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I-Optimal designs for third degree kronecker model mixture experiments

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Abstract
Mixture experiments are special type of response surface designs where the factors under study are proportions of the ingredients of a mixture. In response surface designs, the main interest of the experimenter may be either on precise model estimation or precise predictions of responses. The main aim of I-optimality is to minimize the average prediction variance throughout the region of interest. Although mixtures experiments are usually intended to predict the response for all possible formulations of the mixture and to identify optimal proportions for each of the ingredients, little research has been done on I-optimal third degree Kronecker designs. I-optimal designs were studied in order to predict the response(s) and the optimal formulations for all possible ingredients in the simplex centroid. Weighted Simplex Centroid Designs (WSCD) and Uniformly Weighted Simplex Centroid Designs (UWSCD) mixture experiments were obtained in order to identify optimal proportions for each of the ingredients formulation. Maximal parameters of interest for third degree Kronecker model were considered. The general equivalence theorem for I-optimality was used to test optimality of different mixture formulations. UWSCD was found to perform better than WSCD in terms of average prediction variance with most formulations satisfying general equivalent theorem for I-optimality.

Keywords: Mixture Experiments, Kronecker Model, WSCD, UWSCD, I-optimality, General Equivalent Theorem.

1. Introduction

Mixture experiments are associated with the investigation of the m factors, assumed to influence the response only through proportions in which they are blended together. I-optimal designs minimize the average variance of prediction and therefore more appropriate for mixture experiments for precise predictions of responses. Average prediction variance provides a measure of the precision of the estimated response at any point in the design space. In available literature, the I-optimal designs criterion is often called the V-optimality criterion, Atkinson *et al* (2007) [1], but the names IV- or Q-optimality have been used as well, Borskowski (2003) [2]. Laake (1975) [6] analytically derived the I-optimal weights for the design points in case $q \geq 3$, assuming that the design points are the points of the $(q, 2)$. In experiments with mixtures, Liu and Neudecker (1995) [7] applied Weighted Simplex Centroid (WSC) to obtain V-optimal allocation of observations which was shown to be an optimal design over the entire simplex on Scheffé's polynomial model using the equivalence theorem. Goos *et al* (2016) studied I-optimal designs of mixture experiments for second order, special cubic and q^{th} degree models. They presented I-optimal continuous designs and contrast them with published results. Goos and Syafitri (2014) [4] studied the problem of finding continuous V-optimal mixture designs for the qth degree model. They provided a critical look at the results published in Liu and Neudecker (1995) [7] and found out that their designs were not V-optimal.

The mixture ingredients $t_1, t_2, \ldots, t_m$ are such that $t_i \geq 0$ and further restricted by $\sum t_i = 1$. Thus the experimental domain is the probability simplex

$$T_m = \left\{ t = (t_1 \quad ,..., \quad t_m ,)' \in [0,1]^m : \sum_{i=1}^{m} t_i = 1 \right\} \tag{1}$$

Under experimental condition $t \in T_m$, the response Y_t is taken to be a real-valued random variable. In a polynomial regression model the expected value $E(Y_t)$ is a polynomial function of t. The work done by Draper and Pukelsheim (1998) [3] is being extended to polynomial regression model for third degree mixture model. The S-polynomial is given as,

$$E(Y_t) = f(t)'\theta = \sum_{i=1}^{m} \theta_i t_i + \sum_{\substack{i,j=1 \\ i<j}}^{m} \theta_{ij} t_i t_j + \sum \sum \sum_{i<j<k}^{m} \theta_{ijk} t_i t_j t_k \tag{2}$$

and the homogeneous third-degree K-polynomial is

$$E(Y_t) = f(t)'\theta = (t \otimes t \otimes t)'\theta = \sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{k=1}^{m} \theta_{ijk} t_i t_j t_k \tag{3}$$

in which the Kronecker powers $t^{\otimes^3} = (t \otimes t \otimes t)$, $(\mathrm{m}^3 + 1)$ vectors, consists of pure cubic and three-way interactions of components of t in lexicographic order of the subscripts and with evident that third-degree restrictions are $\theta_{ijk} = \theta_{ikl} = \theta_{jik} = \theta_{jki} = \theta_{kij} = \theta_{kji}$ for all i, j and k

All observations taken in an experiment are assumed to be of equal unknown variance and uncorrelated. The moment matrix $M(\eta) = \sum_{j=1}^{t} w_j(t_j) f(t_j)^t = \int_\eta f(t) f(t)^t d\eta$ for the third degree Kronecker model has all entries homogeneous in degree six and reflects the statistical properties of a design η. The moment matrix can be partition into sub moments according to the number of ingredients in a simplex centroid design as follows

$$M(\eta) = \alpha_1 M(\eta_1) + \alpha_2 M(n_2) + ... + \alpha_m M(n_m) \tag{4}$$

For Uniformly Weighted Simplex Centroid Designs (UWSCD), the weights are assumed to be distributed uniformly in the sub moments matrices. Hence $\alpha_1 = \alpha_2 = ... = \alpha_m = \frac{1}{m}$ and their moment matrix is given as,

$$M(\eta) = \tfrac{1}{m} M(\eta_1) + \tfrac{1}{m} M(n_2) + ... + \tfrac{1}{m} M(n_m) \tag{5}$$

2. Information Matrix

Consider the Euclidean unit vectors in $\Re^m$ denoted by $e_1, e_2, ..., e_m$ and the set for

$$e_{ii\,j} = e_i \otimes e_i \otimes e_j,\ \mathrm{e}_{ijk} = e_i \otimes e_j \otimes e_k \text{ for i<j<k, i,j,k=\{1,2,...,m\}} \tag{6}$$

Let K be a $k \times s$ coefficient matrix such that

$$K = (K_1; K_2; K_3) \in \Re^{m^3 \times (m+1)} \tag{7}$$

where

$$K_1 = \sum_{i=1}^{m} e_{iii} e_i', \qquad K_2 = \tfrac{1}{3(m-1)} [\sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{iij} + e_{iji} + e_{jii}) e_i'] \text{ and } K_3 = \tfrac{1}{m(m-1)(m-2)} \sum_{\substack{i,j,k=1 \\ i \neq j \neq k}}^{m} (e_{ijk})$$

The Kronecker model of the full parameter vector $\theta \in \Re^{m^3}$ is not estimable. When fitting this model, the parameter subsystem considered in this study can be written as

$$K'\theta = \left\{ \begin{array}{l} (\theta_{iii})_{1 \le i \le m} \\ \frac{1}{3(m-1)} \left\{ \sum_{i,j=1}^{m} (\theta_{iij} + \theta_{iji} + \theta_{jii}) \right\} \\ \frac{1}{m(m-1)(m-2)} \sum_{\substack{i,j,k=1 \\ i \neq j \neq k}}^{m} (\theta_{ijk}) \end{array} \right\} \in \Re^{(m+1)} \quad \text{for all } \theta \in \Re^{m^3} \tag{8}$$

where $K \in \Re^{m^3 \times (m+1)}$

The parameter subsystem $K'\theta$ of interest is a maximal parameter system in the full parameter model. The information matrix for the parameter subsystem is given by

$$C_k(M(\eta)) = LM(\eta)L` \in NND(s) \quad (9)$$

where L is the left inverse of coefficient matrix K and is defined by

$$L` = (K`K)^{-1}K` \quad (10)$$

Thus the information matrices for $K`\theta$ are linear transformation of moment matrices.
I-optimal design minimizes average or integrated prediction variance over the experimental region of interest.

$$Average \text{ Variance} = \frac{1}{\int_\chi dt} tr[(t't)^{-1}M] \quad (11)$$

The matrix M is the moment matrix because its elements are proportional to moments of uniform distribution on the design region χ.

In the calculation of average prediction variance (APV), we exploit the following formula

$$Average \text{ Variance} = \int_\tau f'(t)M^{-1}f(t)dt = tr[M^{-1}\int_\tau f(t)f(t)'dt] \quad (12)$$

This expression can be simplified as

$$= \frac{1}{\int_\tau dt} tr[M^{-1}\int_\tau f(t)f'(t)dt] \quad (13)$$

Letting $R = \int_\tau f(t)f'(t)dt$, the AV is expressed as

$$AV = \frac{1}{\int_\tau dt} tr[M^{-1}R] \quad (14)$$

For parameter sub system of interest, inverse of information matrix (9) as,

$$C_k^{-1} = (LM(\eta)L` \in NND(s)\ )^{-1} \quad (15)$$

Assuming that the experimental region η is the full $(q-1)$ dimensional simplex S_{q-1}, the elements of R can be obtained using the formula,

$$R = \int_{S_{q-1}} t_1^{p_1},\ t_2^{p_2}, t_3^{p_3}, \ldots, t_q^{p_q} dt_1, dt_2, dt_3, \ldots, dt_q = \frac{\prod_{i=1}^{q}\Gamma(p_i+1)}{\Gamma(q+\sum_{i=1}^{q}p_i)} = \frac{\prod_{i=1}^{q}(p_i!)}{(\sum_{i=1}^{q}p_i+q-1)!} \quad (16)$$

When the experimental region η is the full $(q-1)$ dimensional simplex S_{q-1}, then its its volume is given by

$$volume = \int_\tau dt = \int_{S_{q-1}} dt = \frac{1}{\Gamma(q)} = \frac{1}{(q-1)!} \quad (17)$$

Therefore average prediction variance was obtained by

$$Average \text{ Variance} = (q-1)!\,tr[C_k^{-1}R] \quad (18)$$

3. Equivalence Theorem

The general equivalence theorem provides a methodology to check the optimality of a given continuous design, for any convex and differentiable design optimality criterion. Atkinson (2007) [1] explain that a continuous design with information matrix C is I-optimal if and only if

$$f'(t)C^{-1}LC^{-1}f(t) \le tr(C^{-1}L) \quad (19)$$

for each point t in the experimental region η according to the general equivalence theorem. The equivalence theorem designs is not constructive, but it can be used to check optimality of a given designs.

4. Four Factors Mixture Experiments

Using simplex restrictions, we obtained the optimal weights for WSCD, $\alpha_1, \alpha_2, \alpha_3$ and α_4 as 4/15, 6/15, 4/15 and 1/15 respectively. From equation (4), we have the moment matrix for four factors mixture experiments as,

$$M(\eta) = \tfrac{4}{15}M(\eta_1) + \tfrac{6}{15}M(n_2) + \tfrac{4}{15}M(n_3) + \tfrac{1}{15}M(n_4) \quad (20)$$

where,

$$M(\eta_1) = \tfrac{1}{4}[e_{111}(e_{111})' + e_{222}(e_{222})' + e_{333}(e_{333})' + e_{444}(e_{444})'] \quad (21)$$

$$M(\eta_2) = \tfrac{1}{384}[(d_1 \otimes d_1 \otimes d_1)(d_1 \otimes d_1 \otimes d_1)' + (d_2 \otimes d_2 \otimes d_2)(d_2 \otimes d_2 \otimes d_2)' + (d_3 \otimes d_3 \otimes d_3)(d_3 \otimes d_3 \otimes d_3)' + (d_4 \otimes d_4 \otimes d_4)(d_4 \otimes d_4 \otimes d_4)' + (d_5 \otimes d_5 \otimes d_5)(d_5 \otimes d_5 \otimes d_5)' + (d_6 \otimes d_6 \otimes d_6)(d_6 \otimes d_6 \otimes d_6)'] \quad (22)$$

$$M(\eta_3) = \tfrac{1}{2916}[(f_1 \otimes f_1 \otimes f_1)(f_1 \otimes f_1 \otimes f_1)' + (f_2 \otimes f_2 \otimes f_2)(f_2 \otimes f_2 \otimes f_2)' + (f_3 \otimes f_3 \otimes f_3)(f_3 \otimes f_3 \otimes f_3)' + (f_4 \otimes f_4 \otimes f_4)(f_4 \otimes f_4 \otimes f_4)'] \quad (23)$$

$$M(\eta_4) = \tfrac{1}{4096} J_{64} \quad (24)$$

also,

$d_1 = (1_4 - e_4 - e_3),\ d_2 = (1_4 - e_2 - e_4),\ d_3 = (1_4 - e_1 - e_4),\ d_4 = (1_4 - e_1 - e_3),$

$d_4 = (1_4 - e_1 - e_3),\ d_5 = (1_4 - e_1 - e_2)\ , d_6 = (1_4 - e_2 - e_3)$

$f_1 = (1_4 - e_4),\ f_2 = (1_4 - e_2),\ f_3 = (1_4 - e_3),\ \ f_4 = (1_4 - e_1),$

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix},\ e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix},\ e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } e_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The Uniformly Weighted Simplex Centriod Designs (UWSCD) for four ingredients were assumed to assign uniform weights to the four elementary centroid designs, $n_1, n_2,\ n_3$ and n_4, such that all weights are equal. That is,

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0.25 \quad (25)$$

The moment matrix for uniformly weighted simplex centriod designs in (5) for four ingredients is given by

$$M(\eta) = 0.25M(\eta_1) + 0.25M(n_2) + 0.25M(n_3) + 0.25M(n_3) \quad (26)$$

where,

$M(\eta_1)$, $M(n_2)$, $M(n_3)$ and $M(n_4)$ are given in (21), (22), (23) and (24) respectively.

The coefficient matrix K for the four ingredients parameter subsystems of interest in (7) and (8) is given as

$$K = (\mathrm{K}_1, K_2, K_3) \quad (27)$$

where

$$K_1 = \sum_{i=1}^{4} e_{iii} e_i' = e_{111} e_1' + e_{222} e_2' + e_{333} e_3' + + e_{444} e_4'$$

$$K_2 = \tfrac{1}{9}\left\{ \sum_{\substack{ij=1 \\ i \neq j}}^{3} (e_{iij} + e_{iji} + e_{jii}) e_i' \right\}$$

and

$$K_3 = \tfrac{1}{24}\left\{ \sum_{\substack{ijk=1 \\ i \neq j \neq k}}^{4} e_{ijk} \right\}$$

The left inverse L in (10) for four ingredients is given as,

$$L' = (\mathrm{K}_1, 6K_2, 24K_3\ ) \quad (28)$$

5. Application of I-Optimal in Four Ingredients

Using (11) and (28), we obtained the information matrix for Weighted Simplex Centroid Designs (WSCD) as

$$C_2 = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{12} & c_{22} & c_{23} \\ c'_{13} & c'_{23} & c_{33} \end{pmatrix} \quad (29)$$

where,

$c_{11} = x_{11}I_4 + y_{11}J_4$; $x_{11} = 688.4\times10^{-4}$, $y_{11} = 12.40842\times10^{-4}$

$c_{12} = x_{12}I_4 + y_{11}J_4$; $x_{12} = 67.98697\times10^{-4}$, $y_{12} = 43.68878\times10^{-4}$

$c_{22} = x_{22}I_4 + y_{22}J_4$; $x_{22} = 220.42181\times10^{-4}$, $y_{22} = 172.77722\times10^{-4}$

$c_{13} = x_{13}1_4$; $x_{13} = 20.36716\times10^{-4}$

$c_{23} = x_{23}I_4$; $x_{23} = 133.92168\times10^{-4}$

$c_{33} = x_{22}$; $x_{22} = 225.43724\times10^{-4}$

Using (17) and (28), we obtained the information matrix for uniform weighted simplex centroid designs as,

$$C_{2u} = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c'_{13} & c'_{23} & c_{33} \end{pmatrix} \tag{30}$$

where c_{11}, c_{12}, c_{13}, c_{22}, c_{23} and c_{33} are given as

$c_{11} = x_{11}I_4 + y_{11}J_4$; $x_{11} = 638.8782\times10^{-4}$, $y_{11} = 8.8354\times10^{-4}$

$c_{12} = c'_{21} = x_{12}I_4 + y_{11}J_4$; $x_{12} = 44.2062\times10^{-4}$, $y_{12} = 35.3124\times10^{-4}$

$c_{22} = x_{22}I_4 + y_{22}J_4$; $x_{22} = 148.05\times10^{-4}$, $y_{22} = 169.7616\times10^{-4}$

$c_{13} = c'_{31} = x_{13}1_4$; $x_{13} = 30.0810\times10^{-4}$

$c_{23} = c'_{32} = x_{23}1_4$; $x_{23} = 224.4348\times10^{-4}$

$c_{33} = x_{22}$; $x_{22} = 475.0416\times10^{-4}$

In four ingredients designs, we obtained the inverse of the information matrix (29) for parameter sub system of interest as,

$$C_2^{-1} = \begin{pmatrix} 14.9825(I_4) + 0.0023(J_4) & -4.6212(I_4) - 0.72399(J_4) & 1.5628(1_4) \\ -4.6212(I_4) - 0.72399(J_4) & 46.79292(I_4) - 7.08239148(J_4) & -10.52455(1_4) \\ 1.5628(1'_4) & -10.52455(1'_4) & 39629.9676 \end{pmatrix} \tag{31}$$

We now obtained the matrix L through integration of the parameter subsystem of interest of the Kronecker model as given in (16). Thus, L becomes,

$$L = \begin{pmatrix} 0.0113(I_4) + 0.0006(J_4) & 0.00158(I_4) + 0.0004(J_4) & 0.00032(1_4) \\ 0.00158(I_4) + 0.0004(J_4) & 0.00033(I_4) + 0.0002(J_4) & 0.00014(1_4) \\ 0.00032(1'_4) & 0.00014(1'_4) & 0.00008 \end{pmatrix} \tag{32}$$

Now using (31) and (32), we obtained $C_2^{-1}L$ as

$$C_2^{-1}L = \begin{pmatrix} 0.1621098(I_4) + 0.007390487(J_4) & 0.0222535(I_4) + 0.005174219(J_4) & 0.004272272(1_4) \\ 0.0222535(I_4) + 0.005174219(J_4) & 0.008138595(I_4) - 0.002221494(J_4) & 0.0001414522(1_4) \\ 0.004272272(1'_4) & 0.0001414522(1'_4) & 0.0017869842 \end{pmatrix} \tag{33}$$

Therefore, the average prediction variance is given by the trace of (33). Hence,

$$APV = tr[C_2^{-1}L] = 0.7034569 \tag{34}$$

Similarly, we obtained the inverse of the information matrix (30) for the parameter subsystem of interest as,

$$C_{2u}^{-1} = \begin{pmatrix} 15.982644(I_4) + 0.0007984(J_4) & -4.77225248(I_4) - 0.08245342(J_4) & 1.398217(1_4) \\ -4.77225248(I_4) - 0.08245342(J_4) & 68.96969(I_4) - 10.63118966(J_4) & -12.17091(1_4) \\ 1.398217(1'_4) & -12.17091(1'_4) & 43.69736 \end{pmatrix} \tag{35}$$

Using (32) and (35), we obtained the matrix $C_{2u}{}^{-1}L$, for the I-optimal design, such that,

$$C_{2u}{}^{-1}L = \begin{pmatrix} 0.1173181095I_4 + 0.007819716J_4 & 0.0237911151I_4 + 0.005501782J_4 & 0.004552701(1_4) \\ 0.0555038I_4 - 0.014274488J_4 & 0.01523243I_4 - 0.002134630J_4 & 0.001065428(1_4) \\ -0.005406623(1'_4) & -0.003104111(1'_4) & -0.001426310 \end{pmatrix} \tag{36}$$

Thus, the average prediction variance becomes,

$$tr[C_{2u}^{-1}L] = 0.7749682 \tag{37}$$

Comparing (34) and (37), WSCD performed better than UWSCD due to its smaller average prediction variance leading to more accurate prediction of responses in mixture experiments.

6. Equivalence Theorem for Weighted Simplex Centroid Designs

For four ingredients, the design is said to be I-optimal, if it satisfy the following inequality at a given design points of the simplex centroid.

$$f^{'}(t)C_2^{-1}LC_2^{-1}f(t) \leq 0.7034569 \tag{38}$$

Table 1: Equivalence Theorem for Four Ingredients (WSCD).

	Average Prediction Variances			
BLENDS	$f^{'}(t)C_1^{-1}LC_1^{-1}f(t)$		$tr[C_1^{-1}L]$	**Optimality**
1, 0, 0, 0	2.41681	>	0.7034569	Not I Optimal
½, ½, 0, 0	0.07862874	<	0.7034569	I-Optimal
1/3, 1/3, 1/3, 0	0.01026738	<	0.7034569	I-Optimal
¼, ¼, ¼, ¼	0.002332298	<	0.7034569	I-Optimal

7. Equivalence Theorem for Uniform Weighted Simplex Centroid Kronecker

For four ingredients, the design is said to be I-optimal if and only if it satisfy,

$$f^{'}(t)C_{2u}^{-1}LC_{2u}^{-1}f(t) \leq 0.7749682 \tag{39}$$

at a given design points of the simplex centroid designs.

Table 2: Equivalence Theorem for Four Ingredients (WSCD)

	Average Prediction Variances			
BLENDS	$f^{'}(t)C_2^{-1}LC_2^{-1}f(t)$		$tr[C_2^{-1}L]$	**Optimality**
1, 0, 0, 0	2.755831	>	0.7749682	Not I Optimal
½, ½, 0, 0	0.09881055	<	0.7749682	I-Optimal
1/3, 1/3, 1/3, 0	0.01341913	<	0.7749682	I-Optimal
¼, ¼, ¼, ¼	0.002813837	<	0.7749682	I-Optimal

It was observed that the pure blends in both WSCD and UWSCD did not satisfy the general equivalence theorem for I-optimality (38) and (39) respectively. The binary, ternary and quaternary blends were found to satisfy the general equivalence theorem, therefore, I-optimal. However, centre point mixtures (¼, ¼, ¼, ¼) were better than all the binary and ternary mixtures due to their smaller average prediction variance, therefore, prediction of responses at this point was accurately achieved than any other point in the simplex centroid designs.

8. Conclusion

The average prediction variances for WSC designs were slightly lower than those of UWSC designs, therefore yielding more accurate results. All mixtures formulations except pure blend satisfied the general equivalence theorem for I-optimality at different points of the simplex centroid designs. On mixture formulations, the centroid point also yield accurate prediction than any other point in the simplex.

9. References

1. Atkinson AC, Donev AN, Tobias RD. Optimum Experimental Designs, with *SAS*, Oxford University Press. 2007.
2. Borkowski JJ. A Comparison of Prediction Variance Criteria for Response Surface Designs. Journal of Quality Technology. 2003; 35(1):70-77.
3. Draper NR, Pukelsheim F. Mixture models based on homogeneous polynomials. J. Statist. Plann. Inference. 1998; 71:303-311.
4. Goos P, Syafitri U. V-optimal mixture designs for the qth degree model. Chemometrics and Intelligent Laboratory Systems, 2014; 136:173-178.
5. Goos P, Jones B, Syafitri U. I-optimal Mixtures designs. Journal of the American Statistical Association. 2016; 111(154):899-911.
6. Laake P. On the optimal allocation of observation in experiments with mixtures, Scandinavian Journal of Statistics, 1975; 2:153-157.
7. Liu S, Neudecker H. A V-Optimal design for Scheffé's Polynomial model. Statistics and Probability letters. 1995; 23:253-258.