Measure of Slope Rotatability for Second Order Response Surface Designs Under Tri-Diagonal Correlation Error Structure Using Central Composite Designs

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ABSTRACT

In the design of experiments for estimating the slope of the response surface, slope rotatability is a desirable property. In this paper, measure of slope rotatability for second order response surface designs using central composite designs under tri-diagonal correlation error structure is suggested and illustrated with examples.

Key words and Phrases: Response surface design, slope-rotatability, tri-diagonal correlation error structure, central composite designs, weak slope rotatability region. 2010 AMS Subject Classification : 62K05.

1 Introduction

Response surface methodology is a collection of mathematical and statistical techniques useful for analyzing problems where several independent variables influence

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a dependent variable. The independent variables are often called the input or explanatory variables and the dependent variable is often the response variable. An important step in development of response surface designs was the introduction of rotatable designs by Box and Hunter (1957). Das and Narasimham (1962) constructed rotatable designs using balanced incomplete block designs (BIBD). The study of rotatable designs mainly emphasized on the estimation of absolute response. Estimation of response at two different points in the factor space will often be of great importance. If differences at two points close together, estimation of local slope (rate of change) of the response is of interest. Hader and Park (1978) extended the notion of rotatability to slope rotatability for the case of second order models. In view of slope rotatability of response surface methodology, a good estimation of derivatives of the response function is more important than estimation of mean response. Estimation of slopes occurs frequently in practical situations. For instance, there are cases in which we want to estimate rate of reaction in chemical experiment, rate of change in the yield of a crop to various fertilizer doses, rate of disintegration of radioactive material in animal etc. (cf. Park 1987). Victorbabu and Narasimham (1991) studied second order slope rotatable designs (SOSRD) using BIBD. Victorbabu (2007) suggested a review on SOSRD. To access the degree of slope rotatability Park and Kim (1992) introduced a measure for second order response surface designs. Victorbabu and surekha (2011) studied measure of slope rotatability for second order response surface designs using central composite designs (CCD).

Many authors have studied rotatable designs and slope rotatable designs assuming errors to be uncorrelated and homoscedastic. However, it is not uncommon to come across practical situations when the errors are correlated, violating the usual assumptions. Das (1997, 2003a) introduced and studied robust second order rotatable designs. Das (2003b) introduced slope rotatability with correlated errors and gave conditions for the different variance-covariance error structures. To access the degree of slope rotatability for correlated errors a new measure for second order response surface designs was introduced by Das and Park (2009). Rajyalakshmi and Victorbabu (2014, 15, 18, 19) studied SOSRD under tri-diagonal structure of errors using CCD, pairwise balanced designs, symmetrical unequal block arrangements (SUBA) with two unequal block sizes and BIBD respectively. Sulochana and Victorbabu (2020a, 2020b) studied SOSRD under tri-diagonal correlated structure of errors using a pair of SUBA with two unequal block sizes and a pair of BIBD respectively. Sulochana and Victorbabu (2020c, 2021a, 21b, 21c) studied measure of slope rotatability for second order response surface designs under intra-class correlated structure of errors using PBD,CCD, BIBD and SUBA with two unequal block sizes respectively.

In this paper, following the works of Park and Kim (1992), Das (2003a, 2003b, 2014), Das and Park (2009), Surekha and Victorbabu (2011), Rajyalakshmi and Victorbabu (2014), the measure of slope-rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD for $\rho(0.9 \le \rho \le 0.9)$ for $2 \le v \le 8$ (v number of factors) is suggested.

2 Preliminaries

2.1 Tri-diagonal correlation structure

The tri-diagonal structure of errors arises when the variance is same (σ^2) and the correlation between any two errors having lag n is ρ , and 0 (zero) otherwise. The tri-diagonal error structure with 2n observations is given below. (cf. Das (2014) p.30).

$$W = \left\{ D(e) = \sigma^2 \left[\begin{bmatrix} I_n & I_n \\ I_n & I_n \end{bmatrix} \times \frac{1+\rho}{2} + \begin{bmatrix} I_n & -I_n \\ -I_n & I_n \end{bmatrix} \times \frac{1-\rho}{2} \right] = W_{2n \times 2n}(\rho), \text{say} \right\}$$

$$W_{2n\times 2n}^{-1}(\rho) = \left(\sigma^2\right)^{-1} \left[\begin{bmatrix} I_n & I_n \\ I_n & I_n \end{bmatrix} \times \frac{1}{2(1+\rho)} + \begin{bmatrix} I_n & -I_n \\ -I_n & I_n \end{bmatrix} \times \frac{1}{2(1+\rho)} \right]$$

2.2 Conditions of slope rotatability for second order response surface designs with tridiagonal correlation error structure (Das 2003a, 2003b, 2014)

A second order response surface design $D = (X_{ui})$ for fitting,

$$Y_u(X) = b_0 + \sum_{i=1}^{v} b_i X_{ui} + \sum_{i=1}^{v} b_{ii} X_{ui}^2 + \sum_{i \le j=1}^{n} b_{ij} X_{ui} X_{uj} + e_u; \ 1 \le u \le 2n$$
(2.1)

where X_{ui} denotes the level the ith factor (i = 1, 2, ..., v) in the u^{th} run (u = 1, 2, ..., 2n) of the experiment, e_u 's are correlated random errors, is said to be a SOSRD under tri-diagonal correlated structure of errors, if the variance of the estimate of first order partial derivative of $Y_u(X_{u1}, X_{u2}, X_{u3} ..., X_{uv})$ with respect to each independent variable (X_i) is only a function of the distance $(d^2 = \sum_{i=1}^{v} X_i^2)$ of the point $(X_{u1}, X_{u2}, X_{u3} ..., X_{uv})$ from the origin (center of the design). i.e., $V\left(\frac{\partial \hat{Y}_u}{\partial X_i}\right) = h(d^2)$. Such a spherical variance function $h(d^2)$ for estimation of slopes in the second order response surface is achieved if the design points satisfy the following conditions (see, Das 2003a, 2003b and 2014, Rajyalakshmi and Victorbabu 2014, 2015, 2018, 2019).

Following Box and Hunter (1957), Hader and Park (1978), Victorbabu and Narasimham (1991a), Das (2003a, 2003b and 2014), Rajyalakshmi and Victorbabu (2014, 2015, 2018, 2019) the general conditions for second order slope rotatability under the tri-diagonal correlated structure of errors can be obtained as follows. To simplify the fit of the second order polynomial from design points D through the method of least squares, we impose the following simple symmetry conditions on Dto facilitate easy solutions of the normal equations. (cf. Das, 2014, p. 67, 112-114).

$$\begin{aligned} &(I) \\ &(i) \sum_{u=1}^{2} nX_{uj} = 0; \ 1 \le j \le v, \\ &(ii) \sum_{u=1}^{2} nX_{uj}X_{ui} = 0; \ 1 \le j < 1 \le v, \\ &(iii) \sum_{u=1}^{2} nX_{ui}X_{uj} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}X_{uj} + \sum_{u=1}^{n} X_{ui}X_{(n+u)j} \right\} = 0, \ 1 \le i \ne j \le v, \\ &(iv) \sum_{u=1}^{2} nX_{ui}^{2}X_{uj} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}^{2}X_{uj} + \sum_{u=1}^{n} X_{ui}^{2}X_{(n+u)j} \right\} = 0, \ 1 \le i \ne j \le v, \\ &(v) \sum_{u=1}^{2n} X_{ui}X_{uj}X_{ul} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}X_{(n+u)j}X_{ul} + \sum_{u=1}^{n} X_{ui}X_{uj}X_{(n+u)l} \right\} = 0, \\ &(v) \sum_{u=1}^{2n} X_{ui}^{2}X_{uj}X_{ul} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}^{2}X_{(n+u)j}X_{ul} + \sum_{u=1}^{n} X_{ui}^{2}X_{uj}X_{(n+u)l} \right\} = 0, \\ &(vi) \sum_{u=1}^{2n} X_{ui}^{2}X_{uj}X_{ul} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}^{2}X_{(n+u)j}X_{ul} + \sum_{u=1}^{n} X_{ui}^{2}X_{uj}X_{(n+u)l} \right\} = 0, \\ &(vi) \sum_{u=1}^{2n} X_{ui}X_{uj}X_{ul} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}X_{(n+u)j}X_{ul} + \sum_{u=1}^{n} X_{ui}X_{uj}X_{(n+u)l}X_{(n+u)l} \right\} = 0, \\ &(vii) \sum_{u=1}^{2n} X_{ui}X_{uj}X_{ul}X_{ul} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}X_{(n+u)j}X_{ul}X_{ul} + \sum_{u=1}^{n} X_{ui}X_{uj}X_{(n+u)l}X_{(n+u)l} \right\} \\ &(vii) \sum_{u=1}^{2n} X_{ui}X_{uj}X_{ul}X_{ul} - \rho \left\{ \sum_{u=1}^{n} X_{(n+u)i}X_{(n+u)j}X_{ul}X_{ul} + \sum_{u=1}^{n} X_{ui}X_{uj}X_{u}X_{(n+u)l}X_{(n+u)l} \right\} \\ &(z < l < j \le v, 1 < t \le v; (i, j) \ne (1, t) \ne j \le v, 1 \le l \le v, \end{aligned}$$

$$\sum_{u=1}^{2n} X_{ui}^2 = \text{a constant} = 2n\lambda_2, \text{ for all } i, \qquad (2.5)$$

$$\sum_{u=1}^{2n} X_{ui}^4 = \text{constant} = c2n\lambda_2, \text{ for all } i, \qquad (2.6)$$

$$\sum_{u=1}^{2n} X_{ui}^2 X_{uj}^2 = \text{constant} = 2n\lambda_4, \text{ for all values } i \neq j$$
(2.7)

$$\sum_{u=1}^{2} nX_{ui}^{4} = c \sum_{u=1}^{2} nX_{ui}^{2}X_{uj}^{2}$$
(2.8)

Using (2.3), (2.4) and (2.5) the design parameters of the tri-diagonal correlated structure are as follows:

 $\begin{aligned} (II) \\ (i)(1-\rho)\left\{\sigma^{2}(1-\rho^{2})\right\}^{-1} \sum_{u=1}^{2n} X_{ui}^{2} &= \frac{2n\lambda_{2}(1-\rho)}{\sigma^{2}(1-\rho^{2})} (>0), 1 \leq j \leq v, \\ (ii)\left\{\sigma^{2}(1-\rho^{2})\right\}^{-1} \left[\sum_{u=1}^{2n} X_{ui}^{2} - 2\rho \sum_{u=1}^{n} X_{ui} X_{(n+u)i}\right] &= \frac{2n\lambda_{2}}{\sigma^{2}(1-\rho^{2})} (>0), 1 \leq i \leq v, \\ (iii)\left\{\sigma^{2}(1-\rho^{2})\right\}^{-1} \left[\sum_{u=1}^{2n} X_{ui}^{4} - 2\rho \sum_{u=1}^{n} X_{ui}^{2} X_{(n+u)i}^{2}\right] &= c \left[\frac{2n\lambda_{4}}{\sigma^{2}(1-\rho^{2})}\right] (>0), 1 \leq i \leq v, \\ (iv)\left\{\sigma^{2}(1-\rho^{2})\right\}^{-1} \left[\sum_{u=1}^{2n} X_{ui}^{2} X_{uj}^{2} - \rho \left[\sum_{u=1}^{n} X_{(n+u)i}^{2} X_{uj}^{2} - \sum_{u=1}^{n} X_{ui}^{2} X_{(n+u)j}^{2}\right]\right] &= \\ \left[\frac{2n\lambda_{4}}{\sigma^{2}(1-\rho^{2})}\right] (>0), 1 \leq i \neq j \leq v, \\ (v)\left\{\sigma^{2}(1-\rho^{2})\right\}^{-1} \left[\sum_{u=1}^{2n} X_{ui}^{2} X_{uj}^{2} - 2\rho \left[\sum_{u=1}^{n} X_{ui} X_{uj} X_{(n+u)i} X_{(n+u)j}\right]\right] &= \\ \left[\frac{2n\lambda_{4}}{\sigma^{2}(1-\rho^{2})}\right] (>0), 1 \leq i \neq j \leq v, \end{aligned}$

From (II) of (iii), (iv) and (v)

$$\left\{ \sigma^{2}(1-\rho^{2}) \right\}^{-1} \qquad \left[\sum_{u=1}^{2n} X_{ui}^{4} - 1\rho \sum_{u=1}^{n} X_{ui}^{2} X_{(n+u)i}^{2} \right] = 2 \left(\left\{ \sigma^{2}(1-\rho^{2}) \right\}^{-1} \right) \\ \left[\sum_{u=1}^{2n} X_{ui}^{2} X_{uj}^{2} - 2\rho \left[\sum_{u=1}^{n} X_{ui} X_{uj} X_{(n+u)i} X_{(n+u)j} \right] \right] \\ + \left\{ \sigma^{2}(1-\rho^{2}) \right\}^{-1} \\ \left[\sum_{u=1}^{2n} X_{ui}^{2} X_{uj}^{2} - \rho \left[\sum_{u=1}^{n} X_{(n+u)i}^{2} X_{uj}^{2} - \sum_{u=1}^{n} X_{ui}^{2} X_{(n+u)j}^{2} \right] \right]$$

which implies to

$$c\left(\frac{2n\lambda_4}{\sigma^2(1-\rho^2)}\right) = \eta \left[2\left(\frac{2n\lambda_4}{\sigma^2(1-\rho^2)}\right) + \left(\frac{2n\lambda_4}{\sigma^2(1-\rho^2)}\right)\right]$$

where $c = 3\eta$, n = 2n, η , λ_2 and λ_4 are constants. The summation is over the designs points, and ρ is the correlation coefficient.

The variance and covariances of the estimated parameters under the tri-diagonal

correlated structure of errors are as follows:

$$V\left(\hat{b}_{0}\right) = \frac{\sigma^{2}\lambda_{4}(c+v-1)(1+\rho)}{2n\Delta}$$

$$(2.9)$$

$$V\left(\hat{b}_{i}\right) = \frac{\sigma^{2}(1-\rho^{2})}{2n\lambda_{2}}$$

$$(2.10)$$

$$V\left(\hat{b}_{ij}\right) = \frac{\sigma^2(1-\rho^2)}{2n\lambda_4} \tag{2.11}$$

$$V(\hat{b}_{ii}) = \frac{\sigma^2(1-\rho^2) \left[\lambda_4(c+v-2) - (v-1)\lambda_2^2(1-\rho)\right]}{(c-1)(2n)\lambda_4\Delta}$$
(2.12)

$$Cov\left(\hat{b}_{0},\hat{b}_{ii}\right) = -\frac{\sigma^{2}\lambda_{2}^{2}(1-\rho^{2})}{2n\Delta}$$

$$(2.13)$$

$$Cov\left(\hat{b}_{ii}, \hat{b}_{ij}\right) = \frac{\sigma^2 (1-\rho^2) \left[\lambda_2^2 (1-\rho) - \lambda_4\right]}{(c-1)(2n)\lambda_4 \Delta}$$
(2.14)

where $\Delta = [\lambda_4(c+v-1) - v\lambda_2^2(1-\rho)]$ and the other covariances are zero.

An inspection of the variance of \hat{b}_0 shows that a necessary condition for the existence of a nonsingular second order slope rotatable design with tri-diagonal correlated structure is

$$\left[\lambda_4(c+v-1) - v\lambda_2^2(1-\rho)\right] > 0$$
(2.15)

$$\frac{\lambda_4}{\lambda_2^2} > \frac{v(1-\rho)}{c+v-1} \qquad (\text{non-singularity condition}) \qquad (2.16)$$

If the non-singularity condition (2.14) exists, then only the design exists. For the second model

$$\frac{\partial \hat{Y}_{u}}{\partial X_{i}} = \hat{b}_{i} + 2\hat{b}_{ii}X_{i} + \sum_{i=j\neq i}^{v} \hat{b}_{ij}X_{j},$$

$$V\left(\frac{\partial \hat{Y}_{u}}{\partial X_{i}}\right) = V\left(\hat{b}_{i}\right) + 4X_{i}^{2}V\left(\hat{b}_{ii}\right) + \sum_{i=j\neq i}^{v} X_{j}^{2}V\left(\hat{b}_{ij}\right)$$
(2.17)

The condition for right hand side of equation (2.15) to be a function of $(d^2 = \sum_{i=1}^{v} X_i^2)$ alone (for slope rotatability) is clearly,

$$V\left(\hat{b}_{ii}\right) = \frac{1}{4}V\left(\hat{b}_{ii}\right) \tag{2.18}$$

Equation (2.16) leads to condition,

$$\frac{cN\lambda_4}{(1-\rho^2)(1+\rho)} \left[4N - (c+v-2)N + v\left(\frac{N\lambda_2^2(1-\rho)}{\lambda_4}\right) \right] + \frac{N^2\lambda_4}{(1-\rho^2)(1+\rho)} [5v-9] - N^2\lambda_2^2 \left[\frac{5v-4}{(1+\rho)^2}\right] = 0$$

$$(2.19)$$

where N = 2n. Simplifying (2.17) gives rise,

$$\lambda_4[v(5-c) - (c-3)^2] + \lambda_2^2[v(c-5) + 4](1-\rho) = 0$$
(2.20)

For $\rho = 0$, equation (2.18) reduces to

$$\lambda_4[v(5-c) - (c-3)^2] + \lambda_2^2[v(c-5) + 4] = 0$$
(2.21)

Equation (2.19) is similar to the SOSRD condition of Victorbabu and Narasimham (1991a).

Therefore, equations (2.2) to (2.12), (2.14) to (2.18) give a set of conditions for SOSRD under tri-diagonal correlated structure of errors for any general second order response surface design.

On simplification of (2.15) using (2.7) to (2.12) and (2.16), we have,

$$V\left(\frac{\partial \hat{Y}_{u}}{\partial X_{i}}\right) = V(\hat{b}_{i}) + 4X_{i}^{2}\frac{V\left(\hat{b}_{ij}\right)}{4} + \sum_{i=1, j \neq i}^{v}X_{j}^{2}V\left(\hat{b}_{ij}\right)$$
$$V\left(\frac{\partial \hat{Y}_{u}}{\partial X_{i}}\right) = V(\hat{b}_{i}) + \sum_{i=1}^{v}X_{i}^{2}V\left(\hat{b}_{ij}\right)$$
$$V\left(\frac{\partial \hat{Y}_{u}}{\partial X_{i}}\right) = V(\hat{b}_{i})V\left(\hat{b}_{ij}\right)d^{2}$$

where $d^2 = \sum_{i=1}^{v} X_i^2$ and $V(\hat{b}_i)$, $V(\hat{b}_ij)$ are stated in (2.8) and (2.9). Further, we have

$$V\left(\frac{\partial \hat{Y}_u}{\partial X_i}\right) = \frac{1-\rho^2}{N} \left(\frac{1}{\lambda_2} + \frac{d^2}{\lambda_4}\right) \sigma^2$$
(2.22)

where N = 2n.

2.3 Slope rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD (Rajyalakshmi and Victorbabu (2014))

Following the works of Hader and Park (1978), Victorbabu and Narasimham (1991), Das (2003a, 03b, 2014), Rajyalakshmi and Victorbabu (2014), the method construction of slope rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD is given below. Central composite designs are obtained by adding suitable factorial combinations $(\pm 1, \pm 1, \ldots, \pm 1)$ to those obtained from $2^{t(v)}$ fractional (or a suitable fractional replicate of 2^v in which no interaction less than five factors is confounded). The 2v additional fractional combinations in CCD are $(\pm \alpha, 0, \ldots, 0)$, $(0, \pm \alpha, 0, \ldots, 0)$, $\ldots (0, 0, \ldots, \pm \alpha)$ and n_0 central points $(0, 0, \ldots, 0)$ if necessary. The total number of factorial combinations in the design can be written as N = F + T. Here F is total number of factorial number of factorial points. i.e., $F = 2^{t(v)}$ and $T = 2v + n_0$.

Here we consider a slope rotatable central composite designs of Hader and Park (1978) having n'(n = F + 2v) non-central design points involving v-factors. The set of n' - non central design points are extended to 2n design points by adding $n'(n_0 = n)$ central points just below or above the n' non-central design points. Hence 2n(= N) be the total number of design points of the slope rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD.

Result (2.1): The design points $(\pm 1, \pm 1, \dots, \pm 1)F \cup (\pm \alpha, \dots, 0)2^1 \cup n_0$ will give a *v*-dimensional SOSRD with tri-diagonal correlation error structure using CCD in design points N = F + T, where α^2 is positive real root of the fourth degree polynomial equation,

$$[(8v(1-\rho)-4N)]\alpha^{8} + [8Fv(1-\rho)]\alpha^{6} + [(2F(4-v)N+2F^{2}v(1-\rho)+16F(1-v))]\alpha^{4} + [(16F^{2}(1-v)(1-\rho))]\alpha^{2} + [(4F^{2}(v-1)N+4F^{3}(1-v)(1-\rho))] = 0$$

Note: Values of SOSRD under tri-diagonal correlation error structure using CCD can be obtained by solving the above equation.

3 Measure of second order slope rotatability for correlated structure of errors (Das and Park, 2009))

Following Das and Park (2009), equations (2.2) to (2.18) give necessary and sufficient conditions for a measure for any second order response surface designs with

correlated errors. Further we have,

 $V(b_i) \text{ equal for all } i,$ $V(b_{ii}) \text{ equal for all } i$ $V(b_{ij}) \text{ equal for all } i, j; \text{ where } i \neq j$ $Cov(b_i, b_{ii}) = Cov(b_i, b_{ij}) = Cov(b_{ii}, b_{ij}) = Cov(b_{ij}, b_{il}) = 0 \text{ for all } i \neq j \neq l \text{ and for all } \rho$ (3.1)

Das and Park (2009) proposed that, if the conditions in (2.2) to (2.18) and (3.1) are met, $M_v(D)$ is the proposed measure of slope rotatability for second order response surface designs for any correlated error structure.

$$M_v(D) = \frac{1}{1 + Q_v(D)}$$

where
$$2(v-1)\sigma^4 Q_v(D) = (v+2)(v+4) \sum_{i=1}^v \left[(V(b_i) - \bar{V}) + \frac{a_i - \bar{a}}{v+2} \right]^2$$

 $+ \frac{4}{v(v+2)} \sum_{i=1}^v (a_i - \bar{a})^2 + 2 \sum_{i=1}^v \left[\left(4V(b_{ii}) \frac{a_i}{v} \right)^2 + \sum_{i=1 \neq j}^v \left(V(b_{ij}) \frac{a_i}{v} \right)^2 \right]$
 $4(v+4) \left[4Cov(b_i, b_{ii})^2 + \sum_{j=1; j \neq i}^v Cov(b_i, b_{ij})^2 \right]$
 $4 \sum_{l=1}^v \left(4 \sum_{j=1; j \neq i}^v Cov(b_{ii}, b_{ij})^2 \right) + \sum_{j < l} \sum_{l \neq i}^v Cov(b_{ij}, b_{lj})^2$ (3.2)
Here $\bar{V} = \frac{1}{v} \sum_{i=1}^v V(b_i), \ a_i = 4V(b_{ii}) + \sum_{j=1; j \neq i}^v V(b_{ij})(1 \le i \le v) \ \text{and} \ \bar{a} =$

Here $V = \frac{1}{v} \sum_{i=1}^{v} V(b_i)$, $a_i = 4V(b_{ii}) + \sum_{j=1; j \neq i}^{v} V(b_{ij}) (1 \le i \le v)$ and $\bar{a} = \frac{1}{v} \sum_{i=1}^{v} a_i$.

It can be easily shown that $Q_v(D)$ in equation (3.2) becomes zero for all values n, if and only if the conditions in equations (3.1) hold. Further, it is simplified to

$$Q_v(D) = \frac{1}{\sigma^4} \left[4V(b_{ii}) - V(b_{ij}) \right]^2.$$
(3.3)

Note that $0 \leq M_v(D) \leq 1$, and it can be easily shown that $M_v(D)$ is one if and only if the design is slope rotatable with any correlated error structure for all values of ρ , and $M_v(D)$ approaches to zero as the design 'D' deviates from the slope-rotatability under specified correlated error structure.

4 Measure of slope rotatability for second order response surface designs with tri-diagonal correlation error structure using central composite designs

Following Park and Kim (1992), Das and Park (2009), Surekha and Victorbabu (2011), Rajyalakshmi and Victorbabu (2014) the proposed measure of slope-rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD is given below.

This well-known type of design consists of $2^{t(v)}$ factorial points $(\pm 1, \pm 1, \ldots, \pm 1)$, 2v axial points of the form $(\pm \alpha, 0, \ldots, 0)$ and a center point $(0, 0, \ldots, 0)$ may be replicated n_0 times if necessary. The total number of factorial combinations in the design can be written as N = F + T. Here F is total number of fractional points. i.e., $F = 2^{t(v)}$ and $T = 2v + n_0$.

Here we consider a slope rotatable central composite designs of Hader and Park (1978) having n(n = F + 2v) non-central design points involving v-factors. The set of n- non central design points are extended to 2n design points by adding $n(n_0 = n)$ central points just below or above the n non-central design points. Hence 2n(= N) be the total number of design points of the slope rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD.

The design points $(\pm 1, \pm 1, ..., \pm 1)F \cup (\pm \alpha, ..., 0)2^1 \cup n_0$, will give measure of slope rotatability for second order response surface designs withtri-diagonal correlation error structure using CCD. Here we have (2.2) are true. Further, from (2.3), (2.4), and (2.5), we have,

$$(I)\sum_{u=1}^{2n} X_{ui}^{2} = F + 2\alpha^{2} = 2n\lambda_{2}$$
$$(II)\sum_{u=1}^{2n} X_{ui}^{4} = F + 2\alpha^{4} = c2n\lambda_{4}$$
$$(III)\sum_{u=1}^{2n} X_{ui}^{2}X_{uj}^{2} = F = 2n\lambda_{4}$$
(4.1)

Measure of slope rotatability of second order response surface designs with tridiagonal correlation error structure using CCD can be obtained by

$$M_{v}(D) = \frac{1}{1 + Q_{v}(D)}$$

$$1 + Q_{v}(D) = \frac{1}{\sigma^{4}} [4V(b_{ii}) - V(b_{jj})]^{2}$$

$$= \frac{1}{\sigma^{4}} [4G - \frac{(1 - \rho^{2})\sigma^{2}}{F}]^{2}$$
(4.2)

where $G = V(b_{ii}) = (1 - \rho^2)\sigma^2 \left[\frac{(v-1)FT - F(v-1)\rho - 4(v-1)F\alpha^2 + 2[N-2(v-1)]\alpha^4}{2\alpha^4 [vFT - Fv\rho - 4vF\alpha^2 + 2[N-2v]\alpha^4]} \right]$

If $M_v(D)$ is one if and only if the design 'D ' is slope rotatable withtri-diagonal correlationerror structure using CCD for all values of ρ and $M_v(D)$ approaches to zero as the design 'D 'deviates from the slope-rotatability withtri-diagonal correlation error structure using CCD.

Example:We illustrate the measure of slope-rotatability for second order response surface designs withtri-diagonal correlated structure of errors with the help of CCD for v=2 factors.

The design points $(\pm 1, \pm 1, \pm 1)2^2 \cup (\pm \alpha, ..., 0)2^1 \cup n_0$, will give slope rotatability for second order response surface designs withtri-diagonal correlation error structure in N = 16 design points for 2 factors. From equations in (4.1), we have

$$(I) \sum X_{ui}^{2} = 4 + 2\alpha^{2} = N\lambda_{2}$$

$$(II) \sum X_{ui}^{4} = 4 + 2\alpha^{4} = cN\lambda_{4}$$

$$(III) \sum X_{ui}^{2}X_{uj}^{2} = 4 = N\lambda_{4}$$
(4.3)

From (I), (II) and (III) of (4.3), we get $\lambda_2 = \frac{4+2\alpha^2}{16}$, $\lambda_4 = \frac{4}{16}$ and $c = \frac{4+2\alpha^4}{4}$ and Substituting λ_2, λ_4 and c in (3.5) and on simplification, we get the following biquadratic equation in α^2 .

$$[16(1-\rho)-64]a^8+64(1-\rho)a^6+[256]a^4-256(1-\rho)a^2+[1024-256(1-\rho)]=0 \quad (4.4)$$

Equation (4.4) has only one positive real root for each value of ρ . This can be alternatively written directly from result (2.1). Solving (4.4), we get $\alpha = 1.7254$. From (4.2) we get $Q_v(D) = 0$, $M_v(D) = 1$ for value of $\rho = 0.1$.

Suppose if we take $\alpha = 1.3$ instead of taking $\alpha = 1.7254$ for 2 factors we get $Q_v(D) = 0.1519$ then $M_v(D) = 0.8790(taking\rho = 0.1)$. Here $M_v(D)$ deviates from slope rotatability for second order response surface designs withtri-diagonal correlation error structure.

4.1 Weak slope rotatability region for correlated errors(cf. Das and Park (2009)

Following Das and Park (2009), we also find weak slope rotatability region (WSRR) for second order response surface designs with tri-diagonal correlation error structure using CCD.

$M_v(D) \ge k$

 $M_v(D)$ involves the correlation parameter $\rho \epsilon W$ and as such, $M_v(D) \ge k$ for all ρ is too strong to be met. On the other hand, for a given v, we can find range of values of ρ for which Das and Park (2009) call this range as the weak slope rotatability region $(WSRR(R_{D(k)}(\rho)))$ of the design 'D'. Naturally, the desirability of using 'D' will rest on the wide nature of $(WSRR(R_{D(k)}(\rho)))$ along with its strength k. Generally, we would require 'v' to be very high say, around 0.95 (cf. Das and Park (2009)).

Table 1 and 2, gives the values of $M_v(D)$ and weak slope rotatability region $(WSRR(R_{D(k)}(\rho)))$ for second order slope rotatable designs with tri-diagonal correlationerror structure using CCD for $\rho(-0.9 \le \rho \le 0.9)$ and $2 \le v \le 8$ (v number of factors) respectively.

Table 1: Measure of slope rotatability for second order response surface designs $(M_V(D))$ with tri-diagonal correlation error structure using CCD $\rho(-0.9 \le \rho \le 0.9)$ and for $2 \le v \le 4$

v = 2, n=8, 2n=N=16									
ρ	α								
	1	1.3	1.6	1.9	2.2	2.5	2.8	3.1	α^*
-0.9	0.7596	0.9009	0.9617	0.9964	0.9995	0.9963	0.9935	0.9917	2.1756
-0.8	0.6353	0.8578	0.9559	0.9974	0.9982	0.9919	0.9872	0.9841	2.105
-0.7	0.5614	0.8385	0.9593	0.9989	0.996	0.9875	0.9812	0.9771	2.0411
-0.6	0.5141	0.8313	0.9652	0.9998	0.9934	0.9831	0.9757	0.971	1.9836
-0.5	0.4831	0.8308	0.9713	0.9999	0.9907	0.9789	0.9708	0.9657	1.9321
-0.4	0.4628	0.8344	0.9769	0.9999	0.9879	0.9753	0.9667	0.9613	1.8863
-0.3	0.4503	0.8406	0.9819	0.9989	0.9853	0.9721	0.9633	0.9577	1.8457
-0.2	0.4439	0.8486	0.9859	0.9979	0.9831	0.9696	0.9607	0.9551	1.8097
-0.1	0.4428	0.8579	0.9894	0.9969	0.9812	0.9677	0.9589	0.9533	1.7781
0	0.4464	0.8681	0.9921	0.9959	0.9798	0.9666	0.9579	0.9525	1.7501
0.1	0.4546	0.8791	0.9942	0.9949	0.9789	0.9661	0.9579	0.9527	1.7254
0.2	0.4676	0.8906	0.9959	0.9942	0.9785	0.9665	0.9587	0.9538	1.7036
0.3	0.4861	0.9027	0.9972	0.9937	0.9788	0.9676	0.9604	0.9558	1.6843
0.4	0.5109	0.9153	0.9982	0.9934	0.9797	0.9695	0.9629	0.9589	1.6671
0.5	0.5438	0.9283	0.9989	0.9935	0.9813	0.9723	0.9666	0.9629	1.6517
0.6	0.5869	0.9417	0.9993	0.9939	0.9835	0.9759	0.9711	0.9681	1.6379
0.7	0.6446	0.9556	0.9997	0.9948	0.9865	0.9805	0.9766	0.9743	1.6255
0.8	0.7229	0.9699	0.9999	0.9961	0.9902	0.986	0.9833	0.9816	1.6143
0.9	0.8339	0.9847	0.9999	0.9978	0.9947	0.9925	0.9911	0.9902	1.6042

v = 3, n=14, 2n=N=28									
ρ	α								
	1	1.3	1.6	1.9	2.2	2.5	2.8	3.1	α^*
-0.9	0.7529	0.9595	0.9904	0.9976	0.9999	0.9998	0.9991	0.9985	2.4616
-0.8	0.6175	0.928	0.9843	0.997	0.9999	0.9994	0.9981	0.9969	2.3772
-0.7	0.5335	0.9035	0.9804	0.9969	0.9999	0.9988	0.997	0.9955	2.3028
-0.6	0.4776	0.8845	0.9779	0.9972	0.9999	0.9982	0.9959	0.9942	2.2386
-0.5	0.4391	0.8699	0.9766	0.9976	0.9999	0.9976	0.9951	0.9931	2.1843
-0.4	0.4122	0.8593	0.9759	0.9979	0.9997	0.9971	0.9942	0.9921	2.139
-0.3	0.3937	0.8519	0.9758	0.9983	0.9995	0.9965	0.9935	0.9913	2.1015
-0.2	0.3816	0.8474	0.9763	0.9986	0.9993	0.9961	0.9929	0.9907	2.0703
-0.1	0.3751	0.8456	0.9769	0.9989	0.9991	0.9957	0.9926	0.9903	2.0444
0	0.3733	0.8464	0.978	0.9991	0.9989	0.9955	0.9923	0.99	2.0226
0.1	0.3763	0.8496	0.9793	0.9993	0.9988	0.9953	0.9922	0.99	2.0226
0.2	0.3841	0.8552	0.9809	0.9995	0.9987	0.9953	0.9924	0.9902	1.9884
0.3	0.3975	0.8632	0.9826	0.9996	0.9987	0.9954	0.9926	0.9907	1.9749
0.4	0.4173	0.8738	0.9846	0.9997	0.9987	0.9956	0.9931	0.9913	1.9632
0.5	0.4457	0.8869	0.9867	0.9998	0.9987	0.9959	0.9938	0.9922	1.9529
0.6	0.4857	0.9028	0.989	0.9999	0.9988	0.9965	0.9946	0.9933	1.9438
0.7	0.5428	0.9217	0.9915	0.9999	0.999	0.9972	0.9957	0.9946	1.9358
0.8	0.6276	0.9439	0.9942	0.9999	0.9993	0.9979	0.9969	0.9962	1.9287
0.9	0.7619	0.9699	0.997	0.9999	0.9996	0.9989	0.9983	0.9979	1.9222

Table 1 continued

v = 4, n=24, 2n=N=48									
ρ	α								
	1	1.3	1.6	1.9	2.2	2.5	2.8	3.1	α^*
-0.9	0.7101	0.9555	0.9922	0.9984	0.9997	0.9999	0.9999	0.9998	2.7796
-0.8	0.5639	0.9191	0.9856	0.9971	0.9996	0.9999	0.9999	0.9996	2.6911
-0.7	0.4773	0.8895	0.98	0.9962	0.9995	0.9999	0.9998	0.9994	2.616
-0.6	0.4213	0.8655	0.9754	0.9955	0.9995	0.9999	0.9997	0.9992	2.5547
-0.5	0.3833	0.8463	0.9717	0.9949	0.9995	0.9999	0.9996	0.9989	2.5057
-0.4	0.3569	0.8314	0.9688	0.9946	0.9995	0.9999	0.9995	0.9988	2.4668
-0.3	0.3389	0.8203	0.9667	0.9944	0.9995	0.9999	0.9994	0.9987	2.4358
-0.2	0.3271	0.8127	0.9653	0.9943	0.9995	0.9999	0.9993	0.9986	2.4109
-0.1	0.3205	0.8084	0.9647	0.9943	0.9996	0.9999	0.9992	0.9985	2.3906
0	0.3184	0.8072	0.9647	0.9944	0.9996	0.9999	0.9992	0.9984	2.3738
0.1	0.3207	0.8091	0.9653	0.9947	0.9997	0.9999	0.9992	0.9984	2.3598
0.2	0.3275	0.8142	0.9666	0.9949	0.9997	0.9999	0.9992	0.9985	2.3479
0.3	0.3395	0.8224	0.9685	0.9953	0.9997	0.9999	0.9992	0.9985	2.3378
0.4	0.3577	0.8341	0.9711	0.9958	0.9998	0.9999	0.9992	0.9986	2.329
0.5	0.3842	0.8495	0.9743	0.9963	0.9999	0.9999	0.9993	0.9987	2.3214
0.6	0.4225	0.8689	0.9781	0.9969	0.9999	0.9999	0.9994	0.9989	2.3147
0.7	0.4787	0.8928	0.9826	0.9976	0.9999	0.9999	0.9995	0.9991	2.3087
0.8	0.5655	0.922	0.9877	0.9983	0.9999	0.9999	0.9996	0.9994	2.3034
0.9	0.7115	0.9573	0.9935	0.9991	0.9999	0.9999	0.9998	0.9997	2.2987

Table 1 continued

Table 2: Values of WSRRs $R_{D(0.95)}(\rho)$ for slope rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD for $\rho(-0.9 \le \rho \le 0.9)$ and fo $2 \le v \le 8$

v	α									
	1	1.3	1.6	1.9	2.2	2.5	2.8	3.1		
2	-	0.7-0.9	0.7-0.9	-1.8	-1.8	-1.8	-1.8	-1.8		
3	-	-	-1.8	-1.8	-1.8	-1.8	-1.8	-1.8		
4	-	-0.9, 0.9	-1.8	-1.8	-1.8	-1.8	-1.8	-1.8		
5	-	-	-1.8	-1.8	-1.8	-1.8	-1.8	-1.8		
6	-	-	-1.8	-1.8	-1.8	-1.8	-1.8	-1.8		
7	-	-	-1.8	-1.8	-1.8	-1.8	-1.8	-1.8		
8	-	-	-1.8	-1.8	-1.8	-1.8	-1.8	-1.8		

Note 1: Here indicates that the values of slope rotatability for second order response surface designs with tri-diagonal correlation error structure using CCD. For each value of α^* , the $M_V(D)$ is equal to 1.

Note 2: Measure of slope rotatability for second order response surface designs $(M_V(D))$ with tri-diagonal correlation error structure using CCD $\rho(-0.9 \le \rho \le 0.9)$ and for $2 \le v \le 4$ are available at the authors.

5 Conclusion

In this paper, the measure of slope rotatability for second order response surface designs with tri-diagonal correlationerror structure using CCD is studied. The degree of slope rotatability of the given design can be calculated for different values of $\rho(-0.9 \le \rho \le 0.9)$ and for $2 \le v \le 8$ (v number of factors). By increasing α and ρ values for different factors (v) the measure of slope rotatability values for second order response surface design withtri-diagonal correlation error structure using CCD are increased.

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103

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