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D- and A-Optimal Design for Mixture Experiments Using some Trigonometric Models

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ABSTRACT
This paper is devoted to study D- and A-Optimal Design for Mixture Experiments with q components

$x_1 = p_1, x_2 = p_2, \ldots\ldots x_q = p_k$

When trigonometric models are used. These models are linear in $m \times 1$ vector of parameters $\bar{\beta} = (\beta_{1,\ldots\ldots,\beta_m})$. Although, these models are extensively investigated by many authors in the literature yet none have been done for mixture experiment . Two numerical methods have been applied to calculate the A- and D -Optimal Design for q=3 components, the first method is a numerical algorithm known as a Multiplicative Algorithm established by Torsney (1988). The other method is a basic grid search to check the solution using the first method, which cannot be done for q>3 . The design points used in this paper are permutations of q constant $p_1, p_2, \ldots\ldots p_q$.

Keywords: A- and D -Optimal Design , Trigonometric Models, Mixture ExperimentsDesign, Multiplicative Algorithm.

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I. INTRODUCTION

The main feature of mixture experiment which distinguishit from other experiments is that

$x_i \geq 0 \quad , \quad i = 1, 2, \ldots\ldots q$

$$\sum_{i=1}^{q} x_i = 1$$

,

Two optimal criterions areA- and D –Optimal. These are can be expressed as a function $\phi(M)$ of the Fisher information matrix M these defined as follows,

D –Optimal : maximize $\phi_{\det}(M) = \log|M|$, A–Optimal: maximize $\phi_{trace}(M) = trace(M)$

A trigonometric model can be written as

$$\eta = \beta_o + \sum_{i=1}^{q} \beta_{ci} \cos(x_i)$$

$$\eta = \beta_o + \sum_{i=1}^{q} \beta_{si} \sin(x_i)$$

$$y = \beta_0 + \sum_{i=1}^{q} \beta_{si} \sin(x_i) + \sum_{i=1}^{q} \beta_{ci} \cos(x_i)$$

Whereas:

η :Expected response

β_o : General average

$\sin(x_i) \quad , i = 1, \ldots q$ trigonometricmodel parameters containing β_{si}

β_{ci} trigonometricmodel parameters containing $\cos(x_i) \quad , i = 1, \ldots q$

They are constant and unknown parameters

The design matrix for 3 and 4 components are

$$X = \begin{bmatrix} p_1 & p_2 & p_3 \\ p_2 & p_3 & p_1 \\ p_3 & p_1 & p_2 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ p_1 & p_3 & p_2 \\ p_2 & p_1 & p_3 \\ p_3 & p_2 & p_1 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix} \quad X = \begin{bmatrix} p_1 & p_2 & p_3 & p_4 \\ p_2 & p_1 & p_4 & p_3 \\ p_3 & p_4 & p_2 & p_1 \\ p_4 & p_3 & p_1 & p_2 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ p_1 & p_2 & p_4 & p_3 \\ p_2 & p_1 & p_3 & p_4 \\ p_3 & p_4 & p_1 & p_2 \\ p_4 & p_3 & p_2 & p_1 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}$$

We have simply , determine theA- and D –Optimal design through the Multiplicative Algorithm which consist of the following iteration to update the value of the q components

$$p_j^{(r+1)} = \frac{p_j^{(r)} f\left(F_j^{(r)}\right)}{\sum_{i=1}^{q} p_i^{(r)} f\left(F_i^{(r)}\right)}$$

Where F is the j^{th} vertex directional derivative for A- and D –Optimal

$$F_\psi\{\underline{p},\underline{e}_j\} = \text{tr}\left\{M^{-2}(\underline{p})\,\frac{\partial M(\underline{p})}{\partial p_j}\right\} - \sum_{i=1}^{q} p_i\,\text{tr}\left\{M^{-2}(\underline{p})\,\frac{\partial}{-}\right.$$

$$F_\psi\{\underline{p},\underline{e}_j\} = \text{tr}\left\{M^{-1}(\underline{p})\,\frac{\partial M(\underline{p})}{\partial p_j}\right\} - \sum_{i=1}^{q} p_i\,\text{tr}\left\{M^{-1}(\underline{p})\,\frac{\partial}{-}\right.$$

F is an increasing positive function.

II. RESULT AND DISCUSSIONS

the Multiplicative Algorithm and the grid search for the D- and A–Optimal design, shows agreements about the solution for Model (3) in the case of 3 component at the vertices as shown in Figures 1 and 2 . For q=4 , using the Multiplicative Algorithm we find out that the solutions are again given at the four vertices i.e. $p_1 = 1,\ p_2 = p_3 = p_4 = 0$ or any permutation of it .

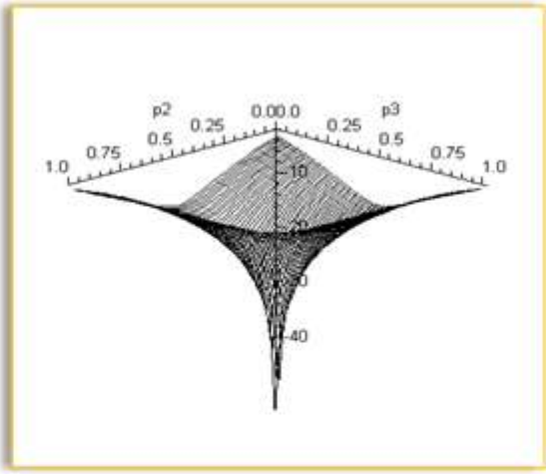

Fig.1: The graph of theD –Optimal design, q=3

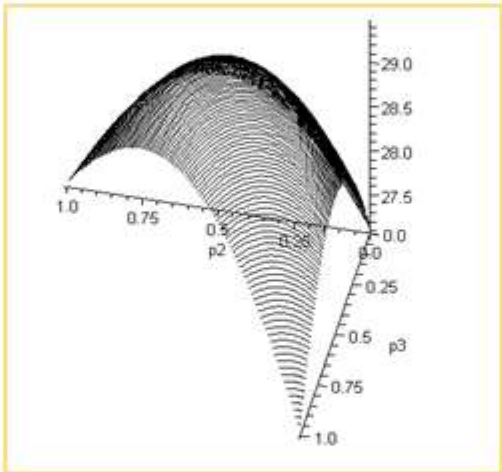

Fig.2: The graph of theA –Optimal design, q=3

Finding optimal values based on the two criteria for some of the proposed triangulation models by applying the algorithm using the S-plus program for Model (3) in the case of 3 componentWe get the following results in table 1 and 2

P Value of components			F Directional derivation			The optimum value for the selected standard
P_1	P_2	P_3	F_1	F_2	F_3	D- Optimal
1	0	0	0	-13.0352179	-13.0352179	-2.7806432
0	1	0	-13.0352179	0	-13.0352179	-2.7806432
0	0	1	-13.0352179	-13.0352179	0	-2.7806432

Table 1: shows the D –Optimal **design, q=3**

P Value of components			F Directional derivation			The optimum value for the selected standard
P_1	P_2	P_3	F_1	F_2	F_3	A- Optimal
1	0	0	0	-474.2848970	-474.2848970	-27.10922
0	1	0	-474.2848970	0	-474.2848970	-27.10922
0	0	1	-474.2848970	-474.2848970	0	-27.10922

Table 2: shows the A –Optimal **design, q=3**

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