



# Nearly A- and E-Optimal Orthogonally Blocked Designs for Scheffe's Quadratic Mixture Model with Three Components

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**Abstract:** Prescott et al. (Technometrics 78: 268-276, 1993) proposed D-optimal orthogonally blocked designs in two blocks for Scheffé's quadratic mixture model with four components. Chan and Sandhu (J.Appl.Statist.26 (1):19-34, 1999) discussed the properties of D-, A- and E-optimal designs for Scheffe's quadratic mixture model in three components. Prescott (Comm.Stat.Theory Methods, 27(10):2259-2580, 1998) introduced nearly D-optimal orthogonally blocked designs for Scheffé's quadratic mixture model in three and four components. In this paper, we propose nearly A- and E-optimal orthogonally blocked designs in two blocks for Scheffé's quadratic mixture model, in three components. The robustness of nearly optimal orthogonally blocked designs, with respect to D-, A- and E-optimality criteria, is checked.

**Keywords:** Latin squares, orthogonal blocks, process variables, Scheffé mixture model.

## 1. INTRODUCTION

In mixture experiments 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  $x_1 + x_2 + \dots + x_q = 1$ . The response depends only on the mixture and not on the total amount of mixture. The factor space is a  $(q-1)$  - dimensional regular simplex  $S_{q-1}$ ,

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

Scheffé [1-2] introduced the model for mixture experiments. Scheffé's quadratic mixture model for experiments with mixtures is given by:

$$E(Y) = \sum_{i=1}^q \beta_i x_i + \sum_{1 \leq i < j \leq q} \beta_{ij} x_i x_j$$

During practical situation we face some other sources of variations which are not part of the mixture but may affect the response. Such sources are tackled by making the orthogonal blocks of runs, which allow the mixture model parameters to be estimated independently from block effects. Orthogonal blocking conditions were derived by Nigam [3] and were further modified by John [4]. In terms of blocking variable  $z_u$  the Scheffé's quadratic mixture model is given by,

$$Y_u = \sum_{i=1}^q \beta_i x_{iu} + \sum_{1 \leq i < j \leq q} \beta_{ij} x_{iu} x_{ju} + \gamma z_u + e_u$$

$$u = 1, 2, \dots, n$$

where  $z_u = -1$  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  $\sigma^2$ . In matrix form the model can be written as,

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} + \gamma\mathbf{z} \tag{1.1}$$

where  $\mathbf{X}$  is the  $n \times q(q+1)/2$  matrix related to the mixture part,  $\boldsymbol{\beta}$  is the  $q(q+1)/2 \times 1$  column vector of unknown parameters,  $\gamma$  is the block effect parameter,  $\mathbf{y}$  is the  $n \times 1$  column vector of observations and  $\mathbf{z}$  is the  $n \times 1$  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  $\mathbf{X}'\mathbf{z} = 0$ , that is the following conditions proposed by John [4] are satisfied.

$$\sum_{u=1}^{n_w} x_{iu} = k_i, \quad \sum_{u=1}^{n_w} x_{iu} x_{ju} = k_{ij} \quad \forall w = 1, 2 \tag{1.2}$$

where  $k_i$  and  $k_{ij}$  are constants,  $i < j$ ,  $i, j = 1, 2, \dots, q$ ,  $w$  shows the block number and  $n_w$  be the number of blends in  $w$ th block

such that  $n_1 + n_2 = n$ , the total number of blends in the mixture.

Prescott et al. [5] proposed D-optimal designs for four components in orthogonal blocks. Chan and Sandhu [6] discussed the properties of D-, A- and E-optimal orthogonal designs in two blocks for Scheffe’s quadratic mixture model with three components. Their A- and E-optimal designs had six binary blends of the form  $(a, 1-a, 0)$  with the optimal value  $a = 0.8167$  and  $a = 0.8454$  respectively, and two centroids, one in each block as repeated blends. For practical investigation we modify the designs, discussed by Chan and Sandhu [6], so that some or all blends that we include contain a minimum proportion of each component and orthogonality holds in blocks.

## 2. RE-PARAMETERIZATION OF THE CO-ORDINATE SYSTEM

The co-ordinates of the points in the  $(q-1)$ -dimensional simplex region are generally denoted by the symbols  $a, b, c, \dots$  such that  $a + b + c + \dots = 1$ . The Latin square based orthogonal block designs provide the algebraic expression for the information matrix  $X'X$  in terms of the symbols  $a, b, c, \dots$ . By using any optimal criteria, we can determine the optimal values of  $a, b, c, \dots$ . Prescott [7] discussed re-parameterization of the co-ordinates for the simplification of problem and investigated the properties of alternative designs formed by shrinking the optimal designs in three and four components, towards the centroid.

Consider a two-dimensional simplex formed by three components, given in Fig.1. Take any design point  $P(a, b, c)$  in the simplex such that  $a \geq b \geq c$ ,  $O(1/3, 1/3, 1/3)$  is the centroid of the simplex,  $Q(f, 1-f, 0)$  is a point on the extension of the line  $OP$  to the edge of the simplex, shown in Fig.1. This figure is reproduced from Prescott [7].

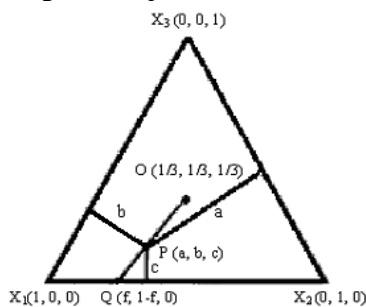


Fig. 1. Re-parameterization of the co-ordinates  $(a, b, c)$ , with  $a \geq b \geq c$ , to  $(f, s)$ .

If  $P$  is located at the proportion  $s = QP/QO$ , along the line  $QO$  then,

$$\begin{aligned} a &= (1-s)f + s/3 \\ b &= (1-s)(1-f) + s/3 \\ c &= s/3 \end{aligned}$$

So the point  $P$  is now in terms of  $f$  and  $s$ , where  $f$  identifies the point  $Q$  on the edge of the simplex and  $s$  is a shrinkage parameter that moves  $Q$  towards the centroid  $O$ . Therefore, by re-parameterization we examine the properties of optimal designs by shrinking it towards the centroid of the simplex.

## 3. NEARLY OPTIMAL ORTHOGONALLY BLOCKED DESIGNS FOR $q = 3$

Consider Scheffé’s quadratic mixture model in three components. We require seven distinct runs to estimate parameters in equation (1.1). We use the designs with a single pair and two pairs of Latin squares.

### 3.1. Designs Formed by using a Single Pair of Latin Square

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 [4] for Scheffé’s quadratic mixture model in three components, Czitrom [8] for D-optimality, Chan and Sandhu [6] for D-, A- and E-optimality in Scheffé’s quadratic mixture model in three components, and Prescott [7] for near optimality in Scheffé’s quadratic mixture model in three and four components.

Table 1. Latin Square orthogonal block design for  $q = 3$ .

Block I				Block II			
Run	$x_1$	$x_2$	$x_3$	Run	$x_1$	$x_2$	$x_3$
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	$1/3$	$1/3$	$1/3$

With equal number of observations in each block of the design in Table.1, the orthogonality conditions given in (1.2) are satisfied, so this is an orthogonal block design in two blocks. Therefore it is unnecessary to consider the process variable  $\mathbf{z}$  while optimizing the design. Only the matrix  $X'X$  is considered where  $X$  is

the extended design matrix for Scheffé's quadratic mixture model.

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

**Table 2.** Properties of nearly A-optimal designs with shrinkage parameter  $s$  applied to design in Table 1.

$s$	Opt $f$	Min(T)	$T_0$	Efficiency
0	0.817	146.975	146.975	100
0.05	0.817	180.818	146.975	81.28
0.1	0.817	224.995	146.975	65.32
0.2	0.817	362.305	146.975	41.00

For A-optimal design, we minimize T, where  $T = \text{trace}(X'X)^{-1}$ , and for E-optimal design we maximize the minimum of the eigenvalues of  $X'X$ . The trace of a matrix is the sum of its eigenvalues. The matrix  $X'X$  of the design in Table.1, for Scheffé's quadratic mixture model has six eigenvalues, as given by Chan and Sandhu [6]. All the eigenvalues are functions of components  $a$ ,  $b$ ,  $c$  and two eigenvalues  $\lambda_1, \lambda_2$  are of multiplicity 2. Thus  $T = 2\lambda_1^{-1} + 2\lambda_2^{-1} + \lambda_3^{-1} + \lambda_4^{-1}$ . The minimum value of T (146.97), for Scheffé's quadratic model, is attained on the boundary of the simplex with  $a = 0.8167$ ,  $b = 0.1833$ ,  $c = 0$ , as given by Chan and Sandhu [6]. The general design in Table.1 may be considered as shrinkage of the design with  $a = f$ ,  $b = 1-f$ ,  $c = 0$  by a factor  $s$ . So, for any fixed value  $s$ , T is minimized and is observed that T is a strictly increasing function of  $s$  as  $s \rightarrow 1$ . Chan and Guan [9] gave a formula of finding the efficiency of A-optimal designs.

$$\text{A-efficiency} = T_0 / \text{Min}(T) \times 100$$

where  $T_0$  is the minimum T obtained by substituting optimal value of  $f$  in original T obtained from the design in Table 1.

**Table 3.** Properties of nearly E-optimal designs with shrinkage parameter  $s$  applied to design in Table 1.

$s$	Opt $f$	Absolute maximum	Absolute maximum (original model)	Efficiency
0	0.845	0.019	0.019	100
0.05	0.845	0.016	0.019	81.24
0.1	0.845	0.013	0.019	65.26
0.2	0.845	0.008	0.019	41.00

We see that, by shrinking A-optimal design towards the centroid, it becomes more efficient. For instance when  $s = 0.05$ , the optimal  $f$  is 0.816 and the design has some loss in efficiency. But we get a least proportion of all available ingredients to form a mixture.

The six eigenvalues for the matrix  $X'X$  are in the order  $\lambda_1 > \lambda_3 > \lambda_4 > \lambda_2$ , with  $a \in [0, 1]$ , as given by Chan and Sandhu [6]. The maximum of the minimum eigenvalue, that is of  $\lambda_2$  was 0.01988 at  $a = 0.8454$ ,  $b = 0.1546$ ,  $c = 0$ . Again by re-parameterization of the co-ordinates ( $a$ ,  $b$ ,  $c$ ) in terms of ( $f$ ,  $s$ ), we get the general form of the minimum eigenvalue,  $\lambda_2$  in this case. For the specific values of  $s$ , we get the maximum of  $\lambda_2$ . The efficiency of E-optimal designs with the different values of  $s$  are obtained by,

$$\text{E-efficiency} = \frac{\text{Abs}\{\text{Max}(\text{MinEigenvalue})\}}{\text{Abs}\{\text{Max}(\text{MinEigenvalue})\}_0} \times 100$$

### 3.2. Designs using Two Pairs of Squares for $q = 3$

Prescott [7] used one extra Latin Square in each block for  $q = 3$ , to get more flexibility in the construction of nearly D-optimal designs. We use it to find nearly A- and E-optimal designs. The design with two Latin squares in each block, as given in Prescott [7], is given in Table.4.

**Table 4.** Latin Square orthogonal block design with two squares in each block for  $q = 3$ .

Run	Block I			Run	Block II		
	$x_1$	$x_2$	$x_3$		$x_1$	$x_2$	$x_3$
1	$a$	$b$	$c$	8	$a$	$c$	$b$
2	$b$	$c$	$a$	9	$b$	$a$	$c$
3	$c$	$a$	$b$	10	$c$	$b$	$a$
4	$a'$	$c'$	$b'$	11	$a'$	$b'$	$c'$
5	$b'$	$a'$	$c'$	12	$b'$	$c'$	$a'$
6	$c'$	$b'$	$a'$	13	$c'$	$a'$	$b'$
7	1/3	1/3	1/3	14	1/3	1/3	1/3

### 3.2.1. Design formed by shrinking both pairs of Latin Square

Consider the case when both pairs of Latin squares in Table.4 have same values i.e.  $a' = a$ ,  $b' = b$ ,  $c' = c$  and as a result we obtain a symmetric design. We shrink both pairs of Latin squares towards the centroid of the design. By re-parameterization of the coordinates, as it is done in section 3.1, nearly A-optimal designs are constructed. For  $s = 0$ , A-optimal design provides the minimum value of T (94.61) for Scheffe's quadratic mixture model on the boundary of the simplex at  $a = f = 0.836$ ,  $b = 1-f = 0.164$ ,  $c = 0$ . The efficiencies of other nearly A-optimal designs are given in Table.5.

**Table 5.** Properties of nearly A-optimal designs with shrinkage parameter  $s$  applied to design 3.2.1.

$s$	Opt $f$	Min(T)	$T_0$	Efficiency
0	0.836	94.611	94.611	100
0.05	0.836	116.474	94.611	81.23
0.1	0.836	145.034	94.611	65.23
0.2	0.836	233.905	94.611	41.00

E-optimal design, by shrinking both Latin Squares towards centroid provides the maximum of minimum eigenvalue value  $\lambda_0 = \lambda_2 = 0.028738$  at  $a = f = 0.878$ ,  $b = 1-f = 0.122$ ,  $c = 0$ . Again by re-parameterization, we get the general form of the minimum eigenvalue i.e. of  $\lambda_2$  in this case. Table.6 provides the maximum of the minimum eigenvalue for some specific values of  $s$  and the respective efficiencies of nearly E-optimal designs.

**Table 6.** Properties of nearly E-optimal designs with shrinkage parameter  $s$  applied to design 3.2.1.

$s$	Opt $f$	Absolute maximum	Absolute maximum (original model)	Efficiency
0	0.878	0.029	0.029	100
0.05	0.878	0.023	0.029	81.27
0.1	0.878	0.019	0.029	65.31
0.2	0.878	0.012	0.029	41.00

### 3.2.2. Design formed by shrinking one pair of Latin Squares

Prescott [7] also proposed the construction of nearly D-optimal designs by shrinking only one Latin square in each block of the design listed in Table.4. We use it to construct nearly A- and E-optimal designs. When only one Latin Square is shrunk towards the centroid of the design, other Latin square is left on the edges of simplex. For instance take blends 1, 2, 3, 8, 9, 10 as binary blends and shrink blends 4, 5, 6, 11, 12, 13 towards the centroid of the design in Table.4. Thus a nearly optimal design here provides some binary blends and some three ingredient blends. The properties of proposed nearly A-optimal designs are given in Table 7.

**Table 7.** Properties of nearly A-optimal designs with shrinkage parameter  $s$  applied to design 3.2.2.

$s$	Opt $f$	Min(T)	$T_0$	Efficiency
0	0.836	94.611	94.611	100
0.05	0.836	103.534	94.611	91.38
0.1	0.835	110.685	94.616	85.48
0.2	0.831	118.532	94.711	79.90

Next for the design 3.2.2 we compute a nearly E-optimal design. The Table.8 below gives the properties of nearly E-optimal designs.

**Table 8.** Properties of nearly E-optimal designs with shrinkage parameter  $s$  applied to design 3.2.2.

$s$	Opt $f$	Absolute maximum	Absolute maximum (original model)	Efficiency
0	0.878	0.029	0.029	100
0.05	0.878	0.026	0.029	91.00
0.1	0.876	0.025	0.029	83.94
0.2	0.868	0.024	0.032	74.00

## 4. ROBUSTNESS WITH RESPECT TO D-, A- AND E-OPTIMALITY CRITERIA

Chan and Sandhu [6] concluded that the design proposed by John [4], given in Table.1, is robust with respect to D-, A- and E-optimality criteria, in the sense that  $\Phi_p$  values do not change much when the component  $a$  varies from 0.15 and

0.19. The efficiency of the design is measured in terms of  $\Phi_p$ -optimality criteria, which changes as  $p$  changes.

$$\Phi_p(X'X) = \left( \sum_{k=1}^r \lambda_k^{-p} / r \right)^{1/p}$$

Here  $r$  shows the number of eigenvalues of the matrix  $X'X$  and  $p > 0$ .  $p \rightarrow 0+$ ,  $p = 1$  and  $p \rightarrow \infty$  corresponds to the D-, A- and E-optimality criteria. Here we extend the same work for checking the robustness with respect to nearly D-, A- and E-optimal designs.

For this, first we use the nearly optimal orthogonally blocked design 3.1, with  $s = 0.05$ . It is nearly D-optimal for  $p \rightarrow 0+$ , with the optimal  $f = 0.832$  as given by Prescott [7]. Table.9 shows that for D-optimality, efficiency of the design i.e.  $\Phi_p$  differs from the minimum value by about 5% or less when  $f \in [0.81, 0.85]$ . For A-optimality, with  $p = 1$ , values of  $\Phi_p$  differ from minimum by about 6% or less when  $f \in [0.81, 0.85]$ . The difference increases as  $p$  increases. For E-optimality, with  $p \rightarrow \infty$ , values of  $\Phi_p$  differ from the minimum by about 29% or less when  $f \in [0.81, 0.85]$ . This shows that the nearly optimal design with  $s = 0.05$  is

robust with respect to D- A-, and E-optimality criteria because  $\Phi_p$  does not change as much when  $f \in [0.81, 0.85]$ . Note from Table.9 that as  $p$  increases robustness decreases and still the robustness is in the acceptable range, when  $p \rightarrow \infty$  and  $f \in [0.81, 0.85]$ . This decrease in robustness, as the optimality criterion changes, is due to the fact that D- and A-optimality criterion involve all eigenvalues whereas E-optimality criteria consider only one eigenvalue.

For nearly optimal orthogonally blocked designs 3.2.1, with  $s = 0.05$ , values of  $\Phi_p$  for D-optimality differ from the minimum value by about 30% or less when  $f \in [0.83, 0.88]$ . For A-optimality with  $p = 1$ , values of  $\Phi_p$  differ from the minimum value by 13% or less when  $f \in [0.83, 0.88]$ . For E-optimality, values of  $\Phi_p$  differ from the minimum value by 40% or less when  $f \in [0.83, 0.88]$ . The same results hold for nearly optimal orthogonally blocked designs 3.2.2, with  $s = 0.05$ . Hence the robustness, with respect to D-, A- and E-optimality criteria, does not hold for the nearly optimal orthogonally blocked designs with two pairs of Latin squares in each block. This robustness is also checked for further values of  $s$  and the same results hold in each case.

**Table 9.** Values of  $\Phi_p$  for different  $p$  and  $f$  with  $s = 0.05$ .

$p$	$f$							
	0.800	0.810	$(f_A =)$ 0.817	0.824	$(f_D =)$ 0.832	$(f_E =)$ 0.845	0.850	0.860
$\rightarrow 0+$	74197.95	70943.65	69405.66	68460.14	68111.28	69431.75	70433.09	73946.54
1	30.47	30.19	30.14	30.21	30.44	31.37	31.81	33.15
2	44.39	43.33	42.88	42.64	42.73	43.85	44.51	46.64
3	51.92	49.99	49.06	48.39	48.19	49.22	44.98	52.61
4	57.08	54.36	52.96	51.82	51.31	52.15	52.98	55.99
5	60.99	57.63	55.80	54.23	53.39	53.99	54.87	58.20
6	64.07	60.21	58.04	56.07	54.91	55.25	56.18	59.79
7	66.54	62.32	59.87	57.56	56.10	56.17	57.14	60.99
8	68.54	64.06	61.40	58.81	57.07	56.87	57.88	61.94
9	70.19	65.51	62.69	59.87	57.89	57.42	58.46	62.72
10	71.56	66.74	63.80	60.80	58.61	57.86	58.94	63.37
20	78.22	72.88	69.52	65.87	62.72	59.90	61.24	66.63
$\rightarrow \infty$	85.56	79.71	76.03	72.03	68.48	61.91	69.30	70.37

### 5. DISCUSSION

In the proposed nearly optimal designs some or all blends have at least a minimum proportion of each ingredient available, with preserving orthogonality in blocks. Further it is observed that by shrinking only one of the Latin squares in each block towards the centroid, as in design 3.2.2, the design points spread more and the design has higher efficiency as compared to design 3.2.1. It is also more efficient than the design 3.1 with single Latin square in each block. For instance when  $s = 0.05$ , nearly A- and E-optimal designs constructed from the design 3.2.1 are not as efficient as those for design 3.2.2. Their A- and E-efficiencies are 81.23%, 81.27% respectively for the design 3.2.1, and 91.38%, 91.0% respectively for the design 3.2.2.

Therefore, nearly A- and E-optimal designs obtain through the design 3.2.2 are preferable to obtain through the design 3.2.1, for Scheffe’s quadratic mixture model. The same result holds for nearly D-optimal designs, as given by Prescott [7]. Further it is concluded that nearly D-, A- and E-optimal designs with single Latin square in each block are robust and this robustness does not hold when an extra Latin square is added in each block.

Here below we provide the layouts of nearly A- and E-optimal designs obtain through the design 3.2.2.

**Table 10.** Nearly A-optimal Orthogonal Block design with  $f = 0.836$  and  $s = 0.05$ .

Block I				Block II			
Run	$x_1$	$x_2$	$x_3$	Run	$x_1$	$x_2$	$x_3$
1	0.836	0.164	0	8	0.836	0	0.164
2	0.164	0	0.836	9	0.164	0.836	0
3	0	0.836	0.164	10	0	0.164	0.836
4	0.811	0.017	0.172	11	0.811	0.172	0.017
5	0.172	0.811	0.017	12	0.172	0.017	0.811
6	0.017	0.172	0.811	13	0.017	0.811	0.172
7	1/3	1/3	1/3	14	1/3	1/3	1/3

**Table 11.** Nearly E-optimal Orthogonal Block design with  $f = 0.878$  and  $s = 0.05$ .

Block I				Block II			
Run	$x_1$	$x_2$	$x_3$	Run	$x_1$	$x_2$	$x_3$
1	0.878	0.122	0	8	0.878	0	0.122
2	0.122	0	0.878	9	0.122	0.878	0
3	0	0.878	0.122	10	0	0.122	0.878
4	0.851	0.017	0.132	11	0.851	0.132	0.017
5	0.132	0.851	0.017	12	0.132	0.017	0.851
6	0.017	0.132	0.851	13	0.017	0.851	0.132
7	1/3	1/3	1/3	14	1/3	1/3	1/3

The same idea can be extended for the designs based on  $q \geq 4$  components and for the designs consisting of three or more Latin Squares in each block. Results for the general case of  $q$  components is difficult to solve but will be very useful.

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