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SLOPE ROTATABLE DESIGNS FOR SECOND ORDER RESPONSE SURFACE MODELS WITH BLOCK EFFECTS†

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ABSTRACT

In this article it is considered that how the slope-rotatability property of a second order design for response surface model is affected by block effects and how the design points are assigned into the blocks so that the blocked design may have the property of slope-rotatability. If an unblocked design is blocked properly, it could be a slope-rotatable design with block effects and this property is named as block slope-rotatability. We approach this problem from the moment matrix of the blocked design, which plays an important role to get the variances of the estimates, and suggest conditions of block slope-rotatability.

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1. INTRODUCTION

A second order mean response surface model with p variables can be written as

$$\eta(\mathbf{x}) = \beta_0 + \sum_{i=1}^{p} \beta_i x_i + \sum_{i=1}^{p} \beta_{ii} x_i^2 + \sum_{i<j}^{p} \beta_{ij} x_i x_j, \tag{1.1}$$

which may be written in matrix form as $\eta(\mathbf{x}) = \mathbf{x}'\boldsymbol{\beta}$ where

$$\mathbf{x} = (1, x_1, x_2, \ldots, x_p, x_1^2, x_2^2, \ldots, x_p^2, x_1x_2, x_1x_3, \ldots, x_{p-1}x_p)',$$
$$\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2, \ldots, \beta_p, \beta_{11}, \beta_{22}, \ldots, \beta_{pp}, \beta_{12}, \beta_{13}, \ldots, \beta_{p-1p})'.$$

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Observations, $y_u(\mathbf{x}) = \eta(\mathbf{x}) + e_u$, $u = 1, 2, \ldots, n$, are taken at n selected combinations of the x variables. The e_u's are assumed to be uncorrelated random errors with zero mean and constant variance, σ^2. The β's are then estimated by the least squares method, $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$, where $\mathbf{X}$ is the matrix of values of the elements of $\mathbf{x}'$s taken at the design points and $\mathbf{Y}$ is the vector of y observations, and the prediction of response at $\mathbf{x}$ is given by: $\hat{y}(\mathbf{x}) = \mathbf{x}'\hat{\boldsymbol{\beta}}$. The prediction variance, or a variance of a predicted value, is given by:

$$\mathrm{Var}(\hat{y}(\mathbf{x})) = \mathrm{Var}(\mathbf{x}'\hat{\boldsymbol{\beta}}) = \mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}\sigma^2.$$

One of the important design criteria is the rotatability which was suggested by Box and Hunter (1957). It means that by restricting the moment matrix of a design it is possible for the design to have the same variance of the predicted value at all points which are equidistant from the design center.

Recently, in the design of experiments for response surface analysis, attention has been focused on the estimation of differences in response rather than absolute value of the response mean itself. If differences at points close together in the design region are involved, estimation of the local slopes of the response surface is of interest. This problem, estimation of slopes, occurs frequently in practical situations. For instance, there are the cases in which one wants to estimate rates of reaction in chemical experiments, rates of change in the yield of a crop to various fertilizers, rates of disintegration of radioactive material in an animal, and so forth. Then the concept of rotatability needs to be extended to the slope-rotatability when the object of experiment is estimation of the derivative of the predicted response with respect to independent variables.

Hader and Park (1978) suggested the slope-rotatable property. This property means that the derivatives of the estimates with respect to each independent variables are equally good (same variance) at all combinations of the independent variables at the point equidistant from the design center, that is, a design is slope-rotatable if the variances of partial derivatives are only a function of ρ, distance from the design center. This property is called slope-rotatability over axial directions by Park (1987).

By Park and Kim (1992), the conditions for slope-rotatability over axial directions are given by

- Condition 1 :

$$\mathrm{Var}(\hat{\beta}_1) = \mathrm{Var}(\hat{\beta}_2) = \cdots = \mathrm{Var}(\hat{\beta}_p),$$

- Condition 2 :

$$\begin{aligned} 4\mathrm{Var}(\hat{\beta}_{11}) &= 4\mathrm{Var}(\hat{\beta}_{22}) = \cdots = 4\mathrm{Var}(\hat{\beta}_{pp}) \\ &= \mathrm{Var}(\hat{\beta}_{12}) = \mathrm{Var}(\hat{\beta}_{13}) = \cdots = \mathrm{Var}(\hat{\beta}_{p-1p}), \end{aligned}$$

- Condition 3 :

$$\mathrm{Cov}(\hat{\beta}_i, \hat{\beta}_{ii}) = \mathrm{Cov}(\hat{\beta}_i, \hat{\beta}_{ij}) = \mathrm{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{ij}) = \mathrm{Cov}(\hat{\beta}_{ij}, \hat{\beta}_{jk}) = 0,$$

for all i, j, k $(i \neq j \neq k \neq i)$.

And quite often, the experimental runs of a design for response surface model are to be assigned in blocks, in order to account for sources of variation caused by heterogeneous experimental conditions such as experimental time, batches used in experiment and so on. But when the blocking scheme is involved in the experimental design, some properties of the design without blocking may be lost. Hence there have been plenty of studies concerned with blocked design. To name a few, there are Khuri (1988, 1991, 1992) and Park and Kim (2002). In this paper we consider the conditions under which a certain design would be a blocked design that still has the slope-rotatability. And we call this design a block slope-rotatable design.

2. VARIANCES OF SECOND ORDER DESIGN UNDER BLOCKING

Consider the second order models with p variables and n observations. And suppose that experimental runs are assigned into b blocks. Then we have the blocked model

$$y_u = \beta_o + \sum_{i=1}^{p} \beta_i x_{iu} + \sum_{i=1}^{p} \beta_{ii} x_{iu}^2 + \sum_{i<j}^{p} \beta_{ij} x_{iu} x_{ju} + \sum_{l=1}^{b} z_{ul}\gamma_l + \epsilon_u, \quad u = 1, 2, \ldots, n, \tag{2.1}$$

where γ_l is an unknown parameter that denotes the effect of the l^{th} block($l = 1, 2, \ldots, b$), and z_{ul} is a dummy variable which is equal to one if the u^{th} experimental run is in the l^{th} block or zero if not, and ϵ_u is a u^{th} error term whose mean is 0 and variance is σ^2. Note that the model (2.1) is given by the following vector form,

$$\mathbf{y} = \beta_0 \mathbf{1}_n + \mathbf{X}^* \tilde{\boldsymbol{\beta}} + \sum_{l=1}^{b} \gamma_l \mathbf{z}_l + \boldsymbol{\epsilon}, \tag{2.2}$$

where $\mathbf{y} = (y_1, y_2, \ldots, y_n)'$, $\mathbf{z}_l = (z_{1l}, z_{2l}, \ldots, z_{nl})'$ and $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2, \ldots, \epsilon_n)'$. Notice that here $\mathbf{X}^*$ matrix and $\tilde{\boldsymbol{\beta}}$ do not contain $\mathbf{1}_n$ column and intercept β_0, respectively.

But the model (2.2) is not of full rank because of $\mathbf{1}_n = \sum_{l=1}^{b} \mathbf{z}_l$. Then let us now reparameterize this model so that it becomes of full rank. Consider the parameters $\tau_0, \tau_1, \ldots, \tau_{b-1}$ where

$$\begin{aligned} \tau_0 &= \beta_0 + \gamma_1, \\ \tau_{l-1} &= \gamma_l - \gamma_1, \quad l = 2, 3, \ldots, b. \end{aligned}$$

Then we obtain the model

$$\mathbf{y} = \tau_0 \mathbf{1}_n + \mathbf{X}^* \tilde{\boldsymbol{\beta}} + \mathbf{Z}\boldsymbol{\tau} + \boldsymbol{\epsilon}, \tag{2.3}$$

where $\boldsymbol{\tau} = (\tau_1, \tau_2, \ldots, \tau_{b-1})'$ and $\mathbf{Z}$ is a matrix of order $n \times (b-1)$ which is given by

$$\mathbf{Z} = \begin{pmatrix} \mathbf{0} \\ \mathbf{L} \end{pmatrix},$$

where $\mathbf{0}$ is a zero matrix of order $n_1 \times (b-1)$ and $\mathbf{L} = \mathrm{Diag}(\mathbf{1}_{n_2}, \mathbf{1}_{n_3}, \ldots, \mathbf{1}_{n_b})$. Here n_l denotes the number of experimental runs in the l^{th} block $(l = 1, 2, \ldots, b)$ and $\mathbf{1}_{n_l}$ means the vector of ones with n_l elements.

It is convenient to write the model (2.3) as

$$\begin{aligned} \mathbf{y} &= \psi_0 \mathbf{1_n} + \mathbf{X}^* \tilde{\boldsymbol{\beta}} + \mathbf{W}\boldsymbol{\tau} + \boldsymbol{\epsilon} \\ &= \mathbf{X}\boldsymbol{\beta}^* + \mathbf{W}\boldsymbol{\tau} + \boldsymbol{\epsilon}, \end{aligned} \tag{2.4}$$

where

$$\mathbf{X} = (\mathbf{1}_n, \mathbf{X}^*),$$

$$\psi_0 = \tau_0 + \mathbf{1}_n' \mathbf{Z}\boldsymbol{\tau}/n,$$

$$\mathbf{W} = (\mathbf{I}_n - \mathbf{J}_n/n)\mathbf{Z},$$

$$\boldsymbol{\beta}^* = (\psi_0, \tilde{\boldsymbol{\beta}}),$$

here $\mathbf{I}_n$ is the identity matrix and $\mathbf{J}_n$ is the matrix of ones, both of order $n \times n$. Note that $\mathbf{W}$ is of full column rank. The advantage of using $\mathbf{W}$ instead of $\mathbf{Z}$ is that the columns of $\mathbf{W}$ sum to zero, that is,

$$\mathbf{1}_n' \mathbf{W} = \mathbf{0}'.$$

In Khuri (1988) it is shown that the design blocks orthogonally if and only if

$$\mathbf{X}'\mathbf{W} = \mathbf{0},$$

or equivalently

$$\mathbf{X}'(\mathbf{I}_n - \mathbf{J}_n/n)\mathbf{Z} = \mathbf{0}.$$

To obtain estimators of the response surface coefficients from the blocked model (2.4), let

$$\boldsymbol{\theta} = \begin{pmatrix} \boldsymbol{\beta}^* \\ \boldsymbol{\tau} \end{pmatrix}, \quad \boldsymbol{\Gamma} = (\mathbf{X} \mid \mathbf{W}).$$

Then we get the least squares estimator of $\boldsymbol{\theta}$, that is given by,

$$\hat{\boldsymbol{\theta}} = (\boldsymbol{\Gamma}'\boldsymbol{\Gamma})^{-1}\boldsymbol{\Gamma}'\mathbf{y}. \tag{2.5}$$

The u^{th} fitted response from the model (2.4) is :

$$\hat{y}_u(\mathbf{x}) = \hat{\psi}_0 + \sum_{i=1}^{p} \hat{\beta}_i x_{iu} + \sum_{i=1}^{p} \hat{\beta}_{ii} x_{iu}^2 + \sum_{i<j}^{p} \hat{\beta}_{ij} x_{iu} x_{ju} + \sum_{l=1}^{b-1} w_{ul}\hat{\tau}_l, \quad u = 1, 2, \ldots, n,$$

where w_{ul} is the u^{th} row and l^{th} column element of $\mathbf{W}$ and $\hat{\tau}_l$ is the l^{th} element of $\hat{\boldsymbol{\tau}}$. Then the first derivative with respect to i^{th} independent variable is given by :

$$\frac{\partial \hat{y}(\mathbf{x})}{\partial x_i} = \hat{\beta}_i + 2\hat{\beta}_{ii} x_i + \sum_{j \neq i}^{p} \hat{\beta}_{ij} x_j, \quad i = 1, 2, \ldots, p. \tag{2.6}$$

Note that only the variance of $\hat{\boldsymbol{\beta}}^*$ is concerned with the variance of $\partial \hat{y}(\mathbf{x})/\partial x_i$. If we know $\mathrm{Var}(\hat{\boldsymbol{\beta}}^*)$ of a blocked design, the conditions of slope-rotatability would be drawn for a blocked model.

From (2.5) it can be shown that :

$$\begin{aligned} \mathrm{Var}(\hat{\boldsymbol{\theta}}) &= (\boldsymbol{\Gamma}'\boldsymbol{\Gamma}\,)^{-1}\sigma^2 \\ &= \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{12}' & \mathbf{A}_{22} \end{pmatrix}^{-1} \sigma^2 = \begin{pmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{12}' & \mathbf{B}_{22} \end{pmatrix} \sigma^2, \end{aligned} \tag{2.7}$$

where

$$\boldsymbol{\Gamma}'\boldsymbol{\Gamma} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{12}' & \mathbf{A}_{22}, \end{pmatrix},$$

and

$$\mathbf{A}_{11} = \begin{pmatrix} n & \mathbf{1}_n'\mathbf{X}^* \\ \mathbf{X}^{*\prime}\mathbf{1}_n & \mathbf{X}^{*\prime}\mathbf{X}^* \end{pmatrix}, \quad \mathbf{A}_{12} = \begin{pmatrix} 0' \\ \mathbf{X}^{*\prime}\mathbf{W} \end{pmatrix}, \quad \mathbf{A}_{22} = \mathbf{W}'\mathbf{W}.$$

Here it is known that:

$$\begin{aligned} \mathbf{B}_{11} &= (\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{12}')^{-1}, \\ \mathbf{B}_{12} &= -(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{12}')^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1}, \\ \mathbf{B}_{22} &= \mathbf{A}_{22}^{-1} + \mathbf{A}_{22}^{-1}\mathbf{A}_{12}'(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{12}')^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1}. \end{aligned} \tag{2.8}$$

It is noticed that only $\mathbf{B}_{11}$ part is needed to calculate $\mathrm{Var}(\hat{\boldsymbol{\beta}}^*)$, and the other parts of the variance ($\mathbf{B}_{12}$, $\mathbf{B}_{22}$) do not affect the variance of the derivative of (2.6).

If a design has the property of slope-rotatability over axial directions when the experimental runs of it are assigned in blocks, it is defined as a block slope-rotatable design over axial directions. Now we derive the conditions of block slope-rotatability over axial directions, by using the $\mathrm{Var}(\hat{\boldsymbol{\beta}}^*)$ of the blocked design.

3. Block Slope-Rotatability

Now consider an experimental design which has a symmetric moment matrix for a second order model such as:

$$\frac{1}{n}\mathbf{X}'\mathbf{X} = \begin{pmatrix} 1 & \cdot & \lambda_2\mathbf{1}_p' & \cdot \\ \cdot & \lambda_2\mathbf{I}_p & \cdot & \cdot \\ \lambda_2\mathbf{1}_p & \cdot & (c-1)\lambda_4\mathbf{I}_p + \lambda_4\mathbf{J}_p & \cdot \\ \cdot & \cdot & \cdot & \lambda_4\mathbf{I}_{\frac{p(p-1)}{2}} \end{pmatrix},$$

where $\lambda_2 = [i^2]$, $\lambda_4 = [i^2j^2]$, $c\lambda_4 = [i^4]$, $[i^2]=\sum_{u=1}^n x_{iu}^2/n$, $[i^2j^2]=\sum_{u=1}^n x_{iu}^2x_{ju}^2/n$, $[i^4] = \sum_{u=1}^n x_{iu}^4/n$, for all $i,j = 1,\ldots,p$, and $\cdot$ means zero vector or zero matrix. Many types of experimental designs including factorial design and central composite design (CCD) have a symmetric moment matrix. From now on, we only concentrate on the designs with symmetric moment matrix.

THEOREM 3.1. *Consider an unblocked design which has a symmetric moment matrix. If the blocking rule satisfies the following conditions, the design is a block slope-rotatable design over axial directions.*

For all $l = 1, \dots, b$,

$$[i]_l = 0, \text{ for all } i = 1, \dots, p, \tag{3.1}$$

$$[ij]_l = 0, \text{ for all } i, j \ (i \neq j) = 1, \dots, p, \tag{3.2}$$

$$\mathbf{U}'\mathbf{W}(\mathbf{W}'\mathbf{W})^{-1}\mathbf{W}'\mathbf{U} = \mu_1 \mathbf{I}_p + \mu_2 \mathbf{J}_p, \tag{3.3}$$

$$\left(1 - \frac{1}{p}\right)\frac{1}{(c-1)\lambda_4 - \mu_1} + \frac{1}{p}\frac{1}{-np\lambda_2^2 + (c+p-1)\lambda_4 - \mu_1 - p\mu_2} = \frac{1}{4n\lambda_4}, \tag{3.4}$$

where $[i]_l$ and $[ij]_l$ mean block design moments of variable i and variables i and j in block l, that is, $[i]_l = \sum_{u \in l} x_{iu}$ and $[ij]_l = \sum_{u \in l} x_{iu}x_{ju}$, respectively. And $\mathbf{U}$ is the pure quadratic part of $\mathbf{X}$ which is an $n \times p$ matrix and μ_1, μ_2 are given constants. The condition (3.3) means that partial moment matrix of the pure quadratic part of the blocked design is to be a symmetric matrix with identical diagonal elements and identical off-diagonal elements.

PROOF. By the conditions (3.1) and (3.2),

$$\mathbf{X}'\mathbf{W} = \begin{pmatrix} \mathbf{0}_{p+1} \\ \mathbf{U}'\mathbf{W} \\ \mathbf{0}_{\frac{p(p-1)}{2}} \end{pmatrix}. \tag{3.5}$$

Hence by using (2.8), $\mathbf{B}_{11}$ of the equation (2.7) is given by,

$$\mathbf{B}_{11} = (\mathbf{A}_{11} - \mathbf{X}'\mathbf{W}(\mathbf{W}'\mathbf{W})^{-1}\mathbf{W}\mathbf{X})^{-1}.$$

By the condition (3.3), we can show that $\mathbf{A}_{11} - \mathbf{X}'\mathbf{W}(\mathbf{W}'\mathbf{W})^{-1}\mathbf{W}\mathbf{X}$ is

$$\begin{pmatrix} n & \cdot & n\lambda_2 \mathbf{1}_p' & \cdot \\ \cdot & n\lambda_2 \mathbf{I}_p & \cdot & \cdot \\ n\lambda_2 \mathbf{1}_p & \cdot & \xi_1 \mathbf{I}_p + \xi_2 \mathbf{J}_p & \cdot \\ \cdot & \cdot & \cdot & n\lambda_4 \mathbf{I}_{\frac{p(p-1)}{2}} \end{pmatrix},$$

where $\xi_1 = (c-1)\lambda_4 - \mu_1$ and $\xi_2 = \lambda_4 - \mu_2$. Thus, it can be shown that $\mathbf{B}_{11}$ is given by :

$$\begin{pmatrix} \delta_0 & \cdot & n\delta_1 \mathbf{1}_p' & \cdot \\ \cdot & \frac{1}{n\lambda_2}\mathbf{I}_p & \cdot & \cdot \\ n\delta_1 \mathbf{1}_p & \cdot & \delta_2 \mathbf{I}_p + \delta_3 \mathbf{J}_p & \cdot \\ \cdot & \cdot & \cdot & \frac{1}{n\lambda_4}\mathbf{I}_{\frac{p(p-1)}{2}} \end{pmatrix},$$

where

$$\delta_0 = \frac{1}{n\phi}(\xi_1 + p\xi_2),\ \delta_1 = \frac{1}{\phi}(-\lambda_2),\ \delta_2 = \frac{1}{\xi_1},\ \delta_3 = \frac{1}{p}\left(\frac{1}{\phi} - \frac{1}{\xi_1}\right),$$
$$\phi = -np\lambda_2^2 + \xi_1 + p\xi_2.$$

From the equation (2.7), we have $\mathrm{Var}(\hat{\boldsymbol{\beta}}^*) = \mathbf{B}_{11}\sigma^2$. Observing the elements of $\mathbf{B}_{11}$, we can verify the fact that the variances of $\hat{\beta}_i$ and $\hat{\beta}_{ij}$ are invariant under this type of blocking, and covariances of $(\hat{\beta}_i, \hat{\beta}_{ii})$, $(\hat{\beta}_i, \hat{\beta}_{ij})$ and $(\hat{\beta}_{ii}, \hat{\beta}_{ij})$ still remain zero. Only the variances of $\hat{\beta}_{ii}$ and covariances of $(\hat{\beta}_{ii}, \hat{\beta}_{jj})$ are changed. *i.e.*, the conditions 1 and 3 of slope-rotatability over axial directions for the blocked design are satisfied. We have only to check out the Condition 2.

Among the variances of the blocked design, $\mathrm{Var}(\hat{\beta}_{ii})$ and $\mathrm{Var}(\hat{\beta}_{ij})$ are given by,

$$\begin{aligned}
\mathrm{Var}(\hat{\beta}_{ii}) &= (\delta_2 + \delta_3)\sigma^2, \quad i = 1, 2, \ldots, p,\\
\mathrm{Var}(\hat{\beta}_{ij}) &= \frac{1}{n\lambda_4}\sigma^2, \quad i, j = 1, 2, \ldots, p,\ (i \neq j).
\end{aligned}$$

and then by the condition (3.4)

$$\begin{aligned}
4\mathrm{Var}(\hat{\beta}_{ii}) &= 4\mathrm{Var}(\delta_2 + \delta_3)\sigma^2 = 4\mathrm{Var}\left(\frac{1}{\xi_1} + \frac{1}{p}\left(\frac{1}{\phi} - \frac{1}{\xi_1}\right)\right)\sigma^2\\
&= 4\mathrm{Var}\left(\left(1 - \frac{1}{p}\right)\frac{1}{(c-1)\lambda_4 - \mu_1} + \frac{1}{p}\frac{1}{-np\lambda_2^2 + (c+p-1)\lambda_4 - \mu_1 - p\mu_2}\right)\sigma^2\\
&= \mathrm{Var}(\hat{\beta}_{ij}).
\end{aligned}$$

Hence, a design satisfies the conditions of slope-rotatability over axial directions for the blocked design. Thus the design which satisfies all the above conditions is a block slope-rotatable design over axial directions. In addition, if a design is blocked orthogonally, it becomes also a block slope-rotatable design over axial directions with $\mathbf{X}'\mathbf{W} = \mathbf{0}$ ($\because$ $\mathbf{U}'\mathbf{W} = \mathbf{0}$ in (3.5)). □

4. Rotatability and Slope-Rotatability for Central Composite Designs

The central composite design(CCD) is a design widely used for estimating second order response surface. It is perhaps the most popular class of second order designs. It involves the use of a two-level factorial (or fractional factorial) combined with $2p$ axial points and center points such as:

Factorial Points			
x_1	x_2	$\cdots$	x_p
-1	-1	$\cdots$	-1
-1	-1	$\cdots$	1
-1	-1	$\cdots$	-1
-1	-1	$\cdots$	1
$\vdots$	$\vdots$	$\ddots$	$\vdots$
1	1	$\cdots$	-1
1	1	$\cdots$	1

Axial Points			
x_1	x_2	$\cdots$	x_p
$-\alpha$	0	$\cdots$	0
α	0	$\cdots$	0
0	$-\alpha$	$\cdots$	0
0	$-\alpha$	$\cdots$	0
$\vdots$	$\vdots$	$\ddots$	$\vdots$
0	0	$\cdots$	$-\alpha$
0	0	$\cdots$	α

Center Points			
x_1	x_2	$\cdots$	x_p
0	0	$\cdots$	0
$\vdots$	$\vdots$	$\ddots$	$\vdots$
0	0	$\cdots$	0

As a result, the design involves, say, $F = 2^p$ factorial points (or $F = 2^{p-k}$ fractional factorial points), $2p$ axial points and n_0 center points. The CCDs were first introduced by Box and Wilson (1951).

A rotatable design is one for which $\text{NVar}[\hat{y}(\mathbf{x})]/\sigma^2$ has the same value at any two locations that have the same distance from the design center. In other words, $\text{NVar}[\hat{y}(\mathbf{x})]/\sigma^2$ is constant on spheres. The rotatability property was first introduced by Box and Hunter (1957).

It is well-known that the condition for a CCD to be rotatable is that

$$\alpha = F^{1/4}.$$

This means that the value of α for a rotatable CCD dose not depend on the number of center points.

Hader and Park (1978) proposed an analog of the Box and Hunter rotatability criterion, which requires that the variance of $\partial\hat{y}(\mathbf{x})/\partial x_i$ be constant on circles ($k = 2$), spheres ($k = 3$), or hyperspheres ($k = 4$) centered at the design origin.

Estimates of the derivative over axial directions would then be equally reliable for all points $\mathbf{x}$ equidistant from the design origin. They referred to this property as slope rotatability, and showed that the condition for a CCD to be a slope-rotatable design is as follows:

$$\begin{aligned}&[2(F+n_0)]\alpha^8 - (4pF)\alpha^6 - F[n(4-p) + pF - 8(p-1)]\alpha^4\\&+[8(p-1)F^2]\alpha^2 - 2F^2(p-1)(n-F) = 0.\end{aligned}$$

5. SLOPE-ROTATABILITY FOR CENTRAL COMPOSITE DESIGNS UNDER BLOCKING

Especially by adjusting the axial value α, a CCD would have a certain property, such as rotatability or slope-rotatability. It is of interest to find out such α

that makes the block slope-rotatable design over axial directions.

Let us consider a CCD with 3 variables and 2 blocks in which the factorial points are assigned in block 1, and the axial points and 2 center points are assigned in block 2. The design matrix is given by

Block 1			*Block 2*		
x_1	x_2	x_3	x_1	x_2	x_3
-1	-1	-1	$-\alpha$	0	0
-1	-1	1	α	0	0
-1	1	-1	0	$-\alpha$	0
-1	1	1	0	α	0
1	-1	-1	0	0	$-\alpha$
1	-1	1	0	0	α
1	1	-1	0	0	0
1	1	1	0	0	0

By the condition (3.3) of block slope-rotatability,

$$\mathbf{U}'\mathbf{W}(\mathbf{W}'\mathbf{W})^{-1}\mathbf{W}'\mathbf{U} = \frac{1}{4}(\alpha^2 - 4)^2\mathbf{J}_3,$$

and we can find that $\mu_1 = 0$ and $\mu_2 = (1/4)(\alpha^2 - 4)^2$. If the axial point coordinate value α is the solution of the equation $4\mathrm{Var}(\hat{\beta}_{ii}) = \mathrm{Var}(\hat{\beta}_{ij})$, it can be a block slope-rotatable design over axial directions. For this example $\alpha = 2\sqrt[4]{2}$ satisfies the condition of block slope-rotatability over axial directions. The $\mathbf{B}_{11}$ matrix for this example is given by

$$\mathbf{B}_{11} = \begin{pmatrix} \frac{5}{32} + \frac{3}{2\alpha^4} + \frac{3}{4\alpha^2} & \cdot & -\frac{4+\alpha^2}{4\alpha^4}\mathbf{1}_3' & \cdot \\ \cdot & \frac{1}{8+2\alpha^2}\mathbf{I}_3 & \cdot & \cdot \\ -\frac{4+\alpha^2}{4\alpha^4}\mathbf{1}_3 & \cdot & \frac{1}{2\alpha^4}\mathbf{I}_3 + \frac{1}{2\alpha^4}\mathbf{J}_3 & \cdot \\ \cdot & \cdot & \cdot & \frac{1}{8}\mathbf{I}_3 \end{pmatrix}.$$

For the CCD with two blocks like the above example, the value of α, which makes a block slope-rotatable design over axial directions, can be easily obtained from the following equation in Theorem 5.1.

THEOREM 5.1. *Suppose the experimental points of a CCD are assigned in two blocks as follows :*

	x_1	x_2	$\cdots$	x_p	
	-1	-1	$\cdots$	-1	
	-1	-1	$\cdots$	1	
	-1	-1	$\cdots$	-1	
Block 1	-1	-1	$\cdots$	1	2^p *factorial points*
	$\vdots$	$\vdots$	$\ddots$	$\vdots$	
	1	1	$\cdots$	-1	
	1	1	$\cdots$	1	
	$\mathbf{0}$	$\mathbf{0}$	$\cdots$	$\mathbf{0}$	n_{0_1} *center points*
	$-\alpha$	0	$\cdots$	0	
	α	0	$\cdots$	0	
	0	$-\alpha$	$\cdots$	0	
Block 2	0	α	$\cdots$	0	$2p$ *axial points*
	$\vdots$	$\vdots$	$\ddots$	$\vdots$	
	0	0	$\cdots$	$-\alpha$	
	0	0	$\cdots$	α	
	$\mathbf{0}$	$\mathbf{0}$	$\cdots$	$\mathbf{0}$	n_{0_2} *center points*

where

$$\begin{aligned}
n_{0_i} &= \text{number of center points in Block } i,\ i = 1, 2, (n_{0_i} \geq 0,\ n_{0_1} + n_{0_2} > 0),\\
n_c &= 2^p = \text{number of factorial points (or corner points) of a CCD},\\
n_1 &= 2^p + n_{0_1} = \text{number of points in Block 1},\\
n_2 &= 2p + n_{0_2} = \text{number of points in Block 2},\\
n &= n_1 + n_2 = \text{total number of points.}
\end{aligned}$$

Then the α that makes a CCD be a block slope-rotatable design over axial directions is given by the positive solution of the following, which is the 4^{th} polynomial equation of α :

$$\frac{n[f + (p-2)g] - (p-1)e^2}{(f-g)\{n[f + (p-1)g - pe^2\}} = \frac{1}{4n_c}, \tag{5.1}$$

where

$$\begin{aligned}
e &= n_c + 2\alpha^2,\\
f &= n_c + 2\alpha^4 - \frac{1}{nn_1n_2}(2n_1\alpha^2 - n_2n_c)^2,\\
g &= n_c - \frac{1}{nn_1n_2}(2n_1\alpha^2 - n_2n_c)^2.
\end{aligned}$$

PROOF. From the given blocked design, it can be easily shown that for $l = 1, 2$,

$$
\begin{aligned}
[i]_l &= 0, \text{ for all } i = 1, \ldots, p, \\
[ij]_l &= 0, \text{ for all } i, j \ (i \neq j) = 1, \ldots, p.
\end{aligned}
$$

To show that the given blocked design satisfies the condition of slope-rotatability over axial directions, it is enough to show that $4\mathrm{Var}(\hat{\beta}_{ii}) = \mathrm{Var}(\hat{\beta}_{ij})$.

Here $\mathbf{W}$ matrix is :

$$
\mathbf{W} = (\mathbf{I}_n - \mathbf{J}_n/n)\mathbf{Z} = -\frac{n_2}{n}\begin{pmatrix} \mathbf{1}_{n_1} \\ \mathbf{0}_{n_2} \end{pmatrix} + \frac{n_1}{n}\begin{pmatrix} \mathbf{0}_{n_1} \\ \mathbf{1}_{n_2} \end{pmatrix}
$$

and $\mathbf{W}'\mathbf{W} = n_1 n_2/n$, then from the equations (2.7) – (2.8) we can show that

$$
\begin{aligned}
\mathbf{B}_{11} &= (\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{12}')^{-1} \\
&= (\mathbf{A}_{11} - \mathbf{U}'\mathbf{W}(\mathbf{W}'\mathbf{W})^{-1}\mathbf{W}'\mathbf{U})^{-1}
\end{aligned}
$$

and

$$
\mathbf{A}_{11} - \mathbf{U}'\mathbf{W}(\mathbf{W}'\mathbf{W})^{-1}\mathbf{W}'\mathbf{U} = \begin{pmatrix} n & \cdot & e\mathbf{1}_p' & \cdot \\ \cdot & e\mathbf{I}_p & \cdot & \cdot \\ e\mathbf{1}_p & \cdot & (f-g)\mathbf{I}_p + g\mathbf{J}_p & \cdot \\ \cdot & \cdot & \cdot & n_c\mathbf{I}_{\frac{p(p-1)}{2}} \end{pmatrix},
$$

which makes the symmetric form. After taking the inverse of the above matrix, from $\mathbf{B}_{11}$ we can derive the fact that :

$$
\begin{aligned}
\mathrm{Var}(\hat{\beta}_{ii}) &= \frac{n[f + (p-2)g] - (p-1)e^2}{(f-g)\{n[f + (p-1)g] - pe^2\}}\sigma^2, \\
\mathrm{Var}(\hat{\beta}_{ij}) &= \frac{1}{n_c}\sigma^2.
\end{aligned}
$$

It is obvious that α, which is the positive solution of (5.1), satisfies the condition:

$$
4\mathrm{Var}(\hat{\beta}_{ii}) = \mathrm{Var}(\hat{\beta}_{ij}).
$$

Thus it makes a block slope-rotatable design over axial directions. □

Table 5.1 and Table 5.2 show the values of α which satisfies the conditions of the block slope-rotatability over axial directions with two variables and three variables respectively. In the table '-' means that there exists no value for the corresponding case. From these tables we derive the fact that the value of α for block slope-rotatable over axial directions for CCD is a function of the number of blocks as well as a function of the number of center points. By increasing the number of center points, the value of α can be decreased.

TABLE 5.1 *The values of α for CCD with $b = 2$ and $p = 2$*

n	n_0	*Rotatable*	*Slope-rotatable*	n_1	n_2	*Block-slope-rotatable*
9	1	1.414	2.090	5	4	-
				4	5	2.213
10	2	1.414	1.984	6	4	-
				5	5	2.135
				4	6	2.000
11	3	1.414	1.911	7	4	-
				6	5	2.081
				5	6	1.944
				4	7	1.911
12	4	1.414	1.859	8	4	-
				7	5	2.042
				6	6	1.906
				5	7	1.864
				4	8	1.861
13	5	1.414	1.820	9	4	-
				8	5	2.013
				7	6	1.880
				6	7	1.834
				5	8	1.820
				4	9	1.829
14	6	1.414	1.791	10	4	-
				9	5	1.991
				8	6	1.861
				7	7	1.813
				6	8	1.794
				5	9	1.792
				4	10	1.807

TABLE 5.2 *The values of α for CCD with $b = 2$ and $p = 3$*

n	n_0	*Rotatable*	*Slope-rotatable*	n_1	n_2	*Block-slope-rotatable*
15	1	1.682	2.432	9	6	-
				8	7	2.632
16	2	1.682	2.339	10	6	-
				9	7	2.532
				8	8	2.378
17	3	1.682	2.268	11	6	-
				10	7	2.452
				9	8	2.314
				8	9	2.272
18	4	1.682	2.213	12	6	-
				11	7	2.389
				10	8	2.264
				9	9	2.223
				8	10	2.213
19	5	1.682	2.172	13	6	-
				12	7	2.340
				11	8	2.227
				10	9	2.186
				9	10	2.172
				8	11	2.176
20	6	1.682	2.139	14	6	-
				13	7	2.300
				12	8	2.197
				11	9	2.158
				10	10	2.142
				9	11	2.140
				8	12	2.149

6. COMPARISON WITH BLOCK ROTATABLE CENTRAL COMPOSITE DESIGNS

Khuri (1991) researched the conditions of block rotatability which means that the blocked design has a rotatable property. It was focused on the conditions of block rotatability when the unblocked design is rotatable central composite design. As a result, since the specific α is already selected for the unblocked rotatable CCD, the value of α is not changed under the blocking. A CCD with 3 variables and 6 center points is given as an example, which can be written as :

$$\mathbf{D} = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ \alpha & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & \alpha \\ 0 & 0 & -\alpha \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{array}$$

Note that this CCD is rotatable when the value of α is 1.682. On the other hand, the condition of slope-rotatability is satisfied only when $\alpha = 2.139$ as shown in Table 5.2.

By Khuri (1991), the following blocked design is a block rotatable CCD with $\alpha = 1.682$.

Block 1		
x_1	x_2	x_3
-1	-1	-1
1	1	-1
1	-1	1
-1	1	1
0	0	0
0	0	0

Block 2		
x_1	x_2	x_3
1	1	1
1	-1	-1
-1	1	-1
-1	-1	1
0	0	0
0	0	0

Block 3		
x_1	x_2	x_3
α	0	0
$-\alpha$	0	0
0	α	0
0	$-\alpha$	0
0	0	α
0	0	$-\alpha$
0	0	0
0	0	0

In comparison with the previous result, under the same blocking rule, the conditions of block slope-rotatability over axial directions are satisfied when α is 2.197. Table 6.1 summarizes the above results.

TABLE 6.1 *Comparison with block rotatable CCD with* $p = 3$

Design property	*Block Size*	n	α
rotatable	-	20	1.682
slope-rotatable	-	20	2.139
block rotatable	$n_1 = 6,\ n_2 = 6,\ n_3 = 8$	20	1.682
block slope-rotatable over axial directions	$n_1 = 6,\ n_2 = 6,\ n_3 = 8$	20	2.197

7. CONCLUDING REMARKS

In general, the slope-rotatability property is not preserved when the experimental points of a design are assigned in blocks. However, there exist the conditions under which the experimental runs of a design are assigned in blocks, then the blocked design has a slope-rotatability property. Such design is defined as a block slope-rotatable design.

When a design which has a symmetric moment matrix, for example, central composite design, icosahedron and dodecahedron with center points, satisfies the conditions of block slope-rotatability, it can be a block slope-rotatable design over axial directions.

Especially if the experimental runs of a central composite design are assigned into the blocks in this way, there exists an axial point coordinate value α that makes this design be a block slope-rotatable design over axial directions.

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