2}\sum_{i=1}^{q}x_i^{\,2}+\frac{-8q^2w_2+q^5w_2}{(q^2w_2-4)^2},\ \|z(\tau;\xi)\|^2=\sum_{i<j}^{q}\delta_{ij}^2(\tau),$$

$$\delta_{ij}(\tau)=\left(\frac{4}{w_1}-c\right)(x_i+x_j)-\frac{4}{w_1}(x_i^2+x_j^2)+\frac{16}{w_1}(x_ix_j),\ \ 1\le j\le q,$$

where and

$$c=\frac{4q}{2+qw_2-q^2w_2}.$$

In the model (11),

$$\psi_{f_1}(\tau;\xi)=\frac{256}{w_2^2}\sum_{i<j}^{q}x_i^{\,2}x_j^{\,2},\ \ \|z(\tau;\xi)\|^2=\sum_{i=1}^{q}\delta_i^2(\tau)$$

where $\delta_i(\tau)=-\dfrac{2}{w_1}\left(2x_i^{\,2}-x_i\right)$, $i=1,2,...,q.$.

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

$$h_i(w_2)=\psi_g(j,\tau_i;\zeta)=sh_{i1}(w_2)+(s^2-s)h_{i2}(w_2)+(1-s)h_{i3}(w_2).$$

In the model (10), we have

$$h_{11}(w_2)=a_0+a_1, h_{12}(w_2)=\frac{16q^2-8q^2w_2+5q^5w_2^2}{(q^2w_2-4)^2}, h_{13}(w_2)=(q-1)c^2;$$

$$h_{21}(w_2)=a_0+\frac{a_1}{2}+\frac{a_2}{4}+\frac{a_3}{4}+\frac{a_4}{16}+\frac{a_5}{16}+\frac{a_6}{8}, h_{22}(w_2)=\frac{8q^2-8q^2w_2+5q^5w_2^2}{(q^2w_2-4)^2},$$

$$h_{23}(w_2)=\left(\frac{4}{w_1}+\frac{4}{w_2}-c\right)^2+(2q-4)\left(\frac{4}{w_1}-\frac{c}{2}\right)^2.$$

In the model (11), $h_{11}(w_2)$ and $h_{21}(w_2)$ are same as model (10), then we have:

$$h_{12}(w_2)=0, h_{13}(w_2)=1/w_1^2; h_{22}(w_2)=16/w_2^2, h_{23}(w_2)=0.$$

Now, we should solve following equation to find the $A-$

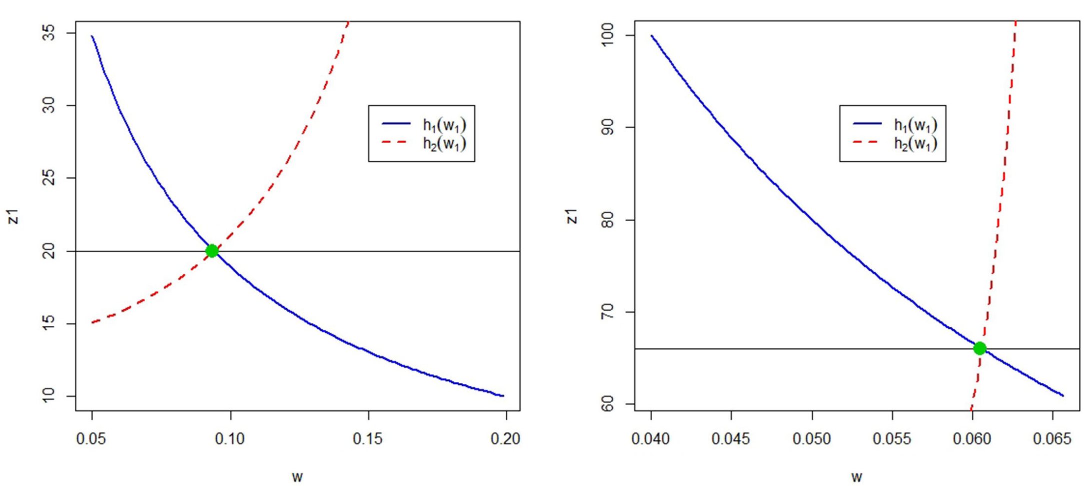

Figure 1. The portrait for A–optimality design in model (10) and model (11).

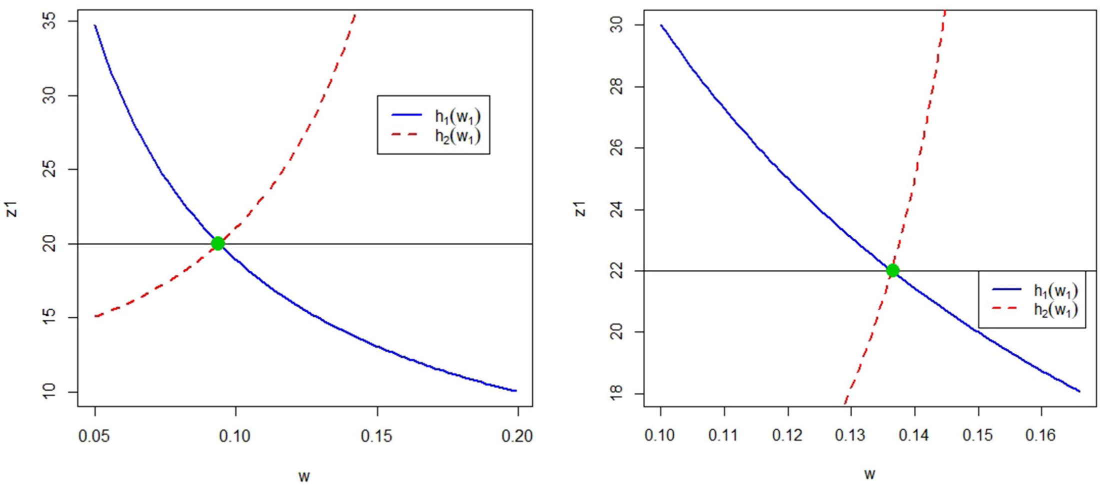

Figure 2. The portrait for A–optimality design in model (10) and model (11).

optimal design ζ^* for the models (10) and (11),

$$\psi_g(j,\tau_1;\zeta^*) = \psi_g(j,\tau_2;\zeta^*). \tag{14}$$

Beside, the solution of equation $w_i = u_i(q,s)$ $i = 1,2$ 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 η^* is a uniform design on X_s, and we can find the optimal design ξ^* on S^{q-1} by calculate $\log h_1(w_2)$ $\log h_2(w_2)$ and $\log t\ (M_g^{-1}(\zeta)$ in $w_2 \in (0,1/Q)$.

For the model (10), we find that $\min\limits_{w_2\in(0,1/Q)} \{\log tr(M_g^{-1}(\zeta))\} = 21.37664$ when

$w_2^* = 0.2911$, so the design

$$\xi^* = (T_1, T_2; 0.0411, 0.2911).$$

For the model (11), we have

$$\min_{w_2\in(0,1/Q)} \{\log tr(M_g^{-1}(\zeta))\} = 26.12341$$

when $w_2^* = 0.0768$, so the design:

$$\xi^* = (T_1, T_2; 0.0077, 0.2577).$$

As we expressed above satisfy equivalence condition (14), we can confirm the design ζ^*, because the three curves $\log h_1(w_2)$ $\log h_2(w_2)$ and $\log t\ (M_g^{-1}(\zeta)$ 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.

$$A_{eff}(\zeta) = \frac{tr\left[M_g^{-1}(\zeta^*)\right]}{tr\left[M_g^{-1}(\zeta)\right]}$$

Table 1. The weights of D -optimal design for $3 \le q \le 6$ and $2 \le s \le 6$

		Model (10)		Model (11)	
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 $\zeta_j^* = \eta^* \times \xi_j^*, j = 1,2,3$ 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 $3 \le q \le 6$ and $2 \le s \le 6$

		ζ_1^*			ζ_2^*	
q	s	(9)	(10)	(11)	(9)	(11)
3	2	0.2154	0.5487	0.0450	0.2230	0.5563
4	2	0.1364	0.2576	0.0223	0.1250	0.2500
5	2	0.0936	0.1468	0.0128	0.0799	0.1399
6	2	0.0686	0.0941	0.0082	0.0555	0.0889
3	3	0.2439	0.5772	0.0425	0.2496	0.5829
4	3	0.1585	0.2723	0.0226	0.1364	0.2576
5	3	0.1132	0.1566	0.0136	0.0858	0.1429
6	3	0.0838	0.1002	0.0089	0.0589	0.0902
3	4	0.2610	0.5943	0.0390	0.2673	0.6006
4	4	0.1746	0.2831	0.0219	0.1428	0.2619
5	4	0.1267	0.1634	0.0136	0.0888	0.1444
6	4	0.0967	0.1053	0.0091	0.0604	0.0908
3	5	0.2724	0.6057	0.0356	0.2791	0.6124
4	5	0.1866	0.2911	0.0207	0.1466	0.2644
5	5	0.1372	0.1686	0.0133	0.0906	0.1453
6	5	0.1049	0.1086	0.0091	0.0617	0.0913
3	6	0.2810	0.6143	0.0325	0.2850	0.6183
4	6	0.1947	0.2965	0.0195	0.1504	0.2669
5	6	0.1448	0.1724	0.0128	0.0924	0.1462
6	6	0.1119	0.1114	0.0082	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 τ be a product design with the marginal designs η and ξ on X_s and X , respectively.

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

$$\det(M_g(\zeta)) = \left(\prod_{s=1}^{S}\eta(s)\right)^{P_1}[\det(M_1\ (\xi)\ ]^{S-1}\det(M_f(\xi) \quad (15)$$

where ρ_1 shows the dimension of M_{11}.

The above lemma indicates the marginal design ρ is defined as an unique design on χ_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:

$$d_h(z;\tau) := h^T(z)M_h^{-1}(\tau)h(z) \qquad for\ z \in Q \quad (16)$$

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:

$$d_g(j,x^T;\tau) = d_f(x;\xi) + \left(\frac{1}{\eta(s)} - 1\right)\Delta_{f_1}(x;\xi) \qquad for(j,x) \in X_j * X_!$$

(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,

$$\Delta_{f_1}(x;\xi) = f_1^T(x)M_1^{-1}(\xi)f_1(x) \quad (18)$$

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.

6. References

1. Bondari K. Mixture Experiments and their applications in Agricultural research. SAS Users Group International Conference; 2005. p. 1–8.
2. Huang MNL, Lee CP, Chen RB, Klein T. Exact D-optimal designs for a second-order response surface model on a circle with qualitative factors. Computational Statistics and Data Analysis. 2010; 54(2):516–30. https://doi.org/10.1016/j.csda.2009.09.022.
3. Kiefer J. Optimal design: Variation in structure and performance under change of criterion. Biometrika. 1975; 62:277–88. https://doi.org/10.1093/biomet/62.2.277.

4. Kiefer J. General equivalence theory for optimum designs (approximate theory). The Annals of Statistics. 1974; 2(5):849–79. https://doi.org/10.1214/aos/1176342810.
5. Lee CP, Lo Huang MN. D-optimal designs for second-order response surface models with qualitative factors. Journal of Data Science. 2011; 9:139–53.
6. Liu Y, Liu MQ. Construction of uniform designs for Mixture Experiments with complex constraints. Communications in Statistics-theory and Methods. 2016; 45(8):2172–80. https://doi.org/10.1080/03610926.2013.875576.
7. Abdullah MS, Amir IZ, Sharon WXR. Mixture experiment on rheological properties of dark chocolate as influenced by cocoa butter substitution with xanthan gum/corn starch/glycerin blends. International Food Research Journal. 2014; 21(5):1887–92.
8. Yue RX, Liu X, Chatterjee K. D-optimal designs for multi-response linear models with a qualitative factor. Journal of Multivariate Analysis. 2014; 124:57–69. https://doi.org/10.1016/j.jmva.2013.10.011.