

Two Degree Becker Model for Mixture Design: Using D-optimal and A-optimal with Qualitative Factor

Zahra Rasooli Berardehi¹ and Chongqi Zhang^{2*}

¹School of Mathematics and information Sciences, Guangzhou University, Guangzhou, China; z.rasooli@gzhu.edu.cn

²School of Statistics and Economics, Guangzhou University, Guangzhou, China; edu.cncqzhang@gzhu.edu.cn

Abstract

Objectives: To achieve an optimal approximation for two-degree Becker model in mixture design. **Methods/Statistical Analysis:** The problem of mixture design case, based on qualitative factors and finding A-optimal and D-optimal design for two-degree Becker model is investigated. With the aim of this issue, a generalization of Lee method is utilized. We proposed a new procedure of Lee method for approximation of Becker model. Moreover, simulation results are done in R software. **Findings:** There is a direct relation between qualitative factor and A-optimal and D-optimal design, such that, 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; and maximization of the determination of information matrix is essential for D-optimal design. Besides, for a product function, based on 3 sections corresponding to the 2-marginal design, the dispersion function can be detected. In addition, illustrated examples confirm the analytical results. **Application/Improvements:** The application of this work is to be used in engineering and manufacturing which need to an amount of convenient mixture design.

Keywords: Becker Model, Dispersion Function, Information Matrix, Mixture Experiment, Optimality

1. Introduction

Mixture experiment is one of the main procedures of manufacturing of a product and it has a vast range of application in industrial and technology. For instance, in Civil engineering¹ Chemical sciences², medicine³ and so on, one can see the role of mixture design in advance^{4,5}. There are many forms of dietary supplements, for example, tablets, capsules, liquids, powders, and gels. Dietary supplements are different from drugs, and they are nonpatent drugs. The Food and Drug Administration (FDA) defined a dietary supplement as an alternative food containing essential nutrients like vitamins, minerals, and proteins⁶. Subsequently, the Nutrition Labeling and Education Act of 1990 added herb or nutritional substances to the definition. In the pharmaceutical industry, tablets are the most acceptable form for consumers in comparison with other oral dosage forms⁷. Tablet oral dosage has many advantages such as its ease of handling, chemical and physical

stability, and portability. Furthermore, this type of dosage form ensures accuracy and consistency of dosages⁸. There are many examinations that can be done in order to maintain the physical qualities of the tablets, for example, hardness test, percentage of friability test, disintegration test, and dissolution test⁹. Tablets are mixtures of active ingredients and other excipients. Mixtures mean the sum of all the ingredients is 100%. There are many types of excipient with their own function in dosage formulation: diluents or fillers, binders, lubricants, glidants, antiadherents, disintegrates, colorants, and flavor or sweeteners. The mixture design statistical method is the most suitable method used in optimizing the tablet production process. The mixture design method is usually used in mixture formulation.

Here, there is the mean response at the j -th level of a s -level for qualitative factor as follows

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

*Author for correspondence

where, $f_1^T(\tau)$ denote the part of the regression functions having interaction with the qualitative factor and $f_1^T(\tau)$ can be seen as the part of the effect of the level, but $f_2^T(\tau)$ is the part which is invariant at each qualitative level and $f_2^T(\tau)\gamma$ can be mention as the sector of common effect. Also, $\beta_j = (\beta_{j1}, \beta_{j2}, \dots, \beta_{jp_1})^T$, $j = 1, 2, \dots, s$ and $\gamma = (\gamma_1, \gamma_2, \dots, \gamma_{p_2})^T$ are vectors of unknown parameters, respectively. The experimental region of quantitative factors x is the q component mixture system which can be expressed as Where the C' s shows additional constraints condition which is introduced in 10. Also, $f_1(\tau)$ and $f_2(\tau)$, as two parts of regression function, are p_1 - and p_2 - dimension vector including the quantitative effects, respectively. It is clear that, the model 1 is more effective to fixing and demonstrate the relationship between variables.

The fundamental objective of this study is to develop the results of the work¹¹ to the A-optimal designs of mixture model and^{12,13} the D-optimal deign of mixture model. The rest of the article is arranged as follows: In section 2, some basic preliminaries and some notations are provided. Also, calculation of the trace of information matrix of model (1) is provided therein. In addition, the main results are given in section 3. And we find the A-optimal design and D-optimal design for the wo degree Becker model based on different situations of model (1). Finally, section 4 provides concluding remarks.

2. Preliminaries

The general linear model given by $E[y(z)] = g^T(z)\theta$, where $y(z)$ is the response variable, θ is a vector of unknown parameters, $g(z)$ is a given vector of regression functions of $z \in \Omega$. An approximate design is a probability distribution with finite support on the factor space Ω and it is represented by

$\zeta = (z_1, z_2, \dots, z_n; w_1, w_2, \dots, w_n)$ which assigns, respectively. Masses $w_1, w_2, \dots, w_n; w_i > 0$, $\sum w_i = 1$, to the n distinct support points of $z_1, z_2, \dots, z_n$ the design s in the experimental region. The worth of a design is measured by its Fisher information matrix which is given by

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

2.1 A-optimal

A design is defined to be A-optimal if it minimizes the trace of the inverse of the information matrix. The works^{14,15} gave us an effective way to check the A-optimality of arbitrary designs ζ , and for a design ζ which is A-optimal if and only if

$$g^T(z)M^{-2}(\zeta)g(z) - t[M^{-1}(\zeta)] \leq 0 \quad (2)$$

Let the general mode (1) be rewritten as

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

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 denote the Kronecker product of two matrices, let $x_s = \{1, 2, \dots, s\}$ be the index set of the qualitative levels and $\Omega = x_s \times x$ be the experimental region. Note the information matrix of the design ξ is:

$$M_f(\xi) = \begin{bmatrix} M_{11}(\xi) & M_{12}(\xi) \\ M_{21}(\xi) & M_{22}(\xi) \end{bmatrix} \quad (3)$$

which is associated with the model $E[y(\tau)] = [f_1^T(\tau), f_2^T(\tau)](\beta^T, \gamma^T)^T$. An arbitrary design on Ω can be expressed as

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

where, η and ξ_j are the marginal and the conditional designs on $\mathcal{X}_s$ and $\mathcal{X}$, respectively.

If ζ is supposed as a design production and it is presented by $\zeta = \eta \times \xi$, where emphasizes that $\xi_j = \xi$ for all j .

According to the result of¹¹ the information matrix of ζ will present by

$$M_g(\zeta) = \begin{bmatrix} D \otimes M_1(\xi) & \eta \otimes M_2(\xi) \\ \eta^T \otimes M_1(\xi) & M_2(\xi) \end{bmatrix}$$

In which

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

$$D = \text{diag}(\eta(1), \eta(2), K, \eta(s)), \quad \eta = (\eta(1), \eta(2), K, \eta(s))^T$$

calculate the inverse matrix of $M_g(\zeta)$. Now, the following lemma can be obtained.

Lemma 1^{16,17} For, an arbitrary design $\zeta(j, \tau) = \eta(j) \times \xi(\tau)$ where η and ξ there are the conditional designs and the marginal on x_s and x , respectively. Then one can has the following equation of trace for model (1).

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

where,

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

and

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

Proof:

By calculating the inverse matrices of $M_f(\xi)$ and $M_g(\zeta)$, we have

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

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

where, 1_s is $s \times 1$ vector of all ones.

$$D_{11}(\zeta) = D^{-1} \otimes M_1(\xi) + J_s \otimes K_{(1)},$$

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

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

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

So we have

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

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

And this completes the proof.

In particular, while the design $\eta(j)$ is a uniform design on x_s , i.e. $\eta(j) = \frac{1}{s}$, $j = 1, 2, K, s$, then we have

$$\begin{aligned} \text{tr}[M_g^{-1}(\zeta)] &= s^2 \cdot (M_{11}^{-1}(\xi)) + s \cdot \text{tr}(K_{(1)}) + \text{tr}(D_{22}(\xi)) \\ &= s^2 \cdot (M_{11}^{-1}(\xi)) + (s^2 - s) \cdot \text{tr}(M_{11}^{-1}(\xi)) + (1 - s) \cdot \text{tr}(D_{22}(\xi)) \end{aligned}$$

Moreover, it also shows that, if ζ be an A-optimal, then all of the elements of η should be equal, i.e.

$$\eta(j) = \frac{1}{s}, \quad j = 1, 2, K, s.$$

2.2 D-optimal

In a design, if the determine of information matrix be maximizes the with that design, then it is as a D-optimal design. A useful way for checking the D-optimality is attention to this point that a design can be D-optimal if and only if

$$g^T(j, \tau) M_g^{-1}(\xi) g^T(j, \tau) - s p_1 - p_2 \leq 0 \quad (4)$$

where, the information matrix of the design is

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

which, it is shown in (3) and this is same as information matrix with A-optimal design.

In next section we will consider finding of the A-optimal and A-optimal designs for two degree Becker model under the this condition which:

$$\eta(j) = \frac{1}{s}, \quad j = 1, 2, K, s.$$

3. Methodology

In this part, A-optimal and D-optimal method for the two degree Becker model are investigated.

3.1 A-optimal for the Two Degree Becker Model

For proving the A-optimality via the equivalence theorem, we can define the function as

$$\Psi_g(z; \zeta) = g^T(z) M_g^{-2}(\zeta) g(z), \quad z \in \Omega$$

Based on the equivalence condition (2), and for any design ζ , this is an A-optimal design if and only if following condition satisfy

$$\Psi_g(z; \zeta) - t [M_g^{-1}(\zeta)] \leq 0$$

Theorem 2 Suppose that all conditions of Lemma 1 be confirmed and consider $\eta(j) = 1/s$, $j = 1, 2, K, s$, then we have

$$\Psi_g(j, \tau; \xi) = s \cdot \Psi_f(\tau; \xi) + (1-s) \|z(\tau; \xi)\|^2 + (s^2 - s) \Psi_{f_1}(\tau; \xi), \quad (5)$$

and

$$z(\tau; \xi) = [-D_{22}(\xi) M_{21}(\xi) M_{11}^{-1}(\xi), D_{22}(\xi)] f(\tau), \quad f^T(\tau) = [f_1^T(\tau), f_2^T(\tau)].$$

Proof:

For the convenience, we simply write (0.3) as $M_f(\xi) = \{M_j\}_{j=1}^2$, then the following results can be obtained.

$$\begin{aligned} \Psi_g(j, \tau; \xi) &= \frac{1}{\eta(j)} \Psi_f(\tau; \xi) + \left(s - \frac{1}{\eta(j)}\right) \left[\sum_{i=1}^4 A_i(\tau; \xi)\right] \\ &+ \left(1 - \frac{1}{\eta(j)}\right) \left[\sum_{i=1}^4 B_i(\tau; \xi)\right] \\ &+ \left(\frac{1}{\eta^2(j)} - \frac{1}{\eta(j)}\right) \Psi_{f_1}(\tau; \xi) \end{aligned}$$

where,

$$A_1(\tau; \xi) = f_1^T(\tau) K_{(1)}^2 f_1(\tau), \quad A_2(\tau; \xi) = f_1^T(\tau) K_{(1)} M_1^{-1} M_2 D_2 f_2(\tau),$$

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

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

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

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

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

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

$$\sum_{i=1}^4 B_i(\tau; \xi) = \|z(\tau; \xi)\|^2 = \left\| [-D_{22}(\xi) M_{12}(\xi) M_{11}^{-1}(\xi), D_{22}(\xi)] f(\tau) \right\|^2$$

It is obviously that the theorem is hold when

$$\eta(j) = 1/s, \quad j = 1, 2, K, s.$$

So, proof is finished.

Corollary 1 As a result of the lemma 1 and theorem 1, one has

$$\Psi_g(z, \tau; \xi) - t[M_g^{-1}(\xi)] = s t_1(\tau; \xi) + (s^2 - s) t_2(\tau; \xi) + (1-s) t_3(\tau; \xi)$$

where,

$$t_1(\tau; \xi) = \Psi_f(\tau; \xi) - t [M_g^{-1}(\xi)],$$

$$t_2(\tau; \xi) = \Psi_{f_1}(\tau; \xi) - t [M_1^{-1}(\xi)],$$

$$t_3(\tau; \xi) = \|z(\tau; \xi)\|^2 - t [D_2(\xi)],$$

And then by considering of the q components two-degree Becker model symbol as

$$E[y(\tau)] = \sum_{k=1}^q f_{L_k}^T(\tau) \beta_k, \quad \tau \in \mathcal{X} \subseteq s^{q-1}$$

where,

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

$$f_{L_2}(\tau) = (\sqrt{x_1 x_2}, \sqrt{x_2 x_3}, \dots, \sqrt{x_{q-1} x_q})^T$$

$$f_{L_1}(\tau) = (x_1 x_2 x_3, x_2 x_3 x_4, \dots, x_{q-2} x_{q-1} x_q)^T, \dots, f_{L_q}(\tau) = x_1 x_2 x_3 \dots x_q$$

Now, for fixing the ideas, we should focus on the model which is provided on S^{q-1} by

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

Three kinds of model which form as (1) given, must be considered. Means, for the general model of multi-response

$$E[y(j, \tau)] = (f_{L_1}^T(\tau), f_{L_2}^T(\tau))\beta_j, \quad j=1, 2, \dots, s \quad (6)$$

where, on the different levels it has different function, and it doesn't have any qualitative factors.

If we assume the $f_{L_2}^T(\tau)$ be a qualitative factors and suppose that $f_{L_1}^T(\tau)$ having interaction with the qualitative factor, then this model can be presented as

$$E[y(j, \tau)] = f_{L_1}^T(\tau)\beta^{(L_1)}_j + f_{L_2}^T(\tau)\gamma^{(L_2)} \quad (7)$$

Equivalently, the two part of regression function can be exchanged as quantitative and qualitative factors, so the model change as

$$E[y(j, \tau)] = f_{L_2}^T(\tau)\beta^{(L_2)} + f_{L_1}^T(\tau)\gamma^{(L_1)} \quad (8)$$

However, there isn't any main difference between model (6) to model (8). In this study, qualitative and quantitative factors are considered altogether, the problem of design to estimate the unknown parameters will be supposed where it is considered to exist one qualitative factor with s levels. The two degree Becker model mentioned that for models (6),(7) and (8), $\psi_g(j, \tau; \xi)$ gains its maximum just at the barycentres of S^{q-1} . Therefore, just the barycentres can be possible in the support points for designs of A-optimal.

In first step, define M_i as a $C(q, i) \times q$ matrix, such that the first i elements in the first row of M_i are 1 and the other elements in the first row equal to 0, and the other $C(q, i) - 1$ rows of M_i have the different permutations of the first row based on lexicographical order. (For instance, in the case of $i=2$ and $q=4$, M_i is a 6×4 matrix, and its 1st, 2nd, ..., 6th rows should be (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.)

Consider that T_i be definition of the points set which elements are each rows of $i^{-1}M_i$, $i=1, 2, \dots, q$. Then, the T_1 called the set of all vertexes of S^{q-1} , T_2 called

the set of barycenter on the $q-2$ ension boundary. So, the design ξ can be define according to the models (6),(7) and (8) as following equation:

$$\xi = (T_1, T_2; w_1, w_2), \quad (9)$$

where, the weight functions w_1 and w_2 satisfy the condition $qw_1 + C(q, 2)w_2 = 1$.

Therefore, for the information matrix $M_f(\xi)$ which is associated via model (6), one can has

$$M_f(\xi) = \begin{bmatrix} \frac{w_2}{4} M_2^T M_2 I_Q + w_2 I_Q & \frac{w_2}{2} M_2^T M_2 I_Q \\ \frac{w_2}{4} M_2 I_Q & \frac{w_2}{2} I_Q \end{bmatrix}$$

where, $Q = q(q-1)/2$, and I_q is the $q \times q$ identity matrix. According to these notations, the following Lemma can be expressed.

Lemma 2 For any design ξ such as (9) defined, the function $\psi_g(j, \tau; \xi)$ with $f^T(\tau) = [f_1^T(\tau) + f_2^T(\tau)]$ in one of the (7) and (8) models can be displayed as

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

where,

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

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

Also, in the model (7),

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

which

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

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

Moreover, in the model (8),

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

$$\text{which, } \delta_i(\tau) = -\frac{2}{w_1}(2x_i^2 - x_i), \quad i = 1, 2, \dots, q.$$

Proof:

By calculating the inverse matrix of $M_f(\xi)$ is

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

Note $J(k, l) = 1_k 1_l^T$, $J_k = 1_k 1_l^T$ and the matrix

$$M_f^{-2}(\xi) = \{A_j\}_{j,i=1}^2, \text{ where}$$

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

$$A_{22} = \frac{256}{w_2^2} I_Q + \frac{64}{w_1^2} J_Q + \frac{128w_1 + 4(4q-7)w_2}{w_1^2 w_2} M_2 M_2^T.$$

For the model (0.6), the form of information matrix is same as (0.9), then we have

$$M_{11}^{-1}(\xi) = -\frac{4q}{4 - q^2w_2} I_q + \frac{q^2w_2}{4 - q^2w_2} J_q,$$

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

$$M_{11}^{-1}(\xi) M_{12}(\xi) D_{22}(\xi) = c M_2^T,$$

$$\text{where, } c = \frac{4q}{2 + qw_2 - q^2w_2}. \text{ For the model (0.7),}$$

$$\text{note } \bar{M}^{-1}(\xi) = \{\bar{D}_{ij}(\xi)\}_{i,j=1}^2,$$

$$\text{the } f^T(x) = [f_1^T(x), f_2^T(x)] = [f_{L_2}^T(x), f_{L_1}^T(x)], \text{ the}$$

form of information matrix is

$$\bar{M}_f(\xi) = \{\bar{M}_{ij}(\xi)\}_{i,j=1}^2 = \begin{bmatrix} M_{22}(\xi) & M_{21}(\xi) \\ M_{11}(\xi) & M_{11}(\xi) \end{bmatrix}$$

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

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 $[D_2 M_2 M_1^{-1}, D_2] f(x)$, respectively.

Then, the proof is completed.

Now, based on the condition $w_1 = 1/q - w_2(q-1)/2$, Theorem 1 and Lemma 2, consider that $\tau_i \in T_i, i=1, 2$, then the function (5) can be precised as

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

Plus, in the model (7), we get

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

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

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

and in the model (8), $h_1(w_2)$ and $h_2(w_2)$ are same as model (7), then one can has

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

Here, for finding of the A -optimal design ξ^* for the model (7) and (8), solving the following equation is needed.

$$\psi_g(j, \tau_1; \xi^*) = \psi_g(j, \tau_2; \xi^*). \quad (10)$$

Clearly the solution of equation $w_i = u_i(q, s), i = 1, 2$ is too complicated to analysis and symbol, however, the approximate of the optimal design by calculate the result of Lemma 2 can be obtained. For instance, consider $q = 30, s = 20$, one can find the A -optimal design of $\xi^* = \eta^* \times \xi^*$ on the region $X_s \times S^{q-1}$, which on X_s region, the η^* should be uniform design and we can obtain the optimal design ξ^* on S^{q-1} by calculat-

ing of $\log h_1(w_2)$, $\log h_2(w_2)$, and $\log tr(M_g^{-1}(\zeta))$ in $w_2 \in (0, 1/Q)$.

Now, in model (7), one gets that $\min_{w_2 \in (0, 1/Q)} \{\log tr(M_g^{-1}(\zeta))\} = 7.3761$ for $w_2^* = 0.0546$, thus the design

$$\xi^* = (T_1, T_2; 0.0908, 0.0546).$$

Also, in model (8), we obtain $\min_{w_2 \in (0, 1/Q)} \{\log tr(M_g^{-1}(\zeta))\} = 7.0867$ in which $w_2^* = 0.0768$, thus the design

$$\xi^* = (T_1, T_2; 0.1348, 0.0768).$$

the design of ξ^* can be verified as defined above implies equivalence condition (11) since the three curves $\log h_1(w_2)$, $\log h_2(w_2)$ and $\log tr(M_g^{-1}(\zeta))$ intersect at the same point, where these are shown in Figures 1 and 2.

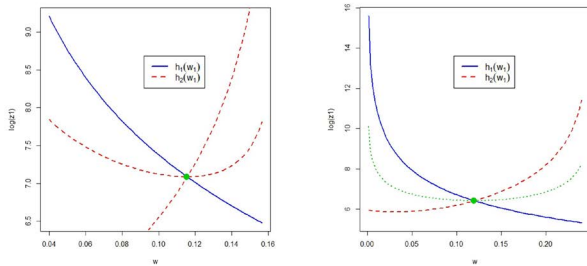


Figure 1. A – optimal design on model (7) and model(8).

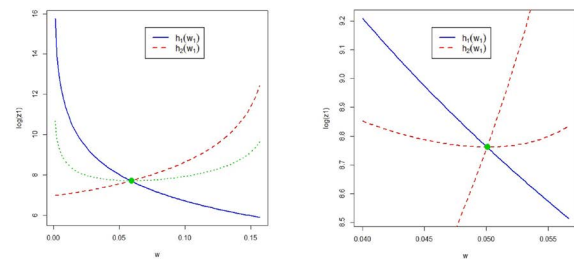


Figure 2. D – optimal design on model (7) and model(8).

Here, the optimal weights for model (6), (7) and (8) are also listed with $q \in \{3, 4, L, 6\}$ and $s \in \{2, 3, L, 6\}$ as one can see in the Tables 1 and 2.

Table 1. The weights of D-optimal design for $3 \leq q \leq 6$ and $2 \leq s \leq 6$ for Model (7)

q	s	Model (7)			
		w_1	w_2	$min(y)$	$log(tr(M_g))$
3	2	0.1735	0.1597	168.981	5.129
4	2	0.1096	0.0935	485.255	6.184
5	2	0.0773	0.0613	1114.969	7.0165
6	2	0.0591	0.0429	2215.092	7.703
3	3	0.1898	0.1433	233.806	5.453
4	3	0.1192	0.0871	611.133	6.4150
5	3	0.0830	0.0584	1324.596	7.188
6	3	0.0623	0.0417	2532.032	7.836
3	4	0.2061	0.1272	318.530	5.763
4	4	0.1289	0.0807	775.176	6.653
5	4	0.0907	0.0546	1597.447	7.3761
6	4	0.0670	0.0398	2944.431	7.9876
3	5	0.2191	0.1141	422.407	6.0459
4	5	0.1386	0.0742	975.466	6.8829
5	5	0.0964	0.0517	1930.49	7.5655
6	5	0.0717	0.0379	3448.009	8.1455
3	6	0.2321	0.1011	545.037	6.3008
4	6	0.1482	0.0678	1210.69	7.0989
5	6	0.1040	0.0479	2321.26	7.7498
6	6	0.0764	0.0360	4038.83	8.3037

The implementation of designs in comparison of the A – optimal design for model $g(\tau)$ are measured by the A -efficiency which is given by

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

It is worth noting that $\zeta_j^* = \eta^* \times \xi_j^*, j = 1, 2, 3$ are A – optimal design for model (6), (7) and (8), respectively. These designs are compared reciprocally with together for $q \in \{3, 4, L, 6\}$ and $s \in \{2, 3, L, 6\}$ and the A – efficiencies are shown in Tables 3 and 4.

Table 2. The weights of D-optimal design for $3 \leq q \leq 6$ and $2 \leq s \leq 6$ for Model (8)

q	s	Model (8)			
		w_1	w_2	$\min(y)$	$\log(\text{tr}(M_g))$
3	2	0.2245	0.1187	350.00	5.857
4	2	0.1154	0.0768	1195.99	7.086
5	2	0.0728	0.0543	3025.01	8.014
6	2	0.0501	0.0414	6383.98	8.761
3	3	0.2317	0.1015	672.74	6.511
4	3	0.1236	0.0644	2366.78	7.769
5	3	0.0768	0.0462	6088.33	8.714
6	3	0.0526	0.0351	12966.00	9.472
3	4	0.2431	0.0901	1089.03	6.993
4	4	0.1283	0.0542	3896.57	8.267
5	4	0.0793	0.0412	10123.57	9.222
6	4	0.0543	0.0308	21775.07	9.987
3	5	0.2489	0.0844	1596.13	7.375
4	5	0.1319	0.0521	5776.14	8.661
5	5	0.0814	0.0371	15107.61	9.622
6	5	0.0553	0.0283	32614.38	10.392
3	6	0.2575	0.0758	2191.95	7.692
4	6	0.0134	0.0485	7988.78	9.987
5	6	0.0829	0.0341	21025.43	9.953
6	6	0.0561	0.0262	45542.74	10.726

Table 3. Comparisons of A – Optimal for $3 \leq q \leq 6$ and $2 \leq s \leq 6$

q	s	Model (7)			
		w_1	w_2	$\min(y)$	$\log(\text{tr}(M_g))$
3	2	0.1735	0.1597	168.981	5.129
4	2	0.1096	0.0935	485.255	6.184
5	2	0.0773	0.0613	1114.969	7.016
6	2	0.0591	0.0429	2215.092	7.703
3	3	0.1898	0.1434	233.806	5.454
4	3	0.1192	0.0871	611.133	6.415
5	3	0.0830	0.0584	1324.596	7.188
6	3	0.0623	0.0417	2532.032	7.836
3	4	0.2061	0.1272	318.530	5.763
4	4	0.1289	0.0807	775.176	6.653
5	4	0.0907	0.0546	1597.447	7.376
6	4	0.0670	0.0398	2944.431	7.987
3	5	0.2191	0.1141	422.407	6.045
4	5	0.1386	0.0742	975.466	6.882
5	5	0.0964	0.0517	1930.49	7.565
6	5	0.0717	0.0379	3448.00	8.145
3	6	0.2321	0.1011	545.037	6.300

4	6	0.1482	0.0678	1210.69	7.098
5	6	0.1040	0.0479	2321.26	7.749
6	6	0.0764	0.0360	4038.87	8.303

Table 4. Comparisons of A – Optimal for $3 \leq q \leq 6$ and $2 \leq s \leq 6$

q	s	Model (8)			
		w_1	w_2	$\min(y)$	$\log(\text{tr}(M_g))$
3	2	0.2145	0.1187	350.00	5.857
4	2	0.1154	0.0768	1195.99	7.086
5	2	0.0728	0.0543	3025.01	8.014
6	2	-	-	-	-
3	3	0.2317	0.1015	672.74	6.511
4	3	0.1236	0.0644	2366.78	7.769
5	3	0.0768	0.0462	6088.33	8.714
6	3	-	-	-	-
3	4	0.2431	0.0901	1089.03	6.993
4	4	0.1283	0.0542	3896.57	8.267
5	4	0.0793	0.0412	10123.57	9.222
6	4	-	-	-	-
3	5	0.2489	0.0844	1596.13	7.375
4	5	0.1319	0.0521	5776.14	8.661
5	5	0.0814	0.0371	15107.61	9.622
6	5	-	-	-	-
3	6	0.2575	0.0758	2191.95	7.692
4	6	0.0134	0.0485	7998.745	8.987
5	6	0.0829	0.0341	21025.43	9.953
6	6	-	-	-	-

4. Conclusion

This study investigates the problem of mixture design case because of efficacy of mixture design in procedure of industrial experiences. In this regard, based on qualitative factors and finding A-optimal and D-optimal design for two-degree Becker model, the condition of production of mixture design is taken into account. It is worth to mention that, there is a direct relation between qualitative factor and A-optimal and D-optimal design. Such that, firstly 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. Secondly, 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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