Journal of the Nigerian Association of Mathematical Physics
***Volume* 17 (November, 2010), pp 359 - 362**
© J. of NAMP

Optimal Orthogonal Second-order Designs

Uchenna C. Nduka

Department of Statistics
University of Nigeria, Nsukka, Nigeria

Abstract

This paper extended the work of Chigbu and Nduka (2006), which obtained interesting results on closed form eigenvalues for comparing both orthogonal and rotatable Central Composite Designs (CCDs), by obtaining a majorization result. The majorization result is based on the principle of Schur's ordering of designs and was used to compare the replicated cube plus one star orthogonal CCD and the replicated star plus one cube CCD. Based on our result the former CCD is better than the latter CCD.

1.0 Introduction

This paper considers the optimal choice between the axial points (star) and non-axial points (cube) replications in the central composite design (CCD) with α-orthogonal structure proposed by [1]. This design has been widely used in agriculture, industrial and scientific investigations, since the design not only reduces experimental cost but also provide more efficient parameter estimation. The CCD is made up of a factorial portion consisting of a 2^k factorial design, axial portion of *k* pairs of points with the *i*th pair consisting of two symmetric points on the *i*th coordinate axis (*i* = 1, 2, …, *k*) at a distance of α from the centre of the design, which coincides with the centre of the coordinates systems by the coding scheme, and $n_0\,(\geq 1)$ centre points. The values of α and n_0 can be chosen so that the CCD acquires certain desirable features; see, for example, [3]. Draper and Draper and Lin ([4] and [5]) have shown that not only the centre points can be replicated but the cube and star as well. In that case, the CCD has a total number of points equal to $2^k n_1 + 2kn_2 + n_0$, where n_1 is the number of cube and n_2 is the number of star.

Replicating the design points in an experiment is so much desirable in the sense that it allows for the estimation of the pure error in the experiment. From the statistician's perspective, a design is deemed good if it ensures small variance of estimates of linear functional. Generally, the value of the variance of linear functional depends on the information matrix of the design as well as on restriction imposed on its combinatorial parameters; see, for example, [6] and [7]. The effects of restrictions, such as orthogonality, rotatability, etc that induce desirable properties in designs, on the variances of quadratic model have been studied by [10]. The study showed that restricted CCD is better than unrestricted CCD. Chigbu and Nduka [2] considered the effect of replicating either the cube or star points of a CCD on some optimality criteria. The paper computationally compared two variations of restricted CCD, namely the replicated cube plus one star and replicated star plus one cube. The information matrix of the restricted CCD was expressed in terms of the number of cube and star and then applied the principle of alphabetical optimality criteria to know the portion of CCD, which optimizes it. Interesting results about closed form eigenvalues for both orthogonally and rotatably restricted CCD were obtained in that work. The results show that replicated cubes plus one star is better than replicated star plus one cube.

In this paper, we go a step further by proving some majorization results for comparing the two variations of orthogonally restricted CCD considered in [2]. Given any two designs η and η' with information matrices $\mathbf{M}$ and

Corresponding author: E-mail; uchenna.nduka@unn.edu.ng or ndukauc@yahoo.com , Tel. +2348063467106

$\mathbf{M}'$ respectively, η is a better design if and only if $\mathbf{M} \geq \mathbf{M}'$; see [6] and [12]. Marshall and Olkin [9] devoted one chapter of the basic book on majorization to multivariate majorization where different orderings such as the one above are presented. The majorization results proved in section 3 are based on the above inequality.

Some other notations used are explained next. Ξ is the set of all designs in a regression model, so η and $\eta' \in \Xi$. Let $\eta \in \Xi$ denote the replicated cube plus one star orthogonal CCD with corresponding information matrix $\mathbf{M}$. Similarly, let $\eta' \in \Xi$ denote the replicated star plus one cube orthogonal CCD with corresponding information matrix $\mathbf{M}'$. Then the ith eigenvalue of $\mathbf{M}$ is denoted by $\lambda_i(\eta)$ and that of $\mathbf{M}'$ is denoted by $\lambda_i(\eta')$.

2.0 THE THEORITICAL FRAMEWORK

For completeness the framework of this study shall follow the same pattern with that of [2] and [10]. In order to show how the orthogonal restriction is made in choosing α, attention will be given to the expanded design matrix, $\mathbf{X}$ and the information matrix, $\mathbf{X'X}$ for the general CCD.

Consider the response surface, say $\varphi(X_1, X_2, \dots, X_k)$, represented in the experimental area $[\pm\alpha, \pm 1]$ by the second-order function

$$y_j = \beta_{00} + \sum_{i=1}^{k} \beta_{i0} X_{ij} + \sum_{i=1}^{k-1} \sum_{i'=i+1}^{k} \beta_{ii'} X_{ij} X_{i'j} + \sum_{i=1}^{k} \beta_{ii} X_{ij}^2 + \varepsilon_j \tag{2.1}$$

where, for orthogonality $\sum_{j=1}^{N} X_{ij} = 0 \quad \forall\ i = 1, 2, \dots, k$, y_j is the jth response, ε_j is the random error component associated with the observation y_j, $\beta_{00}, \beta_{i0}, \beta_{ii'}, \beta_{ii}$ are the unknown parameters of the model and X_1, X_2, …, X_k are the independent variables. Compactly, (2.1) can be written in vector notation as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e} \tag{2.2}$$

where $\mathbf{Y}$ is the $(N \times 1)$ response column vector, $\mathbf{X}$ is the $(N \times P)$ matrix of independent variables of rank P, $\boldsymbol{\beta}$ is the $(P \times 1)$ column vector of the unknown parameters, and $\mathbf{e}$ is the error column vector of order $(N \times 1)$ with $E(\mathbf{e}) = \mathbf{0}$ and $E(\mathbf{ee'}) = \sigma_e^2 \mathbf{I}$. Taking the average of the responses y_j in (2.1), we obtain

$$\bar{y} = \beta_{00} + \sum_{i=1}^{k} \beta_{i0} \bar{X}_i + \sum_{i=1}^{k-1} \sum_{i'=i+1}^{k} \beta_{ii'} \overline{X_i X_{i'}} + \sum_{i=1}^{k} \beta_{ii} \overline{X_i^2} + \bar{\varepsilon}\,. \tag{2.3}$$

By rescaling the response variable y_j, we obtain

$$y_j - \bar{y} = \sum_{i=1}^{k} \beta_{i0} (X_{ij} - \bar{X}_i) + \sum_{i=1}^{k-1} \sum_{i'=i+1}^{k} \beta_{ii'} (X_{ij} X_{i'j} - \overline{X_i X_{i'}}) + \sum_{i=1}^{k} \beta_{ii} (X_{ij}^2 - \overline{X_i^2}) + (\varepsilon_j - \bar{\varepsilon})\,. \tag{2.4}$$

By the same token (2.2) can be rescaled to

$$\mathbf{Y} - \underline{\bar{\mathbf{y}}} = \bar{\mathbf{X}}\boldsymbol{\beta} + (\mathbf{e} - \underline{\bar{\mathbf{e}}})\,, \tag{2.5}$$

where $\underline{\bar{\mathbf{y}}} = (\bar{y}, \bar{y}, \dots, \bar{y})'$, $\underline{\bar{\mathbf{e}}} = (\bar{\mathbf{e}}, \bar{\mathbf{e}}, \dots, \bar{\mathbf{e}})'$ and $\bar{\mathbf{X}}$ is the $(N \times (P-1))$ design matrix with $P = (k+1)(k+2)/2$. The structure of the design matrix $\bar{\mathbf{X}}$ is given in [2]. The corresponding information matrix for the design may be written as

$$\overline{\mathbf{X'X}} = diag(M_1 \mathbf{I}_k,\ M_2 \mathbf{I}_t,\ \mathbf{M}_3)\,. \tag{2.6}$$

In (2.6) $M_1 = 2^k n_1 + 2n_2\alpha^2$, $M_2 = 2^k n_1$ and $\mathbf{M}_3 = (p-q)\mathbf{I}_k + q\mathbf{J}_k$ where $\mathbf{I}_k$ is the $(k \times k)$ identity matrix, $\mathbf{I}_t$ is the $(t \times t)$ identity matrix, $t = k(k-1)/2$ and $\mathbf{J}_k = \underline{1}'\underline{1}$ where $\underline{1}$ is a column vector of ones of k

Corresponding author: E-mail; uchenna.nduka@unn.edu.ng or ndukauc@yahoo.com , Tel. +2348063467106

components. The entries of the sub-matrix $\mathbf{M}_3$, p and q, are given as $q = 2^k n_1 - (2^k n_1 + 2n_2\alpha^2)^2 / N$ and $p = q + 2\alpha^4 n_2$. Clearly by observing $\mathbf{M}_3$, a CCD acquires orthogonal structure if q is equal to zero.

3.0 Ordering Of Orthogonal CCD

Besides the uniform ordering of designs, which is based on the variance of linear functionals defined on the set of all states of the observed object, another ordering can be useful in experimental design; see, [8]. For any information matrix $\mathbf{M}$ with ordered eigenvalues $\lambda_1(\eta) \le \lambda_2(\eta) \le \ldots \le \lambda_k(\eta)$ where multiple eigenvalues appear in the

sequence $\lambda_1(\eta), \lambda_2(\eta), \ldots, \lambda_k(\eta)$ as many as times as their multiplicity is large, a design η is better than the design η' according to Schur's ordering if and only if $\sum_{i=1}^{r} \lambda_i(\eta) \ge \sum_{i=1}^{r} \lambda_i(\eta')$ and if and only if there is strict inequality for at least one r. The designs η and η' are said to be equivalent according to Schur's ordering if and only if there is equality sign for $r \in \{1, \ldots, k\}$.

Following the definition of orthogonal CCD in section 2, that is setting $q = 0$ in p, the information matrix in (2.6) becomes

$$\overline{\mathbf{X}}'\overline{\mathbf{X}} = \mathrm{diag}(M_0\mathbf{I}_k, M_2\mathbf{I}_t, p_0\mathbf{I}_t), \tag{3.1}$$

where $M_0 = (\pi N)^{1/2}$ and $p_0 = (\pi^2 + \pi N - 2\pi(\pi N)^{1/2}) / 2n_2$. The eigenvalues of the information matrix starting with the smallest are p_0 with k multiplicities, π with $k(k-1)/2$ multiplicities, and M_0 with k multiplicities, where $\pi = 2^k n_1$. To compare replicated cube plus one star and replicated star plus one cube, a proposition based on Schur's ordering will be proved for which we will need the following established result.

Proposition 3.1*:* If $\mathbf{A}$ is an $(k \times k)$ symmetric matrix with diagonal elements $a_1, \ldots, a_k$ and ordered eigenvalues $\mu_1 \ge \mu_2 \ge \ldots \ge \mu_k$, then $\sum_{i=1}^{r} a_i \le \sum_{i=1}^{r} \mu_i$ $(i = 1, \ldots, k-1)$; $\sum_{i=1}^{k} a_i = \sum_{i=1}^{k} \mu_i$, see [9].

PROOF:

Denote $\mathbf{D} \equiv \mathrm{diag}(\mu_1, \ldots, \mu_k)$. Let $\mathbf{u}_1, \ldots, \mathbf{u}_k$ be the orthonormal eigenvectors of $\mathbf{A}$ corresponding to $\mu_1, \mu_2, \ldots, \mu_k$, and denote $\mathbf{U} = (\mathbf{u_1}, \ldots, \mathbf{u_k})$. Then $\mathbf{D} = \mathbf{U}'\mathbf{A}\mathbf{U}$, hence $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}'$. It follows that $a_i = \sum_{i=1}^{k} (\{\mathbf{U}\}_{ij})^2 \mu_i$. Obviously,

$$\sum_{i=1}^{k} (\{\mathbf{U}\}_{ij})^2 = \sum_{j=1}^{k} (\{\mathbf{U}\}_{ij})^2 = 1.$$

Take $r \le k-1$ and denote $t_j \equiv \sum_{i=1}^{r} (\{\mathbf{U}\}_{\mathbf{ij}})^2 \le 1$. Clearly, $\sum_{j=1}^{k} t_j = r$, and consequently we can write $\sum_{i=1}^{r} a_i = \sum_{i=1}^{k} t_j \mu_j$, hence

$$\sum_{i=1}^{r} a_i - \sum_{i=1}^{r} \mu_i = \sum_{i=1}^{k} t_j \mu_j - \sum_{i=1}^{r} \mu_j + \mu_r (r - \sum_{j=1}^{k} t_j),$$

which implies that

Corresponding author: E-mail; uchenna.nduka@unn.edu.ng or ndukauc@yahoo.com , Tel. +2348063467106

Optimal Orthogonal Second-order Designs ***Uchenna C. Nduka J of NAMP***

$$\sum_{j=1}^{r}(\mu_j-\mu_r)(t_j-1) + \sum_{j=r+1}^{k} t_j(\mu_j-\mu_r) \le 0.$$

Evidently

$$\sum_{i=1}^{k} a_i = \sum_{i=1}^{k}(\sum_{i=1}^{k}(\{\mathbf{U}\}_{ij})^2\mu_j = \sum_{j=1}^{k}\mu_j .$$

Proposition 3.2: Given the information matrices $\mathbf{M}$ and $\mathbf{M}'$ obtained from using the respective orthogonal CCDs η and η' and the corresponding eigenvalues of the matrices $\lambda_i(\eta)$ and $\lambda_i(\eta')$, then $\sum_{i=1}^{r}\lambda_i(\eta) > \sum_{i=1}^{r}\lambda_i(\eta')$ if and only if $\mathbf{M} = diag(M_0\mathbf{I}_k, M_2\mathbf{I}_t, n_2 p_0\mathbf{I}_t)$ and $\mathbf{M}' = diag(n_1^{-1/2}M_0\mathbf{I}_k, n_1^{-1}M_2\mathbf{I}_t, p_0\mathbf{I}_t)$.

PROOF: Suppose $\mathbf{M} = diag(M_0\mathbf{I}_k, M_2\mathbf{I}_t, n_2 p_0\mathbf{I}_t)$ and $\mathbf{M}' = diag(n_1^{-1/2}M_0\mathbf{I}_k, n_1^{-1}M_2\mathbf{I}_t, p_0\mathbf{I}_t)$, let $\mathbf{u}_1, ..., \mathbf{u}_k$ be the orthonormal eigenvectors of $\mathbf{M}$ corresponding to $\lambda_1(\eta) \le \ldots \le \lambda_k(\eta)$. Then for each *i* $\lambda_i(\eta)$ =

$\mathbf{u}_i'\mathbf{M}\mathbf{u}_i \ge \mathbf{u}_i'\mathbf{M}'\mathbf{u}_i \equiv h_i$. According to Proposition 3.1, we have that

$$\sum_{i=1}^{r}h_i - \sum_{i=1}^{r}\lambda_i(\eta') = \left(\sum_{i=1}^{k}h_i - \sum_{i=1}^{k}\lambda_i(\eta')\right) - \sum_{i=k+1}^{k}h_i + \sum_{i=k+1}^{k}\lambda_i(\eta') \ge 0.$$

Hence

$$\sum_{i=1}^{r}\lambda_i(\eta) \ge \sum_{i=1}^{r}h_i \ge \sum_{i=1}^{r}\lambda_i(\eta')$$

for r = 1, 2, …, k, this implies that η is better in the sense of Schur's ordering than η'.

4.0 Conclusion

Proposition 3.2 shows that the replicated cube plus one star orthogonal CCD is better than replicated star plus one cube orthogonal CCD. This implies that adding more points to the non-axial points will give better estimate of the parameters of second-order model than adding more points to the axial points.

Hence, in choosing points to be replicated in a quadratic design where the adequacy of the design is based on the information matrix, replicated cube plus one star orthogonal CCD is the better choice.

References

Box, G. E. P. and Wilson, K. B. (1951). On the experimental attainment of optimum conditions. *Journal of Royal Statistical Society*, series **B 13(1)**, 1 – 45.

Chigbu, P. E. and Nduka, U. C. (2006). On the optimal choice of the cube and star replications in restricted second-order designs. *The Abdus Salam International Centre for Theoritical Physics*, Trieste, Italy, preprint No, IC/2006/113.

Draper, N.R. and John, J.A., (1998). Response Surface Designs Where Levels of Some Factors are Difficult to Change. *Australian and New Zealand Journal of Statistics*, **40** (4), 487-495.

Draper, N.R. and Lin, D.K.J., (1990). Small Response-Surface Designs. *Technometrics*, **32**, 187-194.

Corresponding author: E-mail; uchenna.nduka@unn.edu.ng or ndukauc@yahoo.com , Tel. +2348063467106

Draper, N.R., (1982). Center Points in Second-order Response Surface Designs. *Technometrics*¸ **24** (2), 127 - 133.

Fedorov, V. V. (1972). Theory of optimal experiments. Academic Press, New York

Galil, Z. and Kiefer, J. (1977). Comparison of rotatable designs for regression on balls, I(Quadratic). *Journal of Statistical Planning and Inference* 1, 27 – 40.

Giovagnoli, A. and Wynn, H. P. (1981). Optimum continuous block designs. *Proc. Roy. Soc. Lond.* **A377**, 405 – 416.

Marshall, A. W. and Olkin, I. (1979). Inequalities: Theory of Majorization and its Applications. Academic Press, New York.

Nwobi, F.N., Okoroafor, A.C., and Onukogu, I.B., (2001). Restricted Second-Order Designs on One and Two Concentric Balls. *Statistica,* **LXI** (1), 103-112.

Onukogu, I. B., (1997). Foundations of Optimal Exploration of Response Surfaces. Eprata Press, Nsukka, Nigeria.

Pazman, A., (1986). Foundations of Optimal Experimental Designs. D. Reidel Publishing Company Dordrecht.

Corresponding author: E-mail; uchenna.nduka@unn.edu.ng or ndukauc@yahoo.com , Tel. +2348063467106