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Understanding the Features of Non-Orthogonality in Quadratic Response Surface Designs

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SUMMARY

Orthogonality is an important concept in design of experiment. Though orthogonal designs exist for multivariate first-degree regression model, such designs do not exist for second- and higher-degree models. In this paper, an attempt has been made to first introduce some measures or indices to non-orthogonality, and then to identify designs with minimum non-orthogonality indices. It is observed that such designs are neither D-optimal nor rotatable. Some examples are given for second degree model with two and three factors.

***Keywords and phrases*:** Response surface design; Orthogonal design; Non-orthogonality measures; D-optimal design; Rotatable design.

Preamble

During the course of revision of the original manuscript, it was rightly pointed out by one of the Editorial Board Members that Late (Professor) M.N. Das, along with two of his research collaborators, had touched upon some aspects of Response Surface Designs [RSDs]. However, while in our work we deal with non-orthogonality of a Quadratic RSD and study the extent of its departure from [hypothetical] orthogonal Quadratic RSD, Das *et al.* (1999) studied departures from rotatability of QRSDs, and yet satisfying an alternative moment condition. Further, they studied both symmetrical and asymmetrical QRSDs. The alternative moment condition was aimed at providing smaller variance of the estimated response at suitably designated points in the response surface. They also suggested some simple methods of construction of such QRSDs.

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1. INTRODUCTION

Consider a k- variate linear regression model:

$$y_i = \boldsymbol{f}'(\boldsymbol{x_i})\boldsymbol{\theta} + e_i, i = 1, 2, \ldots, N, \qquad (1.1)$$

where y_i is the response under study at the point $\boldsymbol{x} = \boldsymbol{x_i}$, $\boldsymbol{x} = (x_1, x_2, \ldots, x_k)$ is a vector of k independent variables, $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)'$ is a vector of unknown parameters, $\boldsymbol{f}(\boldsymbol{x}) = (f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_p(\boldsymbol{x}))'$ is the vector of known functions, and e_i-s are uncorrelated random errors with mean zero and common variance σ^2. Let $\boldsymbol{\chi}$ be the domain of the k independent variables. Generally, two types of domains are considered:

(i) Unit k-ball: $\boldsymbol{\chi} = \{x = (x_1, x_2, \ldots, x_k) \,|\, |\boldsymbol{x}| \le 1, -1 \le x_i \le 1, i = 1, 2, \ldots, k\}$.

(ii) Unit k-cube: $\boldsymbol{\chi} = \{x = (x_1, x_2, \ldots, x_k) \,|\, -1 \le x_i \le 1, i = 1, 2, \ldots, k\}$. (1.2)

For the N observations $y_1, y_2, \ldots, y_N$ corresponding to N points $\boldsymbol{x_i} \in \boldsymbol{\chi}, i=1,2, \ldots, N$, the model (1.1) can be

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written as

$$\boldsymbol{y} = \mathrm{X}\boldsymbol{\theta} + \boldsymbol{e} \tag{1.3}$$

where $\boldsymbol{y} = (y_1, y_2, \ldots, y_N)'$, $\mathrm{X} = (\boldsymbol{f}(\boldsymbol{x}_1), \boldsymbol{f}(\boldsymbol{x}_2), \ldots, \boldsymbol{f}(\boldsymbol{x}_N))'$ and $\boldsymbol{e} = (e_1, e_2, \ldots, e_N)'$, with $\mathrm{E}(\boldsymbol{e}) = \boldsymbol{0}$ and $\mathrm{Disp}(\boldsymbol{e}) = \sigma^2 I_N$.

We assume that the $\boldsymbol{x}_i$-s are specified in such a manner that the matrix X′X is positive definite. As such, all the components of $\boldsymbol{\theta}$ will be estimable.

Under the above assumption, the unique least squares estimator (LSE) of $\boldsymbol{\theta}$ is given by

$$\hat{\boldsymbol{\theta}} = (\mathrm{X}'\mathrm{X})^{-1}\mathrm{X}'\boldsymbol{y}$$

with dispersion matrix $\mathrm{Disp}(\hat{\boldsymbol{\theta}}) = \sigma^2(\mathrm{X}'\mathrm{X})^{-1}$.

The problem of selecting a design is that of choosing N points $\boldsymbol{x}_i \in \chi$, i=1,2, …, N such that the parametric functions of interest are estimated with sufficient accuracy. There are different interpretations of the term ‘sufficient accuracy’ leading to different classes of designs. In the context of response surface design, an *orthogonal design* is one for which the coefficients in the model are estimated with minimum variance, and this is achieved if and only if the estimates of the coefficients are uncorrelated with one another. This means $(\mathrm{X}'\mathrm{X})^{-1}$ or, equivalently $(\mathrm{X}'\mathrm{X})$, should be a diagonal matrix, and hence the moment matrix, to be defined in Section 2, should be diagonal.

Though orthogonal designs exist for the first-degree model, such designs do not exist when the model is of degree more than one. Orthogonal designs of a sort can be obtained, if we express the response function in terms of orthogonal polynomials. However, such designs have limitations in the sense that the coefficients of the new model in terms of the orthogonal polynomials are linear functions of the coefficients of the original model, which involve the design. To overcome this, Box and Hunter (1957) introduced the concept of rotatable designs. Later, several authors worked on the properties and construction of rotatable designs, see e.g., Bose and Draper (1959), Das and Narasimham (1962), Nigam and Das (1966), Herzberg (1967), among others.

Orthogonal designs have great appeal in the sense that lack of orthogonality results in lower efficiency. In fact, for inferring about a vector of parametric functions of interest, an orthogonal design is superior to any non-orthogonal design in terms of Loewner Order Domination (LOD) or Partial Loewner Ordering (PLO) of information matrices under the two designs (cf. Pukelsheim (1993), Liski *et al.* (2002)). Thus, it is desirable to make a design as close to orthogonality as possible when orthogonal designs are not feasible. Since orthogonal designs do not exist for models of degree greater than one, one should look for a design which is ‘less non-orthogonal’ than others in some sense. To compare designs, we, therefore, need some measures of, or indices to non-orthogonality in regression designs.

Mandal (2017) introduced a set of non-orthogonality measures in the set-up of block designs, and investigated block designs which are least non-orthogonal. In this paper, we confine ourselves to second degree multi-factor regression model. In Section 2, we investigate the problem and introduce some indices to non-orthogonality. In Section 3, designs possessing minimum non-orthogonality indices are explored and illustrated through examples for two- and three-factor experiments. Section 4 concludes with a brief discussion on our study.

2. INVESTIGATION OF THE PROBLEM

Consider a k-variate first degree model

$$E(y|\boldsymbol{x}) = \theta_0 + \sum_{i=1}^{k} \theta_i x_i. \tag{2.1}$$

Given an n-point design $D^{n\times k} = (x_{u1}, x_{u2}, \ldots, x_{uk};\ u = 1, 2, \ldots, n)$, the coefficient matrix X is given by X = $(\mathbf{1}_n,\ D)$ and we get the corresponding information matrix as

$$\mathrm{X}'\mathrm{X} = n\begin{bmatrix} 1_{n'}D \\ D'D \end{bmatrix},$$

where $\mathbf{1}_n$ is a $n\times 1$ vector with all elements unity.

The information matrix on a per observation basis, also called the moment matrix, is then given by

$$\mathrm{M} = \mathrm{X}'\mathrm{X}/n = \begin{bmatrix} 1 & [1] & [2] & \ldots & [k] \\ & [11] & [12] & \ldots & [1k] \\ & & [22] & \ldots & [1k] \\ & \ldots & \ldots & \ldots & \ldots \\ & & & & [kk] \end{bmatrix}$$

where

$$[\mathrm{i}] = \sum_{u=1}^{n} \frac{x_{ui}}{n},\ [\mathrm{ii}] = \frac{\sum_{u=1}^{n} x_{ui}^2}{n},\ [\mathrm{ij}] = \sum_{u=1}^{n} \frac{x_{ui}x_{uj}}{n}.$$

We shall work in the framework of a *continuous* (or *approximate*) design introduced by Kiefer (1959) for the study of optimality in regression designs.

A continuous design, written as $\xi = \{ \boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n; w_1, w_2, \ldots, w_n\}$, assigns weights $w_1, w_2, \ldots, w_n$ ($w_u \geq 0$, for u = 1,2,…,n; $\sum_{u=1}^{n} w_u = 1$) to the n design points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$, respectively in the domain $\boldsymbol{\chi}$. The points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ are called the *support points* of ξ. For such a design, the different order moments are given by

$$[i] = \sum_{u=1}^{n} w_u x_{ui}\ , [ii] = \sum_{u=1}^{n} w_u x_{ui}^2\ , [ij] = \sum_{u=1}^{n} w_u x_{ui} x_{uj}\ . \tag{2.2}$$

For the model (2.1), which can be written as $E(y/\boldsymbol{x}) = \boldsymbol{f}'(\boldsymbol{x})\boldsymbol{\theta}$, where $\boldsymbol{f}'(\boldsymbol{x}) = (1, x_1, x_2, \ldots, x_k)$, $\boldsymbol{\theta} = (\theta_0, \theta_1, \theta_2, \ldots, \theta_k)'$, the moment matrix of a continuous design ξ with support points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ and $w_1, w_2, \ldots, w_n$ as the respective weights, can be written as $M = \sum_{u=1}^{n} w_u \boldsymbol{f}(\boldsymbol{x_u}) \boldsymbol{f}'(\boldsymbol{x_u})$.

By definition, the design ξ is orthogonal if and only if $(X'X)^{-1}$, or M^{-1} is diagonal, which holds if and only if

$$[i] = 0,\ i = 1,2,\ldots,k\ ;\ [ij] = 0,\ i,\ j = 1,2,\ldots,k,\ i \neq j\ . \tag{2.3}$$

In the first order case, a design satisfying the moment conditions (2.3) is also rotatable, that is, such a design is both orthogonal and rotatable. Designs satisfying condition (2.3) are available in literature for both the domains in (1.2) (cf. Pukelsheim 1993). For completeness we cite a simple example below:

Example 2.1 Consider a 3-factor experiment in the domain $[-1,+1]^3$. An orthogonal design can be constructed using a 2^3 factorial experiment with levels ±1 as follows, where every row represents a design point:

x_1	x_2	x_3
1	1	1
1	1	-1
1	-1	1
1	-1	-1
-1	1	1
-1	1	-1
-1	-1	1
-1	-1	-1

It is easy to show that $[i] = [ij] = 0$ for all $i\ j = 1,2,3$. Hence the design satisfies condition (2.3) and is first order orthogonal. Because of symmetry and invariance of the design, it satisfies, in addition, $[ii]$ = constant, $i = 1,2,3$. which is not essential for orthogonality.

Now, consider a k-variate second degree model

$$E(y \mid \boldsymbol{x}) = \theta_0 + \sum_{i=1}^{k} \theta_i x_i + \sum_{i=1}^{k} \theta_{ii} x_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{k} \theta_{ij} x_i x_j . \tag{2.4}$$

For convenience's sake, we rewrite the model (2.4) as

$$E(y \mid \boldsymbol{x}) = \theta_0 + \sum_{i=1}^{k} \theta_{ii} x_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{k} \theta_{ij} x_i x_j + \sum_{i=1}^{k} \theta_i x_i . \tag{2.5}$$

Let Δ be the class of all second order designs in (2.2) for the model (2.5). Then the information matrix for the parameter vector $\boldsymbol{\theta} = (\theta_0, \theta_{11}, \theta_{22}, \ldots, \theta_{kk}, \theta_{12}, \ldots, \theta_{k-1,k}, \theta_1, \theta_2, \ldots, \theta_k)'$ based on a $\xi \in \Delta$ can be written as

$$M = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix},$$

where the partitions are based on $(1, x_1^2, x_2^2, \ldots, x_k^2)$, $(x_1x_2, x_1x_3, \ldots, x_{k-1}x_k)$ and $(x_1, x_2, \ldots, x_k)$, so that

$$M_{11} = \begin{bmatrix} 1 & [11] & [22] & \ldots & [kk] \\ & [1111] & [1122] & \ldots & [11kk] \\ & & [2222] & \ldots & [22kk] \\ & \ldots & \ldots & \ldots & \ldots \quad \ldots \\ & & & & [kkkk] \end{bmatrix}$$

$$M_{12} = M_{21}' = \begin{bmatrix} [12] & [13] & \ldots & [1k] & [23] & \ldots & [(k-1)k] \\ [1112] & [1113] & \ldots & [111k] & [1123] & \ldots & [11(k-1)k] \\ [2212] & [2213] & \ldots & [221k] & [2223] & \ldots & [22(k-1)k] \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\ [kk12] & [kk13] & \ldots & [kk1k] & [kk23] & \ldots & [kk(k-1)k] \end{bmatrix}$$

$$M_{13} = M_{31}' = \begin{bmatrix} [1] & [2] & \ldots & [k] \\ [111] & [112] & \ldots & [11k] \\ [221] & [222] & \ldots & [22k] \\ \ldots & \ldots & \ldots & \ldots \\ [kk1] & [kk2] & \ldots & [kkk] \end{bmatrix}$$

$$M_{22} = \begin{bmatrix} [1122] & [1123] & \dots & [12(k-1)k] \\ & [1133] & \dots & [13(k-1)k] \\ \dots & \dots & \dots & \dots \\ & & & [(k-1)(k-1)kk \end{bmatrix}$$

$$M_{23} = \begin{bmatrix} [112] & [122] & \dots & [12k] \\ [113] & [123] & \dots & [13k] \\ \dots & \dots & \dots & \dots \\ [1(k-1)k] & [2(k-1)k] & & [(k-1)kk] \end{bmatrix}$$

$$M_{33} = \begin{bmatrix} [11] & [12] & \dots & [1k] \\ & [22] & \dots & [2k] \\ \dots & \dots & \dots & \dots \\ & & & [kk] \end{bmatrix} \qquad (2.6)$$

Let us write $\mathrm{M}^{-1} = \begin{bmatrix} M^{11} & M^{12} & M^{13} \\ M^{12'} & M^{22} & M^{23} \\ M^{13'} & M^{23'} & M^{33} \end{bmatrix}$.

We define a design to be *block orthogonal* if M_{12}, M_{13} and M_{23} are null matrices of appropriate orders, i.e., the coefficients of one group of parameters are orthogonal to the coefficients of the other groups. Now, by the choice of a design, it is possible to achieve $M_{12} = M_{13} = M_{23} = \mathrm{O}$. Moreover, we can achieve M_{22} and M_{33} as diagonal matrices, which hold iff

$$[ij]=0,\ [iii]=[iij]=[ijl]=0,\ [iiij]=[iijl]=[ijlm]=0,$$

for all $i \neq j \neq l \neq m$. (2.7)

But the structure of M_{11} in (2.6) shows that it cannot be made a diagonal matrix, whatever be the design ξ. Thus, for a second degree model, though we can achieve block orthogonality, there doesn't exist any orthogonal design in the sense that M is a diagonal matrix. This calls for introducing a measure of non-orthogonality of a design.

As mentioned earlier, a design is orthogonal if and only if the dispersion matrix of the best linear unbiased estimator (BLUE) $\hat{\boldsymbol{\theta}}$ of the parameter vector $\boldsymbol{\theta}$ is diagonal. Hence, a measure of non-orthogonality may be introduced as the absolute value of the sum of the off- diagonal elements of the dispersion matrix, that is,

$$\delta_1 = | [\mathbf{1}'\mathrm{M}^{-1}\mathbf{1} - \mathrm{tr}(\mathrm{M}^{-1})]|$$

This may be realized if the design is invariant with respect to sign changes and permutation of factors.

It may be noted that, we can also define an index to non-orthogonality in terms of the information matrix, which will be the sum of the off-diagonal elements of M, i.e.,

$$\delta_2 = | [\mathbf{1}'\mathrm{M}\mathbf{1} - \mathrm{tr.}\ (\mathrm{M})]| = 2(\Sigma_i [ii] + \Sigma_{i<j} [iijj]).$$

Though this criterion and the one defined in (2.9) assume the same value, viz. zero, for orthogonal designs, they differ for non-orthogonal designs. However, we will not be considering it in this paper.

Let us confine our investigations to the sub-class $\Delta_1(\subset\Delta)$ of designs satisfying (2.7).

A design in Δ_1 has M_{ij} =0, for $i, j = 1, 2, 3, i < j$, and hence $M^{ij} = = 0$, for $i, j = 1, 2, 3, i < j$. Moreover, M_{22} and M_{33} are diagonal matrices, so that M^{22} and M^{33} turn out to be diagonal matrices. So, eventually, we need to evaluate the extent of non orthogonality of the partitioned matrix M^{11}.

We, therefore, modify δ_1 as

$$\delta_1 = |[\mathbf{1}'M_{11}^{-1}\mathbf{1} - \mathrm{tr}(M_{11}^{-1})]|. \qquad (2.8)$$

Before proceeding further, let us partition M_{11} as

$$M_{11} = \begin{bmatrix} M_{11.11} & M_{11.12} \\ M_{11.21} & M_{11.22} \end{bmatrix} = \begin{bmatrix} A & B \\ B' & C \end{bmatrix}, \text{ say,}$$

where $A = M_{11.11} = 1$, $B = M_{11.12} = M_{11.21}' = ([11], [22], \ldots, [kk])$,

$$C = M_{11.22} = \begin{bmatrix} [1111] & [1122] & \dots & [11kk] \\ & [2222] & \dots & [22kk] \\ \dots & \dots & \dots & \dots \\ & & & [kkkk] \end{bmatrix},$$

and set

$$M_{11}^{-1} = \begin{bmatrix} A & B \\ B' & C \end{bmatrix}^{-1} = \begin{bmatrix} M^{11.11} M^{11.12} \\ M^{11.21} M^{11.22} \end{bmatrix} = \begin{bmatrix} P & Q \\ Q' & R \end{bmatrix}.$$

Note that, $Q = -BR, AQ + BR = 0, Q = -A^{-1}BR.$

In order to understand the contribution of M_{11}^{-1} towards the non-orthogonality index δ_1, it is noted that the contribution comes from Q and the off-diagonal elements of R. This is because P is a scalar and, the off-diagonal elements of R and the elements of Q, which is a row vector, may be non-zero.

We, therefore, modify δ_1 to get the following as a non-orthogonality index:

$$\delta_1^* = |\mathbf{1}'R\mathbf{1} - \mathrm{tr}(R)| + 2|Q\mathbf{1}|$$

$$= |\mathbf{1}' M^{11.22}\mathbf{1} - \mathrm{tr.}\ (M^{11.22})| + 2|M_{11.12}M^{11.22}\mathbf{1}| \qquad (2.9)$$

The expression (2.9) is derived by substituting the expressions for R and Q, and noting that $A = 1$.

It may be noted that the criterion δ_1^* is invariant with respect to the components and is convex in M_{11}. In view of this, the following theorem is immediate.

Theorem 2.1: *A non-orthogonal design which minimizes* δ_1^* *is necessarily invariant under sign changes and permutation of the factors.*

For an invariant design, $[ii]$ and $[iiii]$-s are constants independent of $i = 1, 2, \ldots, k$, and so also are $[iijj]$-s for all $i \neq j (i, j = 1, 2, \ldots, k)$. So, we can take

$$[ii] = a,\ [iiii] = b,\ [iijj] = c. \tag{2.10}$$

where a, b and c are scalars.

Then, under (2.10), we get

$$\left(M^{11.22}\right)^{-1} = M_{11.22} - M_{11.12}M_{11.21}\ (\text{since}\ M_{11.11} = 1)$$

$$= \begin{bmatrix} [1111]\text{-}[11]^2 & [1122]\text{-}[11][22] & \ldots & [11kk]\text{-}[11][kk] \\ & [2222]\text{-}\ [22]^2 & \ldots & [22kk]\text{-}\ [22][kk] \\ \ldots & \ldots & \ldots & \ldots \\ & & & [kkkk]\text{-}\ [kk]^2 \end{bmatrix}$$

$$= (b - c) I_k + (c - a^2) J.$$

And,

$$M^{11.12} = -M_{11.12}\, M^{11.22} = ([11], [22], \ldots, [kk])\, M^{11.22} = -a1'\, M^{11.12} \tag{2.11}$$

Now $(M^{11.22})^{-1}$ represents the variance-covariance matrix of $(x_1^2, x_2^2, \ldots, x_k^2)$. So, setting $z_i = x_i^2, i = 1, 2, \ldots, k$, the off-diagonal elements of $(M^{11.22})^{-1}$ correspond to the covariance between the respective components of $\boldsymbol{z} = (z_1, z_2, \ldots, z_k)'$. With respect to any two of the components, say z_i and z_j, the covariance term will be zero if and only if

$$[iijj] = [ii][jj] \text{ for all } i \neq j. \tag{2.12}$$

The condition (2.12) can be realized if the values taken by z_i are independent of the values taken by z_j, and vice versa. If this is true for every pair of z_i-s, condition (2.12) makes $(M^{11.22})^{-1}$, and hence $M^{11.22}$ diagonal, but we cannot make $M^{11.12} = \mathbf{0}'$. Thus, though we cannot make M diagonal, it is close to it except for $M^{11.12}$. It should be noted that in making $M^{11.12} = \mathbf{0}'$. $M_{11.22}$ becomes a singular matrix. However, (2.12) may not be a necessary condition for the minimization of δ_1^*.

Using (2.10), for a design $\xi \in \Delta_1$, $M^{11.22}$ reduces to the form

$$M^{11.22} = (g - h) I_k + hJ, \tag{2.13}$$

where

$$g = \frac{b + (k-2)c - (k-1)a^2}{(b-c)\left(b + (k-1)c - ka^2\right)}$$

$$h = -\frac{c - a^2}{(b-c)\left(b + (k-1)c - ka^2\right)}. \tag{2.14}$$

From (2.11), we therefore get

$$M^{11.12} = -a\left(g + (k-1)h\right)1_k'. \tag{2.15}$$

Hence, the non-orthogonality index δ_1^* reduces to

$$\delta_1^* = k(k-1)h + 2ka\left[g + (k-1)h\right]. \tag{2.16}$$

If (2.12) also holds, the non-orthogonality index δ_1^* reduces to

$$\delta_1^* = 2kag = 2ka\frac{b + (k-2)c - (k-1)a^2}{(b-c)\left(b + (k-1)c - ka^2\right)}. \tag{2.17}$$

3. LEAST NON-ORTHOGONAL DESIGNS

In Section 2, we have observed that for a second-degree model (2.5), it is not possible to find an orthogonal design, that is, a design with information matrix M, given by (2.6), or equivalently its inverse M^{-1}, as a diagonal matrix. An index to non-orthogonality has been introduced based on the off-diagonal elements of M^{-1}. It is clear that in the class of symmetric invariant designs Δ_1, if a design satisfies $M_{12} = M_{13} = M_{23} = O$ (see (2.6)) and (2.7), then we can make the off-diagonals of M^{-1} zero except for those in M^{11} [recall that $M^{-1} = \begin{bmatrix} M^{11} & M^{12} & M^{13} \\ M^{12'} & M^{22} & M^{23} \\ M^{13'} & M^{23'} & M^{33} \end{bmatrix}$, where M^{11} is of order $(k+1)\times(k+1)$]. In this section, we discuss finding a design in Δ_1 that minimizes δ_1^*, given by (2.9).

Consider a design in Δ_1 satisfying (2.7) and (2.10). In view of the discussion in the previous section, we note that for any pair (z_i, z_j) where

$z_j = x_j^2, i, j = 1, 2, \ldots, k, i \neq j,$ (2.12) holds in the two-dimensional ***z***-space, if the values taken by z_i are independent of the values taken by z_j. Hence, for the two-factor space, the points must be horizontal and /or vertical along the two axes in the domain [0,1]⊗ [0,1] of the ***z***-space, or equivalently, in the ***x***-space the points must be of the form

$$(0, \pm s), (\pm s, 0), (\pm t, \pm t) \tag{3.2}$$

for some s and t lying in $[-1,+1]$. The same is true for every pair of z_i-s. This, however, does not ensure that M_{11} will be a diagonal matrix, but helps to make $M^{11.22}$ a diagonal matrix.

We consider the cases of $k = 2$, 3 below, confining to the sub-class of designs in Δ_1 satisfying (2.7) and (2.12).

Case 1: *k*=2.

Here the model is given by

$$E(y) = \theta_0 + \theta_1 x_1^2 + \theta_2 x_2^2 + \theta_{12}\theta_1 x_1 x_2 + \theta_1 x_1 + \theta_2 x_2. \tag{3.2}$$

Since there are six parameters in the model, for a design to be non-singular we need at least six distinct support points. From the above discussion, the design in the domain of $\boldsymbol{x} = (x_1, x_2)$ reduces to the following form which is similar to the central composite design (CCD) (c.f. Box and Wilson (1951)):

x_1	x_2	Mass
$\pm t$	$\pm t$	$\alpha_1/4$
0	$\pm s$	$\alpha_2/4$
$\pm s$	0	$\alpha_2/4$

with $0 \leq \alpha_1, \alpha_2 \leq 1, \alpha_1 + \alpha_2 = 1; 0 < s, t \leq 1.$

For a given design ξ, we have to minimize δ_1^* given by (2.16).

Now for the above design we have

$$[11] = t^2\alpha_1 + \frac{s^2\alpha_2}{2} = a$$

$$[1111] = t^4\alpha_1 + \frac{s^4\alpha_2}{2} = [2222] = b$$

$$[1122] = t^4\alpha_1 = c.$$

The moment matrix is, therefore,

$$m = \left[\begin{array}{ccc|c|cc} 1 & t^2a_1 + \frac{s^2a_2}{2} & t^2a_1 + \frac{s^2a_2}{2} & 0 & 0 & 0 \\ & t^4a_1 + \frac{s^4a_2}{2} & t^4a_1 & 0 & 0 & 0 \\ & & t^4a_1 + \frac{s^4a_2}{2} & 0 & 0 & 0 \\ \hline & & & t^4a_1 & 0 & 0 \\ \cline{4-6} & & & & t^2a_1 + \frac{s^2a_2}{2} & 0 \\ & & & & & t^2a_1 + \frac{s^2a_2}{2} \end{array}\right]$$

$$= \left[\begin{array}{c|c|c} M_{11} & M_{12} & M_{13} \\ \hline & M_{22} & M_{23} \\ \hline & & M_{33} \end{array}\right], \text{ where}$$

$$M_{11} = \begin{bmatrix} 1 & a & a \\ a & b & c \\ a & c & b \end{bmatrix},$$

$$M_{11}^{-1} = \frac{1}{(b-c)(b+c-2a^2)} \begin{bmatrix} b^2 - c^2 & ac - ab & ac - ab \\ ac - ab & b - a^2 & a^2 - c \\ ac - ab & a^2 - c & b - a^2 \end{bmatrix}$$

$$= \begin{bmatrix} M^{11.11} & M^{11.12} \\ M^{11.21} & M^{11.22} \end{bmatrix}.$$

Hence,

$$\delta_1^* = \frac{1}{(b-c)(b+c-2a^2)} \left[\left| \left(a^2 - c \right) \right| + 2\left| ac - ab \right| \right].$$

The off-diagonal elements of $M^{11.22}$ are zero if and only if

[1122] = [11]×[22], that is, $a^2 - c = 0.$

This gives,

$$t^2 = \frac{4s^2\alpha_1\alpha_2 + 4s^2\sqrt{\alpha_1}\alpha_2}{8\alpha_1(1-\alpha_1)} = \frac{s^2\alpha_2\left(\sqrt{\alpha_1}+1\right)}{2\sqrt{\alpha_1}(1-\alpha_1)}, \quad \text{since}$$

$t^2 \geq 0$

$$\Rightarrow t = s\sqrt{\frac{\alpha_2\left(\sqrt{\alpha_1}+1\right)}{2\sqrt{\alpha_1}(1-\alpha_1)}} = s\sqrt{\frac{\left(\sqrt{\alpha_1}+1\right)}{2\sqrt{\alpha_1}}}, \tag{3.3}$$

since $t, s \geq 0,$ and $\alpha_2 = 1 - \alpha_1.$

If $\left(\frac{t}{s}\right)^2 = r,$ then (3.3) gives

$$\sqrt{\alpha_1} = \frac{1}{2r-1}$$

$$\Rightarrow \alpha_1 = \left(\frac{1}{2r-1}\right)^2. \tag{3.4}$$

Clearly, since α_1, and hence $\sqrt{\alpha_1}$, lies between 0 and 1, we must have $2r-1>1$, which gives $r>1$, meaning $t^2 > r^2$.

For off-diagonal elements of $M^{11.22}$ all zero, we get

$$\delta_1^* = \frac{2|ac-ab|}{(b-c)(b-a^2)} = \frac{2a}{b-a^2} = \frac{2a}{b-c} \text{ (since } a^2-c=0)$$

$$= 2\frac{t^2\alpha_1 + \frac{s^2\alpha_2}{2}}{\frac{s^4\alpha_2}{2}}$$

$$= \frac{1}{t^2-s^2} + \frac{2}{s^2}. \tag{3.5}$$

This is a decreasing function of *t*, and a convex function of *s*.

The optimal values of *t*, *s* and α_1 minimizing δ_1^* come out to be $t = 1$, $s = \sqrt{\frac{\sqrt{2}}{\sqrt{2}+1}} = 0.7654$, $\alpha_1 = \left(\sqrt{2}+1\right)^{-2.} = 0.1716$, and $\delta_1^* = 5.8284$.

Case 1: *k* =3.

Here the model is given by

$$E(y) = \theta_0 + \sum_{i=1}^{3}\theta_i x_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{3}\theta_{ij}x_i x_j + \sum_{i=1}^{3}\theta_i x_j. \tag{3.6}$$

Since there are ten parameters in the model, for a non-singular design we need at least ten distinct support points. From the above discussion, the design in the domain of $\boldsymbol{x} = (x_1, x_2, x_3)$ has the following form:

x_1	x_2	x_3	Mass
$\pm t$	$\pm t$	$\pm t$	$\alpha_1/8$
$\pm s$	0	0	$\alpha_2/6$
0	$\pm s$	0	$\alpha_2/6$
0	0	$\pm s$	$\alpha_2/6$

with $0 \le \alpha_1, \alpha_2, \alpha_3 \le 1$, $\alpha_1 + \alpha_2 + \alpha_3 = 1$; $0 < s, t \le 1$.

The moment matrix comes out as

$$\mathrm{M} = \begin{bmatrix} M_{11} & O & O \\ O & M_{22} & O \\ O & O & M_{33} \end{bmatrix},$$

where M_{22} and M_{33} are diagonal matrices, and

$$M_{11} = \begin{bmatrix} 1 & a & a & a \\ & b & c & c \\ & c & b & c \\ & & & b \\ & & & \end{bmatrix} = \begin{bmatrix} M_{11.11} & M_{11.12} \\ & M_{11.22} \end{bmatrix}, \text{ say, with}$$

$a = [ii] = t^2\alpha_1 + \frac{s^2\alpha_2}{3}$, $b = [iiii] = t^4\alpha_1 + \frac{s^4\alpha_2}{3}$, $c = [iijj] = t^4\alpha_1 (i \ne j)$. Then,

$$M^{-1} = \begin{bmatrix} M^{11.11} & M^{11.12} \\ & M^{11.22} \end{bmatrix},$$

where each element of $M^{11.12}$ is $-\frac{a(b-c)^2}{(b-c)^2(b+2c-3a^2)} = -\frac{a}{(b+2c-3a^2)}$, and each of the off-diagonal elements of $M^{11.22}$ is $-\frac{(c-a^2)(b-c)}{(b-c)^2(b+2c-3a^2)} = -\frac{(c-a^2)}{(b-c)(b+2c-3a^2)}$.

Using (2.12), we have $c - a^2 = 0$, which is true for

$$r = \frac{1+\sqrt{\alpha_1}}{3\sqrt{\alpha_1}}, \tag{3.7}$$

where $r = \frac{t^2}{s^2} > 0$.

From(3.7) we ger

$$\sqrt{\alpha_1} = \frac{1}{3r-1} \Rightarrow \alpha_1 = \left(\frac{1}{3r-1}\right)^2. \tag{3.4}$$

As α_1, and hence $\sqrt{\alpha_1}$, lies between 0 and 1, we must have $3r-1>1$, which gives $r > \frac{2}{3}$, meaning $t^2 > \frac{2}{3}s^2$.

As off-diagonal elements of $M^{11.22}$ are zero under (2.12), we get

$$\delta_1^* = \frac{3a}{(b+2c-3a^2)} = \frac{3a}{b-c} \text{ (since } c = a^2)$$

$$=3\,\frac{t^2\alpha_1+\dfrac{s^2\alpha_2}{3}}{\dfrac{s^4\alpha_2}{3}}$$

$$=3\left[\frac{1}{3t^2-2s^2}+\frac{1}{s^2}\right]. \qquad (3.5)$$

This is a convex function of s^2, and a decreasing function of t^2.

We obtain the optimal values as $t=1$, $s=\sqrt{\frac{\sqrt{2}}{3}\left(\sqrt{2}+1\right)}$ = 0.3125, $\alpha_1=0.1716$, and $\delta_1^*=31.78964$.

4. COMPARISON WITH PERFORMANCE OF A D-OPTIMAL DESIGN

It is well known that an orthogonal design maximizes det.(M). Hence, we can introduce a non-orthogonality index as

$$\delta_D = \text{det.(M)}/b^k c^{k(k\text{-}1)/2} a^k, \qquad (4.1)$$

where the denominator gives the determinant of the moment matrix M* of a virtual/fictitious design with $M^*=\text{diag}\left(1,\underbrace{b,b,\ldots,b}_{k},\underbrace{c,c,\ldots,c}_{k(k-1)/2},\underbrace{a,a,\ldots,a}_{k}\right)$, that is, the off-diagonal elements are all zero.

It may be noted that the denominator in the expression for δ_D refers to the non-attainable upper bound (U) for any design 'D' with the given design parameters, and 0 [zero] gives the *limiting* lower bound. As such, rescaling a measure of non-orthogonality so that the index lie within the range (0,1) simplifies to (4.1).

Using the properties of log det(M) viz. (i) invariance under permutation and sign changes, and (ii) concavity, one can restrict to the class Δ_1 of designs which satisfy (2.7) and (2.10). This can be achieved through a symmetric design, i.e., by a design which is invariant under sign changes. Though condition (2.12) diagonalizes $M^{11.22}$, it may not be a necessary condition to achieve minimum non-orthogonality index δ_D given by (4.1).We may, therefore, restrict to the class of symmetric designs and minimize (4.1), and also find the design minimizing (3.1) under the condition (2.12). If the two designs differ then we can claim that (2.12) is not a necessary condition for minimizing (3.1).

It is well known that a central composite design (CCD) possesses many important properties and is very popular among practitioners.

5. CONCLUDING REMARKS

In this paper an index is introduced to assess the degree of non-orthogonality in a response surface design for the second-degree model. A class of designs is considered which satisfies a set of necessary conditions. Some designs are suggested which attain minimum value of non-orthogonality index within this class. Since the designs are determined in a subclass of designs satisfying the necessary conditions, it may not be the best in the whole class. However, such designs seem to be a strong contender, if not the best, to be the least non-orthogonal design.

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