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Generalization of E-Optimal Design for Non-Maximal Parameter Subsystem for M-Ingredients

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Abstract
A mixture of two or more ingredients forms several products. In mixture experiments of m ingredients, the measured response is assumed to depend on the relative proportions. This study aims at developing a generalized E-optimal criterion formula for $m \geq 2$ ingredients which can be used to obtain the smallest eigen value for m number of ingredient. Using the Kronecker model by Draper and Pukelsheim, coefficient matrices for non-maximal parameter subsystem is developed. After obtaining coefficient matrix, information matrices for the respective parameter subsystem for two and m ingredient is then obtained. We then derived E-optimal weighted centroid designs for non-maximal parameter subsystem for two to m ingredients. Optimal weights and values for the weighted centroid designs were obtained using R-Package software. Results on non-maximal parameter subsystem, second degree mixture model for two to m ingredient E-optimal weighted centroid design therefore exist. A generalized formula for the computation of the smallest eigenvalues for m≥2 hence exists.

Keywords: Mixture experiments, Kronecker product, Moment matrices, Weighted Centroid Designs, Information matrices.

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I. Introduction

Mixture experiments is made up of mixing several components. The response in a mixture experiment is a function of the proportions of the different ingredients in the mixture. An example of a mixture experiments is applicable in agricultural research. Mixture experiment in agriculture depend on measurements of yield of a crop obtained from applications of various mixtures of fertilizers. The main objective in mixture experiment is to fit a mathematical model depending on the proportions of the components and the amount of the mixture.

Theorem I

Second degree Kronecker model for m-ingredients, the weighted centroid design

$\eta(\alpha^{(E)}) = \alpha_1\eta_1 + \alpha_2\eta_2$ is E-optimal. (1)

The maximum value for E-criterion for $K'\theta$ with m ingredients is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{8m}\left[(-m+3)\alpha_1 + m + 1 \pm \sqrt{D}\right] \tag{2}$$

Where $D = (m^2 + 14m + 1)\alpha_1^2 - (2m^2 + 20m - 22)\alpha_1 + (m^2 + 6m - 7)$

Proof

An Information matrix $C \in sym(s, H)$ can be uniquely represented in the form, Draper and Pukelsheim (1998).

$$C = \begin{pmatrix} aU_1 + bU_2 & dV_1 \\ dV'_1 & c\dfrac{V'V}{m} \end{pmatrix} \tag{3}$$

For the case of m ingredients, the information matrix $C_k(M(\eta(\alpha)))$ can then be written as

$$C = \begin{pmatrix} aU_1 + bU_2 & dV \\ dV' & c\frac{V'V}{m} \end{pmatrix} \tag{4}$$

With coefficients $a, b, c, d \in \Re$,
Where,

$$U_1 = I_m = \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} \tag{5}$$

$$U_2 = I_m I'_m - I_m = \begin{pmatrix} 1 & . & . & . & 1 \\ . & . & & & . \\ . & & . & & . \\ . & & & . & . \\ 1 & . & . & . & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & . & . & . & 1 \\ 0 & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 1 & & . & . & . & 0 \end{pmatrix},$$

(6)
and

$$V = \sum_{\substack{i,j=1 \\ i<j}}^{m} (e_i) \in \Re^{m\times 1} = (e_1 + e_2 + \ldots + e_m) = \begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \end{pmatrix} \tag{7}$$

Hence the information matrix $C_k(M(\eta(\alpha)))$ can be written as

$$C_k(M(\eta(\alpha))) = \begin{pmatrix} aU_1 + bU_2 & dV \\ dV' & c\frac{V'V}{m} \end{pmatrix} = \begin{bmatrix} a\begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 1 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 0 & & . & . & . & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 & . & . & . & 1 \\ 1 & 0 & & & & . \\ . & & . & & & . \\ . & & & . & & . \\ . & & & & . & \\ 1 & & . & . & . & 0 \end{pmatrix} & d\begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \end{pmatrix} \\ d(1 \quad . \quad . \quad . \quad 1) & c(1) \end{bmatrix}$$

$$= \begin{pmatrix} \frac{8\alpha_1 + \alpha_2}{8m}U_1 + \frac{\alpha_2}{8m(m-1)}U_2 & \frac{\alpha_2}{4m}V \\ \frac{\alpha_2}{4m}V' & \frac{\alpha_2}{4}\frac{V'V}{m} \end{pmatrix} \tag{8}$$

Where $a = \frac{8\alpha_1 + \alpha_2}{8m}$, $b = \frac{\alpha_2}{8m(m-1)}$, $c = \frac{\alpha_2}{4}$ and $d = \frac{\alpha_2}{4m}$

From Klein (2004) for m ingredients we have

$$D_1 = [a + (m-1)b - c]^2 + 2(m-1)[2d]^2$$

$$= \left[\frac{8\alpha_1 + \alpha_2}{8m} + \frac{(m-1)\alpha_2}{8m(m-1)} - \frac{\alpha_2}{4}\right]^2 + 2(m-1)\left[2\frac{\alpha_2}{4m}\right]^2$$

$$= \frac{(4m^2 + 56m + 4)\alpha_1^2 - (8m^2 + 80m - 88)\alpha_1 + (4m^2 + 24m - 28)}{64m^2} \quad (9)$$

The eigenvalues are;

$$\lambda_{2,3} = \frac{1}{2}\left[a + (m-1)b + c \pm \sqrt{D_1}\right] \quad (10)$$

$$= \frac{1}{2}\left[\frac{8\alpha_1 + \alpha_2}{8m} + \frac{(m-1)\alpha_2}{8m(m-1)} + \frac{\alpha_2}{4} \pm \sqrt{D_1}\right]$$

$$= \frac{1}{8m}\left[(-m+3)\alpha_1 + (m+1) - \sqrt{D}\right]$$

Where $D = (m^2 + 14m + 1)\alpha_1^2 - (2m^2 + 20m - 22)\alpha_1 + (m^2 + 6m - 7)$ with multiplicity 1.

Hence the smallest eigenvalue is $\lambda_{\min} = \frac{1}{8m}\left[(-m+3)\alpha_1 + (m+1) - \sqrt{D}\right]$ (11)

where *D* is as defined above.

Then $\lambda_{\min}$ is an eigenvalue for C if for corresponding eigenvector, say $\bar{z}$, we have $(C - \lambda I)\bar{z} = \bar{0}$ or $(C\bar{z} = \lambda\bar{z})$ with $\bar{z} \neq \bar{0}$

Now let

$$\bar{z} = \begin{pmatrix} z_1 \\ . \\ . \\ . \\ z_{m+1} \end{pmatrix}$$, be the eigenvector of C corresponding to λ.

We therefore have $(C - \lambda I)$, as

$$\begin{pmatrix} \frac{(m+4)\alpha_1 - m + \sqrt{D}}{8m}U_1 + \frac{\alpha_2}{8m(m-1)}U_2 & \frac{\alpha_2}{4m}V \\ \frac{\alpha_2}{4m}V' & \frac{(-m-3)\alpha_1 + (m-1) + \sqrt{D}}{8m}\frac{V'V}{m} \end{pmatrix}$$

(12)

Let $p_1 = \left[(m+4)\alpha_1 - m + \sqrt{D}\right]$, $q_1 = \alpha_2^2$, $r_1 = \left[(-m-3)\alpha_1 + (m-1) + \sqrt{D}\right]$

Where $D = (m^2 + 14m + 1)\alpha_1^2 - (2m^2 + 20m - 22)\alpha_1 + (m^2 + 6m - 7)$

We get $(C - \lambda I)\bar{z} = \bar{0}$

$$\frac{1}{8m}\begin{pmatrix} (m-1)p_1U_1 + q_1U_2 & 2(m-1)q_1V \\ 2(m-1)q_1V' & (m-1)r_1\frac{V'V}{m} \end{pmatrix}$$

Solving these equations for z_i we get,

$$\bar{z} = \begin{pmatrix} z_1 \\ . \\ . \\ . \\ \\ z_{m+1} \end{pmatrix} = \begin{pmatrix} 1 \\ . \\ . \\ . \\ 1 \\ \frac{-cmq}{r} \end{pmatrix}$$

Where c=2 for even number of ingredients and c=1 for odd number of ingredients as the eigenvector corresponding to $\lambda_{\min}$

Thus

$$\bar{z}\bar{z}' = \begin{pmatrix} U_1 + U_2 & -cmqV \\ \frac{cmq}{r}V' & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix} \quad (13)$$

and

$$\|z\|^2 = \frac{mr^2 + c^2m^2q^2}{r^2} \quad (14)$$

Therefore

$$E = \frac{\bar{z}\bar{z}'}{\|z\|^2} = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} U_1 + U_2 & -cmqV \\ \frac{cmq}{r}V' & \frac{c^2m^2q^2}{r^2}\frac{V'V}{m} \end{pmatrix} \quad (15)$$

From Cherutich (2012)

$$C_1 = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (16)$$

And from equation(15) and (16)

$$C_1E = \frac{r^2}{mr^2 + c^2m^2q^2}\begin{pmatrix} \frac{1}{m}U_1 + \frac{1}{m}U_2 & -cqV \\ 0 & 0 \end{pmatrix} \quad (17)$$

A weighted centroid design $\eta(\alpha)$ is E-optimal for $K'\theta$ in T if and only if $traceC_jE = \lambda_{\min}(C)$.

For j=1

$$traceC_jE = \frac{r^2}{m(mr^2 + c^2m^2q^2)} + ... + .\frac{r^2}{m(mr^2 + c^2m^2q^2)} = \frac{r^2}{(mr^2 + c^2m^2q^2)}$$

Hence $traceC_jE = \lambda_{\min}(C) \Leftrightarrow \frac{r^2}{(mr^2 + c^2m^2q^2)} = \frac{1}{8m}\left[(-m+3)\alpha_1 + (m+1) - \sqrt{D}\right]$ (18)

Putting $q = \alpha_2$, $r_1 = \left[(-m-3)\alpha_1 + (m-1) + \sqrt{D}\right]$ and

$D = (m^2 + 14m + 1)\alpha_1^2 - (2m^2 + 20m - 22)\alpha_1 + (m^2 + 6m - 7)$ reduces equation (18) to

$$-i\alpha_1^6 + j\alpha_1^5 - k\alpha_1^4 + l\alpha_1^3 - m\alpha_1^2 + n\alpha_1^1 - o = 0 \quad (19)$$

Where

$i = -320m^4 - 4672m^3 + 2880m^2 - 1664m^1 + 512$

$j = 1920m^4 + 25728m^3 - 25984m^2 + 17664m^1 - 6144$

$k = -4800m^4 - 58560m^3 + 83648m^2 - 63360m + 23040$

$l = 6400m^4 + 70400m^3 - 132352m^2 + 110080m - 40960$

$m = -4800m^4 - 47040m^3 + 111808m^2 - 101760m + 38400$

$n = 1920m^4 + 16512m^3 - 48512m^2 + 48384m - 18432$

$o = -320m^4 - 2368m^3 + 8512m^2 - 9344m + 3584$

Solving the above polynomial yields the values of α_1 from which we choose α_1,such that $\alpha_1 \in (0,1)$; we substitute this values to $\lambda_{\min}$ and take the values that minimizes the $\lambda_{\min}$, hence the optimal E-criterion is

$$v(\phi_{-\infty}) = \lambda_{\min}(C) = \frac{1}{8m}\left[(-m+3)\alpha_1 + m + 1 - \sqrt{D}\right] \qquad (20)$$

Where $D = (m^2 + 14m + 1)\alpha_1^2 - (2m^2 + 20m - 22)\alpha_1 + (m^2 + 6m - 7)$

II. Conclusion

From the study it is clear that second degree Kronecker model with m ≥2 ingredients a unique E-optimal weighted centroid designs exist for non-maximal parameter subsystem. Most importantly in addition, generalized formula for the computation of the smallest eigenvalues for m≥2 exists based on non-maximal parameter subsystems used in this study.

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