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I-optimal designs for three and four component mixture models in orthogonal blocks

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Abstract

In Industrial and Pharmaceutical experiments it is desired to have best predictions of the response on the basis of small amount of data. Mixture experiment generally aims to predict the response(s) for all possible mixture blends. When we compute optimal design for mixture response surface we must focus on prediction capability of the design. The conventional optimal criteria, such as D-, A- and E-optimality are not suitable for determining the prediction capability of designs. As I-optimal design minimizes the average variance of prediction over the mixture region, so it clearly focuses on prediction capability of the design. Hence I-optimal criterion seems to be more appropriate in this conjecture. In this paper we propose the construction of I-optimal mixture designs for a quadratic Scheffé's and Darroch and Waller's model in three and four components, using two orthogonal blocks. I-efficiency of designs is compared with the I-efficiency of D-optimal designs for Scheffé's and Darroch and Waller's models.

Key Words: Mixture Experiments, Latin Squares, Orthogonal Blocks, I-optimality, Average Prediction variance, D-optimality.

Mathematical Subject Classification: 62k05, 62k10

1. Introduction

In a mixture experiment with q components the proportion of ingredients may be denoted by $x_1, x_2, \dots, x_q$ where $x_i \geq 0$ for $i = 1, 2, \dots, q$ and $x_1 + x_2 + \cdots x_q = 1$. The response only depends upon the mixture and not on the total amount of mixture. The design space is a (q -1) - dimensional regular simplex S_{q-1}, where

$$S_{q-1} = \{ x : (x_1, x_2, \dots, x_q) \mid \sum_{i=1}^{q} x_i = 1, x_i \geq 0 \}$$

The response can be expressed from

$$y(x) = \eta(x) + \varepsilon(x)$$

where $y(x)$ is the observed response at x. $\eta(x)$ and $\varepsilon(x)$ are the expected response and error term at x respectively. Various forms of $\eta(x)$ can be found in literature. These may be the models given by Scheffé' (1958), Becker (1986) ,Darroch and Waller(1985) and Draper and Pukelsheim (1998).

In a practical situation we encounter some other sources of variations which are not part of the mixture but may affect the response. Such variables are called process variables, which may affect response in the experiment. These process variables are tackled by making orthogonal blocks of runs, which allow the mixture model parameters to be estimated independently from block effects. In terms of blocking variable ***z*** the mixture model becomes,

$$y(x,z)=\eta(x)+\phi(z)+\varepsilon(x,z)$$

In order to make blocks orthogonal to the estimates of the model, the conditions were derived by Nigam (1970) which were further modified by John (1984). D-optimal orthogonal designs in two blocks for Scheffé's quadratic model, in three and four components, were discussed by Czitrom (1988, 1989). Draper et al. (1993) discussed an industrial problem of bread making flour in which four component mixture blends were partitioned in two orthogonal blocks and D-optimal value was obtained when quadratic Scheffé's model was used. Chan and Sandhu (1999) discussed the properties of D-, A- and E-optimal orthogonal designs in two blocks for Scheffé mixture model with three components. Singh (2003) discussed D-, A- and E-optimal orthogonal designs in two blocks for Darroch and Waller's additive quadratic mixture model in three and four components.

D-optimality criterion prefers on precision of the estimated coefficients of the assumed model and neglects prediction capability which is a very important property of any design. I-optimality criterion minimizes the average prediction variance over a specified range of interest. Confidence interval for predictions is narrower for I-optimal designs than for conventional optimal designs. Very little published results are available for I-optimal mixture deigns using Scheffé's model. It can be found in Lambrakis (1986b), Laake (1975), Liu and Neudecker (1995) and Sinha, et al. (2014). Goos et al. (2016) studied discrete and continuous I-optimal designs for mixture experiments using quadratic and special cubic Scheffé's model and compared them with the D-optimal mixture designs, available in literature.

I-optimal designs for mixture experiments with orthogonal blocks have not been addressed so far in literature. In this paper we have constructed I-optimal design in two orthogonal block designs in two blocks for quadratic Scheffé and Darroch and Waller's model in three and four mixture components. The I-efficiency of such designs is compared with the I-efficiency of existing D-optimal designs for the relevant models.

The article is organized as follows. First a review on quadratic mixture models with the orthogonal blocking conditions is given. Next an I-optimality and D-optimality criteria are discussed in detail. Further construction of I-optimal orthogonal designs in two blocks for three and four mixture components, using Latin squares, is given for quadratic Scheffé's and Darroch and Waller's model. Finally D-efficiency and I-efficiency of the designs are compared and conclusions are drawn.

2. Mixture Models with orthogonal blocking conditions

2.1 Scheffé's quadratic mixture model

Scheffé (1958) introduced quadratic mixture model for q components.

$$\eta=\sum_{i=1}^{q}\beta_i x_i+\sum_{1\le i<j\le q}^{q}\beta_{ij}x_i x_j$$

Let n mixture blends are distributed in two blocks of same sizes. In terms of blocking variable z_u the Scheffé's quadratic mixture model is given by,

$$Y_u=\sum_{i=1}^{q}\beta_i x_{iu}+\sum_{1\le i<j\le q}^{q}\beta_{ij}x_{iu}x_{ju}+\gamma z_u+e_u \quad u=1,2,...,n \tag{1}$$

The blocking variable z_u = -1 for the blends in the first block and z_u = +1 for the blends in second block. e_u is the error term which is assumed to be normal with zero mean and common variance σ^2. In matrix form the model can be written as,

$$E(\mathbf{y})=\mathbf{X\beta}+\gamma\mathbf{Z} \tag{2}$$

where $\boldsymbol{X}$ is the extended design matrix related to the mixture part, $\boldsymbol{\beta}$ is the column vector of unknown parameters, γ is the block effect parameter, $\mathbf{y}$ is the $n\times1$ column vector of observations and $\mathbf{Z}$ is $n\times1$ column vector corresponding to blocking variable z_u. The two blocks of mixture blends will be orthogonal when the block effects do not affect the estimate of the coefficients in the mixture model. It will be true only when $\boldsymbol{X'Z} = 0$, that is the following conditions proposed by John (1984) are satisfied.

$$\sum_{u=1}^{n_w} x_{iu} = k_i, \ \sum_{u=1}^{n_w} x_{iu} x_{ju} = k_{ij} \quad \forall\, w = 1,2 \tag{3}$$

where k_i and k_{ij} are constants, $i < j, \quad i, j = 1, 2, \ldots, q$, w shows the block number and n_w be the number of blends in wth block such that $n_1 + n_2 = n$, the total number of blends in the mixture.

2.2 Darroch and Waller's (DW) quadratic mixture model

Darroch and Waller's (1985) suggested another form of additive model in which the response variable is expressible as a sum of separate functions of $x_1, x_2, \ldots, x_q$. The additive quadratic mixture model for the expected response η is given by

$$\eta = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \beta_{ii} x_i^2$$

For n mixture blends (not necessarily all distinct) distributed in two orthogonal blocks of same size, Eq. (4) in terms of the blocking variable z_u is

$$Y_u = \sum_{i=1}^{q} \beta_i x_{iu} + \sum_{i=1}^{q} \beta_{ii} x_{iu}{}^2 + \gamma z_u + e_u \qquad u = 1, 2, \ldots, n \tag{4}$$

which can be expressed in matrix notation as in Eq. (2). The orthogonal blocking conditions for Darroch and Waller's model are

$$\sum_{u=1}^{n_w} x_{iu} = k_i, \sum_{u=1}^{n_w} x_{iu}^2 = k_{ii} \quad \forall\, w = 1,2 \tag{5}$$

where k_i and k_{ii} are constants, $i < j, \quad i, j = 1, 2, \ldots, q$

3. I-optimality and D-optimality criteria

An I-optimal design minimizes the average prediction variance (APV) over the experimental region χ.

$$\text{APV} = \frac{\int_\chi f'(x)(X'X)^{-1} f(x)dx}{\int_\chi dx} \tag{6}$$

Here $M = \int_\chi f(x) f'(x) dx$ is the moment matrix, the matrix X is of order $n \times p$, with n the number of blends and p the number of terms in the model. The above formula can be written as

$$\text{APV} = \frac{trace[(X'X)^{-1} \int_\chi f(x) f'(x) dx]}{\int_\chi dx} \tag{7}$$

$$\text{APV} = \frac{trace[(X'X)^{-1} M]}{\int_\chi dx} \tag{8}$$

If P_1 is the APV of Design 1 and P_2 is the APV of Design 2 then the relative I-efficiency of Design 1 versus Design 2 is

$$\text{Relative I-efficiency of Design 1 versus Design 2} = P_2 / P_1 \tag{9}$$

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Kiefer and Wolfowitz (1959) introduced D-optimality criterion. This criterion proposes the decrease in uncertainty of the parameter estimates of the model. In D-optimality we minimize $|(X'X)^{-1}|$, or in other words we maximize the determinant of the information matrix of the design. If D_1 is the determinant of the information matrix of first design and D_2 is the determinant of the information matrix of second design, then the relative D-efficiency of the former design compared to latter is defined as

$$\text{Relative D-efficiency of Design 1 versus Design 2} = (D_1 / D_2)^{(1/P)} \tag{10}$$

where p be the number of parameters in the model.

4. Construction of I-optimal designs in two blocks for three-component mixtures using Latin Square based orthogonal blocking Scheme

For quadratic mixture models in three components we require seven distinct runs to estimate parameters. We use the designs with a single pair of Latin square.

4.1 Design formed by using a quadratic Scheffé's model

We use the design given in Table 1 which has a single Latin square and a common centroid in each block. The same design is proposed by John (1984), Czitrom (1988) for D-optimality, Chan and Sandhu (1999) for D-, A- and E-optimality, Prescott (1998) for nearly D-optimality in Scheffé's quadratic mixture model and Hasan and Khan (2011, 2012) for nearly A-, and E-optimality in k-model and Scheffé's quadratic model.

Table 1: *Latin Square orthogonal block design for q = 3*

Run	Block 1			Run	Block 2		
	x_1	**x_2**	**x_3**		**x_1**	**x_2**	**x_3**
1	*a*	*b*	*c*	5	*a*	*c*	*b*
2	*b*	*c*	*a*	6	*b*	*a*	*c*
3	*c*	*a*	*b*	7	*c*	*b*	*a*
4	1/3	1/3	1/3	8	1/3	1/3	1/3

For Scheffé's quadratic model, with equal number of observations in each block of the design given in Table.1, the orthogonality conditions in Eq. (3) are satisfied. So it is an orthogonal design in two blocks. It is unnecessary to consider the process variable **z** while optimizing the design. Only the matrix $X'X$ is considered where X is the design matrix corresponding to Scheffé's quadratic mixture model.

$$X = \begin{pmatrix} a & b & c & ab & ac & bc \\ b & c & a & bc & ab & ac \\ c & a & b & ac & bc & ab \\ 1/3 & 1/3 & 1/3 & 1/9 & 1/9 & 1/9 \\ a & c & b & ac & ab & bc \\ b & a & c & ab & bc & ac \\ c & b & a & bc & ac & ab \\ 1/3 & 1/3 & 1/3 & 1/9 & 1/9 & 1/9 \end{pmatrix}$$

For I-optimality we minimize APV given in Eq. (10). We have,

$$f'(x) = \begin{pmatrix} x_1 & x_2 & x_3 & x_1x_2 & x_1x_3 & x_2x_3 \end{pmatrix}$$

and $$M = \int_{x\in[0,1]^3} f(x)f'(x)dx$$

$$M = \int_0^1\int_0^1\int_0^1 \begin{pmatrix} x_1^2 & x_1x_2 & x_1x_3 & x_1^2x_2 & x_1^2x_3 & x_1x_2x_3 \\ x_1x_2 & x_2^2 & x_2x_3 & x_1x_2^2 & x_1x_2x_3 & x_2^2x_3 \\ x_1x_3 & x_2x_3 & x_3^2 & x_1x_2x_3 & x_1x_3^2 & x_2x_3^2 \\ x_1^2x_2 & x_1x_2^2 & x_1x_2x_3 & x_1^2x_2^2 & x_1^2x_2x_3 & x_1x_2^2x_3 \\ x_1^2x_3 & x_1x_2x_3 & x_1x_3^2 & x_1^2x_2x_3 & x_1^2x_3^2 & x_1x_3^2x_2 \\ x_1x_2x_3 & x_2^2x_3 & x_2x_3^2 & x_1x_2^2x_3 & x_1x_3^2x_2 & x_2^2x_3^2 \end{pmatrix} dx_1dx_2dx_3$$

$$M = \begin{pmatrix} 1/3 & 1/4 & 14 & 1/6 & 1/6 & 1/8 \\ 1/4 & 1/3 & 1/4 & 1/6 & 1/8 & 1/6 \\ 1/4 & 1/4 & 1/3 & 1/8 & 1/6 & 1/6 \\ 1/6 & 1/6 & 1/8 & 1/9 & 1/12 & 1/12 \\ 1/6 & 1/8 & 1/6 & 1/12 & 1/9 & 1/12 \\ 1/8 & 1/6 & 1/6 & 1/12 & 1/12 & 1/9 \end{pmatrix}$$

The I-optimal design in two blocks for Scheffé’s quadratic model is given in Table.2.

Table 2: I-*optimal orthogonal Block design for three components using Scheffé’s quadratic mixture model.*

Run	Block 1			Run	Block 2		
	x_1	x_2	x_3		x_1	x_2	x_3
1	0.142	0.858	0	5	0.142	0	0.858
2	0.858	0	0.142	6	0.858	0.142	0
3	0	0.142	0.858	7	0	0.858	0.142
4	1/3	1/3	1/3	8	1/3	1/3	1/3

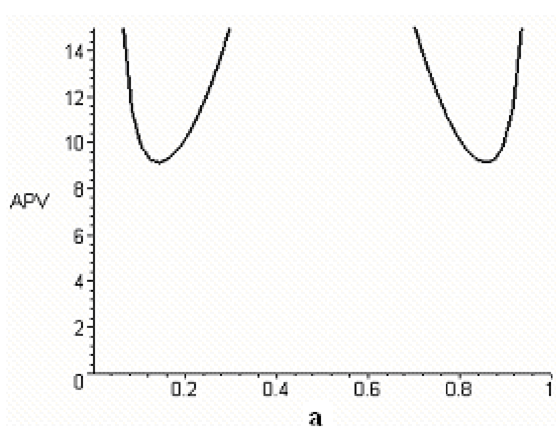

Figure 1: *Graph of APV using Scheffé’s quadratic model*

The above graph of APV is symmetrical about $a = 0.5$ and its minimum value (= 9.1244) is attained at $a = 0.142$,0.858.

4.2 Designs formed by using a quadratic DW model

For quadratic DW model the design in Table 1 with two blocks is orthogonal with respect to its orthogonal blocking conditions given in Eq. (5). The design matrix *X* corresponding to quadratic DW model is

$$X=\begin{pmatrix} a & b & c & a^2 & b^2 & c^2 \\ b & c & a & b^2 & c^2 & a^2 \\ c & a & b & c^2 & a^2 & b^2 \\ 1/3 & 1/3 & 1/3 & 1/9 & 1/9 & 1/9 \\ a & c & b & a^2 & c^2 & b^2 \\ b & a & c & b^2 & a^2 & c^2 \\ c & b & a & c^2 & b^2 & a^2 \\ 1/3 & 1/3 & 1/3 & 1/9 & 1/9 & 1/9 \end{pmatrix}$$

$$f'(x)=\begin{pmatrix} x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^2 \end{pmatrix}$$

$$M=\begin{pmatrix} 1/3 & 1/4 & 1/4 & 1/4 & 1/6 & 1/6 \\ 1/4 & 1/3 & 1/4 & 1/6 & 1/4 & 1/6 \\ 1/4 & 1/4 & 1/3 & 1/6 & 1/6 & 1/4 \\ 1/4 & 1/6 & 1/6 & 1/5 & 1/9 & 1/9 \\ 1/3 & 1/4 & 1/4 & 1/9 & 1/5 & 1/9 \\ 1/4 & 1/3 & 1/4 & 1/9 & 1/9 & 1/5 \end{pmatrix}$$

The I-optimal value is obtained by minimizing APV using Eq. (10). The minimum value of APV is 1.306 which is attained at a = 0.84, b = 0.16 and c = 0. The I-optimal orthogonal design in two blocks for a quadratic DW model in three components is given in Table 3.

Table 3: I-*optimal orthogonal Block design for three components using quadratic Darroch and Waller's model*

Run	Block 1			Run	Block 2		
	x_1	x_2	x_3		x_1	x_2	x_3
1	0.84	0.16	0	5	0.84	0	0.16
2	0.16	0	0.84	6	0.16	0.84	0
3	0	0.84	0.16	7	0	0.16	0.84
4	1/3	1/3	1/3	8	1/3	1/3	1/3

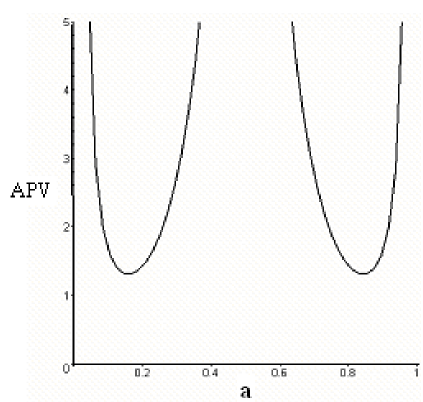

Figure 2: *Graph of APV using DW quadratic model*

The above graph of APV is symmetrical about $a = 0.5$ and its minimum value (= 1.306) is attained at $a = 0.16, 0.84$

4. Construction of I-optimal design in two orthogonal blocks for four-component mixtures

When a single process variable is present with two levels, the orthogonal block design in two blocks, for four components, can be used. Each of the two orthogonal blocks consists of eight binary blends and a full mixture blend having equal proportion for each component. Among sixteen binary blends in two orthogonal blocks four binary blends are common. The class of designs in Table 5 is reproduced from the design in Table 2 of Draper et al. (1993) for general *b* and *d*. Gosh and Liu (1999) applied the same design for the construction of A-optimal design in four components using Scheffé's quadratic mixture model. We consider this class of design to construct I-optimal design for quadratic Scheffé's and DW model in four components.

Table 4: *Four component orthogonally blocked mixture design*

Run	Block 1				**Run**	Block 2			
	x_1	x_2	x_3	x_4		x_1	x_2	x_3	x_4
1	0	*b*	0	*d*	10	0	*b*	0	*d*
2	0	*d*	0	*b*	11	0	*d*	0	*b*
3	*b*	0	*d*	0	12	*b*	0	*d*	0
4	*d*	0	*b*	0	13	*d*	0	*b*	0
5	0	*d*	*b*	0	14	0	*b*	*d*	0
6	*b*	0	0	*d*	15	*d*	0	0	*b*
7	0	0	*d*	*b*	16	0	0	*b*	*d*
8	*d*	*b*	0	0	17	*b*	*d*	0	0
9	1/4	1/4	1/4	1/4	18	1/4	1/4	1/4	1/4

5.1 Design formed by using quadratic Scheffé's model

For quadratic Scheffé's model the design in two blocks, given in Table 5, is orthogonal with respect to its orthogonal blocking conditions given in Eq. (3). The design matrix *X* corresponding to the quadratic Scheffé's model is,

$$X = \begin{pmatrix}
0 & b & 0 & d & 0 & 0 & 0 & 0 & bd & 0 \\
0 & d & 0 & b & 0 & 0 & 0 & 0 & bd & 0 \\
b & 0 & d & 0 & 0 & bd & 0 & 0 & 0 & 0 \\
d & 0 & b & 0 & 0 & bd & 0 & 0 & 0 & 0 \\
0 & d & b & 0 & 0 & 0 & 0 & bd & 0 & 0 \\
b & 0 & 0 & d & 0 & 0 & bd & 0 & 0 & 0 \\
0 & 0 & d & b & 0 & 0 & 0 & 0 & 0 & bd \\
d & b & 0 & 0 & bd & 0 & 0 & 0 & 0 & 0 \\
1/4 & 1/4 & 1/4 & 1/4 & 1/16 & 1/16 & 1/16 & 1/16 & 1/16 & 1/16 \\
0 & b & 0 & d & 0 & 0 & 0 & 0 & bd & 0 \\
0 & d & 0 & b & 0 & 0 & 0 & 0 & bd & 0 \\
b & 0 & d & 0 & 0 & bd & 0 & 0 & 0 & 0 \\
d & 0 & b & 0 & 0 & bd & 0 & 0 & 0 & 0 \\
0 & b & d & 0 & 0 & 0 & 0 & bd & 0 & 0 \\
d & 0 & 0 & b & 0 & 0 & bd & 0 & 0 & 0 \\
0 & 0 & b & d & 0 & 0 & 0 & 0 & 0 & bd \\
b & d & 0 & 0 & bd & 0 & 0 & 0 & 0 & 0 \\
1/4 & 1/4 & 1/4 & 1/4 & 1/16 & 1/16 & 1/16 & 1/16 & 1/16 & 1/16
\end{pmatrix}$$

$$f'(x) = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 & x_1x_2 & x_1x_3 & x_1x_4 & x_2x_3 & x_2x_4 & x_3x_4 \end{pmatrix}$$

$$M = \begin{pmatrix} 1/3 & 1/4 & 1/4 & 1/4 & 1/6 & 1/6 & 1/6 & 1/8 & 1/8 & 1/8 \\ 1/4 & 1/3 & 1/4 & 1/4 & 1/6 & 1/8 & 1/8 & 1/6 & 1/6 & 1/8 \\ 1/4 & 1/4 & 1/3 & 1/4 & 1/8 & 1/6 & 1/8 & 1/6 & 1/8 & 1/6 \\ 1/4 & 1/4 & 1/4 & 1/3 & 1/8 & 1/8 & 1/6 & 1/8 & 1/6 & 1/6 \\ 1/6 & 1/6 & 1/8 & 1/8 & 1/9 & 1/12 & 1/12 & 1/12 & 1/12 & 1/16 \\ 1/6 & 1/8 & 1/6 & 1/8 & 1/12 & 1/9 & 1/12 & 1/12 & 1/16 & 1/12 \\ 1/6 & 1/8 & 1/8 & 1/6 & 1/12 & 1/12 & 1/9 & 1/16 & 1/12 & 1/12 \\ 1/8 & 1/6 & 1/6 & 1/8 & 1/12 & 1/12 & 1/16 & 1/9 & 1/12 & 1/12 \\ 1/8 & 1/6 & 1/8 & 1/6 & 1/12 & 1/16 & 1/12 & 1/12 & 1/9 & 1/12 \\ 1/8 & 1/8 & 1/6 & 1/6 & 1/16 & 1/12 & 1/12 & 1/12 & 1/12 & 1/9 \end{pmatrix}$$

By minimizing APV, using Eq. (10), we get the I-optimal value 25.53 at $b = 0.143$, $d = 0.857$, $a = 0$, and $c = 0$. So I-optimal orthogonal design in two blocks for quadratic Scheffé model with four components is given in Table 5.

Table 5: *Four component I-optimal orthogonally blocked mixture design for quadratic Scheffé's model*

Run	Block 1				Run	Block 2			
	x_1	**x_2**	**x_3**	**x_4**		**x_1**	**x_2**	**x_3**	**x_4**
1	0	0.143	0	0.857	10	0	0.143	0	0.857
2	0	0.857	0	0.143	11	0	0.857	0	0.143
3	0.143	0	0.857	0	12	0.143	0	0.857	0
4	0.857	0	0.143	0	13	0.857	0	0.143	0
5	0	0.857	0.143	0	14	0	0.143	0.857	0
6	0.143	0	0	0.857	15	0.857	0	0	0.143
7	0	0	0.857	0.143	16	0	0	0.143	0.857
8	0.857	0.143	0	0	17	0.143	0.857	0	0
9	0.25	0.25	0.25	0.25	18	0.25	0.25	0.25	0.25

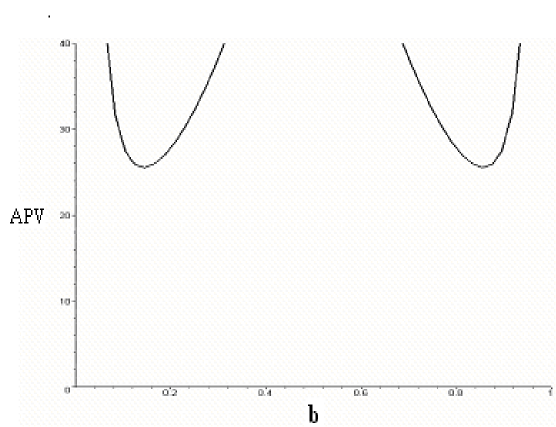

Figure 3: *Graph of APV using Scheffé's quadratic model in four components*

The above graph of APV is symmetrical about $b = 0.5$ and its minimum value (= 25.53) is attained at

$b = 0.143, 0.857$.

5.2 Design formed by using quadratic DW model

For quadratic DW model the design in Table 5 with two blocks is orthogonal with respect to its orthogonal blocking conditions given in Eq. (5). The design matrix X corresponding to the quadratic DW model with four components is,

$$X = \begin{pmatrix} 0 & b & 0 & d & 0 & b^2 & 0 & d^2 \\ 0 & d & 0 & b & 0 & d^2 & 0 & b^2 \\ b & 0 & d & 0 & b^2 & 0 & d^2 & 0 \\ d & 0 & b & 0 & d^2 & 0 & b^2 & 0 \\ 0 & d & b & 0 & 0 & d^2 & b^2 & 0 \\ b & 0 & 0 & d & b^2 & 0 & 0 & d^2 \\ 0 & 0 & d & b & 0 & 0 & d^2 & b^2 \\ d & b & 0 & 0 & d^2 & b^2 & 0 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 & 1/16 & 1/16 & 1/16 & 1/16 \\ 0 & b & 0 & d & 0 & b^2 & 0 & d^2 \\ 0 & d & 0 & b & 0 & d^2 & 0 & b^2 \\ b & 0 & d & 0 & b^2 & 0 & d^2 & 0 \\ d & 0 & b & 0 & d^2 & 0 & b^2 & 0 \\ 0 & b & d & 0 & 0 & b^2 & d^2 & 0 \\ d & 0 & 0 & b & d^2 & 0 & 0 & b^2 \\ 0 & 0 & b & d & 0 & 0 & b^2 & d^2 \\ b & d & 0 & 0 & b^2 & d^2 & 0 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 & 1/16 & 1/16 & 1/16 & 1/16 \end{pmatrix}$$

$$f'(x) = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 & x_1^2 & x_2^2 & x_3^2 & x_4^2 \end{pmatrix}$$

$$M = \begin{pmatrix} 1/5 & 1/9 & 1/9 & 1/9 & 1/4 & 1/6 & 1/6 & 1/6 \\ 1/9 & 1/5 & 1/9 & 1/9 & 1/6 & 1/4 & 1/6 & 1/6 \\ 1/9 & 1/9 & 1/5 & 1/9 & 1/6 & 1/6 & 1/4 & 1/6 \\ 1/9 & 1/9 & 1/9 & 1/5 & 1/6 & 1/6 & 1/6 & 1/4 \\ 1/4 & 1/6 & 1/6 & 1/6 & 1/3 & 1/4 & 1/4 & 1/4 \\ 1/6 & 1/4 & 1/6 & 1/6 & 1/4 & 1/3 & 1/4 & 1/4 \\ 1/6 & 1/6 & 1/4 & 1/6 & 1/4 & 1/4 & 1/3 & 1/4 \\ 1/6 & 1/6 & 1/6 & 1/4 & 1/4 & 1/4 & 1/4 & 1/3 \end{pmatrix}$$

By minimizing APV, using Eq. (10), we get I-optimal value 0.9758 at $b = 0.164$, $d = 0.836$, $a = 0$, and $c = 0$. So, I-optimal orthogonal design in two blocks for three components is given in Table 6.

Table 6: *Four component I-optimal orthogonally blocked mixture design for quadratic DW model*

Run	**Block1**				**Run**	**Block2**			
	x_1	x_2	x_3	x_4		x_1	x_2	x_3	x_4
1	0	0.16	0	0.84	10	0	0.16	0	0.84
2	0	0.84	0	0.16	11	0	0.84	0	0.16
3	0.16	0	0.84	0	12	0.16	0	0.84	0
4	0.84	0	0.16	0	13	0.84	0	0.16	0
5	0	0.84	0.16	0	14	0	0.16	0.84	0
6	0.16	0	0	0.84	15	0.84	0	0	0.16
7	0	0	0.84	0.16	16	0	0	0.16	0.84
8	0.84	0.16	0	0	17	0.16	0.84	0	0
9	1/4	1/4	1/4	1/4	18	1/4	1/4	1/4	1/4

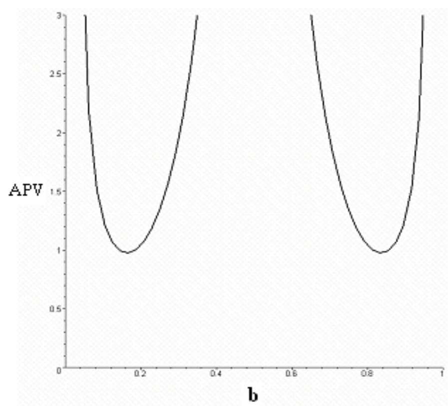

Figure 4: *Graph of APV using DW quadratic model in four components*

The above graph of APV is symmetrical about $b = 0.5$ and its minimum value (= 0.9758) is attained at

b = 0.164 ,0.836.

Discussion

In this article we have constructed I-optimal orthogonal designs in two blocks for three and four mixture components based upon Latin squares orthogonal blocking scheme for quadratic Scheffé and DW model. Czitrom (1988) and Draper et al. (1993) obtained D-optimal orthogonal designs in two blocks for Scheffé's quadratic model with three and four components, using the design given in Table 1 and in Table 5 respectively. The D-optimality for three component mixtures was obtained at $a = 0.168$, $b = 0.832$ and $c = 0$. The relative D-efficiency of the I-optimal design versus D-optimal design equals 98.83%, whereas the relative I-efficiency of the D-optimal design versus I-optimal design equals 97.53%. This shows that I-optimal design performs little better than D-optimal design in terms of D-optimality criterion whereas D-optimal design performs little worse than I-optimal design in terms of I-optimality criterion. Further for four components the D-optimality of the design given in Table 5 was obtained at $a = c = 0$, $b = 0.24$ and $d = 0.76$. The relative D-efficiency of the I-optimal design versus D-optimal design equals 86.06%, whereas the relative I-efficiency of the D-optimal design versus I-optimal design equals 81.87%. This shows that I-optimal design performs better than D-optimal design in terms of D-optimality criterion whereas D-optimal design performs worse than I-optimal design in terms of I-optimality criterion.

Singh (2003) obtained D-optimal designs in two orthogonal blocks for DW quadratic model with three and four components, using the design given in Table 1 and Table 5 respectively. For the design in Table 1 the D-optimality was obtained at a = 0.168, b = 0.832 and c = 0 and for the design in Table 5 the D-optimality was obtained at $a = c$ = 0, b = 0.187 and d = 0.813. For the design in Table 1 the relative D-efficiency of I-optimal design versus D-optimal design equals 99.87%, whereas the relative I-efficiency of D-optimal design versus I-optimal design equals 99.39%. This shows that I-optimal design performs little better than D-optimal design in terms of D-optimality criterion whereas D-optimal design performs little worse than I-optimal design in terms of I-optimality criterion. For the design in Table 5 relative D-efficiency of I-optimal design versus D-optimal design is 99.12% whereas relative I-efficiency of D-optimal design versus I-optimal design is 97.26%. It can be said that I-optimal design outperforms D-optimal design relative to D-optimality criterion whereas D-optimal design performs little worst then I-optimal design relative to I-optimal criterion.

The objective of our research is to minimize the average prediction variance through the design region for a quadratic Scheffé and DW model. Our computational results show that I-optimal orthogonal designs in two blocks for three and four mixture components, using quadratic Scheffé and DW model, are more efficient than D-optimal designs.

Practical Illustration

Draper et al.(1993) provided an example of Spillers Milling, a major producer of bread-making flour in United Kingdom. Four flours each of four varieties of wheat were taken and mixed in to dough with different proportions. The breads were baked from dough with the responses y as their volume (ml/100g). The proportions of four flours in a mixture was x_1, x_2, x_3 and x_4 with $\sum_{i=1}^{4} x_i = 1$. The experiment was run in two orthogonal blocks with nine runs each, given in Table 5. Scheffé's quadratic mixture model was used and the maximum D-criterion value 1.24×10^{-6} was obtained at (a, b, c, d) = (0, 0.24, 0, 0.76). For this D-optimal design, the minimum APV value is 31.18. When we use I-optimal design in two orthogonal blocks, given in Table 6, by the I-optimal criterion, the minimum APV value 25.53 was obtained at (a, b, c, d) = (0, 0.14, 0, 0.86). Hence I-optimal design outperforms D-optimal design with reference to its prediction capability.

Conclusion

In this paper we have constructed I-optimal designs in two orthogonal blocks for quadratic Scheffé and DW model using three and four components. The comparison of I-efficiency and D-efficiency of designs reveals that I-optimal designs in two orthogonal blocks for quadratic Scheffé and DW outperform D-optimal designs available in literature.

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