Slope Rotatability of Second Order Response Surface Regression Models with Correlated Errors[1]

Hyang Sook Jung[2] and Sung Hyun Park[3]

Abstract

In this paper a class of multifactor designs for estimating the slope of second order response surface regression models with correlated errors is considered. General conditions for second order slope rotatability over all directions and also with respect to the maximum directional variance in case of $k=2$ have been derived assuming errors have a general correlated error structure. And we consider the measures for evaluating slope rotatability with correlated errors similar to in case of uncorrelated error structures.

Key words: Response Surface Designs(RSM), Slope Estimation, Slope Rotatability with correlated errors.

1. Introduction

Most of literatures for RSM was given assuming the errors are uncorrelated and homoscedastic. Some authors have focused attention on the estimation of partial derivatives of the response function with respect to the independent variables. Atkinson(1970), Murly and Studden(1972), Otto and Mendenhall(1972), Myers and Lahoda(1975), Hader and Park(1978), Mukkerjee and Huda(1985), and others have considered problems associated with estimation of derivatives of response. In particular, Hader and Park(1978) suggested the concept of slope rotatability and studied slope rotatable central composite designs: the derivatives of the estimates with respect to each independent variables are equally good at the points equidistant from the design center, that is, a design is slope rotatable if the variances of partial derivatives are only a function of ρ, the distance from the design center. It is called slope rotatability over axial directions by Park(1987), who also suggested another version of slope rotatability, slope rotatability over all directions, and examined the class of slope rotatable designs assuming errors in observations are uncorrelated and homoscedastic. However, it is not uncommon to come across practical situations when the errors are correlated, violating the usual assumptions. Panda and Das(1994) initiated a study of rotatable designs with correlated errors and attempted a systematic study of first order rotatable designs for various correlated structures of the errors. A study of slope rotatable designs with

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2) Dept of Statistics, Seoul National Univ., Seoul, 151-742, Korea

3) Professor, Dept of Statistics, Seoul National Univ., Seoul, 151-742, Korea

correlated errors was initiated by Das(2003a) and the conditions of second order slope rotatability over axial directions were derived. In this paper, we consider the problem in case of slope rotatability of second order response surface models with correlated errors. In section 2, the concept of slope rotatability over all directions has been extended in case of assuming the correlated errors and we obtain the measures for evaluating slope rotatability with correlated error structure. In section 3, in case correlated errors of the second order response surface models, the conditions of slope rotatability with equal maximum directional variances will be suggested. Summary is provided in section 4.

2. Slope rotatability over all directions with correlated errors

Suppose there are 'k' independent variables which yield a response of y_u on the response variable y when $x = x_u = (x_{1u}, x_{2u}, \cdots, x_{ku})'$, $1 \le u \le N$. Assuming that a second order response surface regression model is as follows:

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i \le j > 1} \sum^{k} \beta_{ij} x_{iu} x_{ju} + e_u, \quad 1 \le u \le N$$

or $y = X\beta + e$ where $X = (1 \colon Z)$ is the matrix of values of the elements of x's taken at the design points where $x_i = (x_{i1}, x_{i2}, \cdots, x_{iN})'$, $x_i \otimes_1 x_j = (x_{i1}x_{j1}, x_{i2}x_{j2}, \cdots, x_{iN}x_{jN})'$;$1 \le i, j \le k$, and $Z = (x_1 \otimes_1 x_1, x_2 \otimes_1 x_2, \cdots, x_k \otimes_1 x_k, x_1, x_2, \cdots, x_k, x_1 \otimes_1 x_2, x_1 \otimes_1 x_3, \cdots, x_{k-1} \otimes_1 x_k)$. Here $\otimes_1$ denotes the Hadamard product of two matrices of the same order and it is defined as follows. Let $L_1 = ((a_{ij}))$ and $L_2 = ((b_{ij}))$ with $p \times q$. The Hadamard product $L_1 \otimes_1 L_2$ is a matrix H, of order $p \times q$, where $H = ((a_{ij} b_{ij}))$. Further, e is the $N \times 1$ vector of errors which are assumed to be normally distributed with $E(e) = 0$ and $D(e) = V$ with rank(V)=N. The matrix V may represent any structure with correlated errors. The estimated response at a point x is given by $\hat{y}(x) = b_0 + \sum_{i=1}^{k} b_{ii} x_i^2 + \sum_{i=1}^{k} b_i x_i + \sum_{j=1}^{k} \sum_{j \ne i}^{k} b_{ij} x_i x_j$. Let

$g(x) = \left(\frac{\partial \hat{y}}{\partial x_1}, \frac{\partial \hat{y}}{\partial x_2}, \cdots, \frac{\partial \hat{y}}{\partial x_k} \right) = Db$ where D is the $k \times m$ matrix arising from the differentiation of $x_s' b$ with respect to each of the k independent variables. The estimated derivative at any point x in the direction specified by the $k \times 1$ vector of direction cosines $p' = (p_1, p_2, \cdots, p_k)$ is $p' g(x)$, where $\sum_{i=1}^{k} p_i^2 = 1$. Then the variance of this specified slope can be written as $V_p(x) = Var[p' g(x)] = \sigma^2 p' D (X' V^{-1} X)^{-1} D' p$. If we are interested in all possible directions of k with correlated error structures, we want to consider the average of $V_p(x)$ over all possible directions.

Theorem 2.1 The average of $V_p(x)$ over all possible directions with correlated error structure V is $\overline{V}(\boldsymbol{x})=\frac{1}{k}tr[D(X'V^{-1}X)^{-1}D']$.

Proof. Let $M=DVar(b)D'$. The average of $V_p(\boldsymbol{x})$ over all directions with correlated errors is $\overline{V}(\boldsymbol{x})=\underset{\boldsymbol{p}}{avg}(\boldsymbol{p}'M\boldsymbol{p})=tr[M\left(\underset{\boldsymbol{p}}{avg}(\boldsymbol{pp}')\right)]$ and $\underset{\boldsymbol{p}}{avg}(\boldsymbol{pp}')=\phi\int\boldsymbol{pp}'dA$ where dA is the area element of the hypersphere with unit radius, $U_\rho=\left\{(x_1,x_2,\cdots,x_k):\sum_{i=1}^{k}x_i^2=\rho^2\right\}$ and $\phi^{-1}=\int_{U_\rho}dA=2\pi^{k/2}/\Gamma\left(\frac{k}{2}\right)$. Let $\phi\int\boldsymbol{pp}'dA=\nu I_k$, then $\overline{V}(\boldsymbol{x})=tr(M\nu I_k)=\nu\sum_{i=1}^{k}\lambda_i$ where the λ_i's are eigenvalues of M in Park(1987). Then the average of $\boldsymbol{p}'M\boldsymbol{p}$ is 1 and $\lambda_i=1$ for all i. Therefore, $\nu=\frac{1}{k}$ and $\overline{V}(\boldsymbol{x})$ become $\overline{V}(\boldsymbol{x})=\frac{1}{k}tr(D(X'V^{-1}X)^{-1}D')$. □

From Theorem 2.1,

$$\begin{aligned}\overline{V}(\boldsymbol{x})=&\frac{1}{k}\sum_{i=1}^{k}Var(b_i)+\frac{2}{k}\sum_{i=1}^{k}x_i[2Cov(b_i,b_{ii})+\sum_{j=1,j\neq i}^{k}Cov(b_j,b_{ij})]\\&+\frac{2}{k}\sum_{i=1}^{k}\sum_{j=1,j\neq i}^{k}x_ix_j[2(Cov(b_{ii},b_{ij})+Cov(b_{jj},b_{ij}))+\sum_{s=1,s\neq i,j}^{k}Cov(b_{is},b_{js})]\\&+\frac{1}{k}\sum_{i=1}^{k}x_i^2[4Var(b_{ii})+\sum_{j=1,j\neq i}^{k}Var(b_{ij})]\end{aligned}$$

If $\overline{V}(\boldsymbol{x})$ is only a function of $\rho=\sqrt{\sum_{i=1}^{k}x_i^2}$ equidistant from the design center for all $\boldsymbol{x}$, we can call it the slope rotatable design over all directions with correlated errors.

Theorem 2.2 The necessary and sufficient conditions for a design to be slope rotatable over all directions with correlated errors are as follows :

1. $2Cov(b_i,b_{ii})+\sum_{j=1,j\neq i}^{k}Cov(b_j,b_{ij})=0$ for all i

2. $2(Cov(b_{ii},b_{ij})+Cov(b_{jj},b_{ij}))+\sum_{s=1,s\neq i,j}^{k}Cov(b_{is},b_{js})=0$ for any (i,j), when $i\neq j$

3. $4Var(b_{ii})+\sum_{j=1,j\neq i}^{k}Var(b_{ij})=\delta$, say, for all i, where constant. □

Now we consider the measures for evaluating slope rotatability with correlated errorsIn as an analog of a measure of slope rotatability over axial directions proposed by Park and Kim(1992) and Jang and Park(1993), in the k dimensional space $(k\geq 2)$, a point $\boldsymbol{x}'=(x_1,x_2,\cdots,x_k)$ can be expressed in terms of spherical coordinates as $(\rho,\psi_1,\cdots,\psi_{k-2},\theta)$, where $\rho\geq 0,\ 0\leq\psi_1\leq\pi,\cdots,\ 0\leq\psi_{k-2}\leq\pi,\ 0\leq\theta\leq 2\pi$ and $x_1=\rho\cos\psi_1, x_2=\rho\sin\psi_1\cos\psi_2,\cdots x_{k-1}=\rho\sin\psi_1\sin\psi_2\cdots\sin\psi_{k-2}\cos\theta, x_k=\rho\sin\psi_1\sin\psi_2\cdots\sin\psi_{k-2}\sin\theta$.

and (See Edwards (1973)). Let us denote it by $w_i(\rho,\psi_1,\cdots,\psi_{k-2},\theta) = Var(\frac{\partial \hat{y}(x)}{\partial x_i})$. This is then the variance of the first derivative of $\hat{y}(x)$ with respect to x_i, at a point whose spherical coordinate is $(\rho,\psi_1,\cdots,\psi_{k-2},\theta)$. Let us define the following quantities:

$$\overline{w_i}(\rho) = \frac{1}{I_k}\int_0^{2\pi}\int_0^{\pi}\cdots\int_0^{\pi} w_i(\rho,\psi_1\cdots,\psi_{k-2},\theta)\times \sin^{k-2}\psi_1\sin^{k-3}\psi_2\cdots\sin\psi_{k-2}d\psi_1\cdots d\psi_{k-2}d\theta,$$

$\phi^{-1} = I_k = \int_0^{2\pi}\int_0^{\pi}\cdots\int_o^{\pi}\sin^{k-2}\psi_1\sin^{k-3}\psi_2\cdots\sin\psi_{k-2}d\psi_1\cdots d\psi_{k-2}d\theta$ is found to be $2\pi^{k/2}/\Gamma(\frac{k}{2})$ and $\overline{w}(\rho) = \frac{1}{k}\sum_{i=1}^{k}\overline{w_i}(\rho)$. Here, $\Gamma(\alpha) = \int_0^{\infty} t^{\alpha-1}e^{-t}dt$ is the gamma function of $\alpha > 0$. Define

$$h(\rho) = \sum_{i=1}^{k}\int_0^{2\pi}\int_0^{\pi}\cdots\int_0^{\pi}[w_i(\rho,\psi_1,\cdots,\psi_{k-2},\theta) - \overline{w}(\rho)]^2\sin^{k-2}\psi_1\sin^{k-3}\psi_2\cdots\sin\psi_{k-2}d\psi_1\cdots d\psi_{k-2}d\theta.$$

Defining $Q_k(D) = \frac{1}{e_k}\int_0^1 \rho^{k-1}h(\rho)d\rho$ divided by e_k, an appropriate positive constant depending on k, $Q_k(D)$ is similar to the measure of slope rotatability proposed by Park and Kim(1992). It can be shown that $Q_k(D)$ is zero if and only if a design D is slope rotatable over axial directions. The spherical region moments are used in the development of model specific forms for the spherical average slope variance for locations on the surface of a hypersphere defined by $U_\rho = \left\{(x_1,x_2,\cdots,x_k)|\sum_{i=1}^{k}x_i^2 = \rho^2\right\}$. A spherical region moment of order δ is defined to be $\sigma_{\delta_1\delta_2\cdots\delta_k} = \phi\int_{U_\rho} x_1^{\delta_1}x_2^{\delta_2}\cdots x_k^{\delta_k}dx$. Define the spherical region moment matrix S by $S = \phi\int_{U_\rho} D'D\ dx$. Let us define that the spherical average slope variance, $\overline{V}(\rho)$, is a quantity given by $\overline{V}(\rho) = \frac{\phi}{\sigma^2}\int_{U_\rho}\overline{V}(x)dx = \frac{1}{k}tr[S(X'V^{-1}X)^{-1}]$. Then the slope variance dispersion measure, the range of $\overline{V}(x)/\sigma^2$ on the sphere of radius ρ, as $RV(\rho) = V_{\max}(\rho) - V_{\min}(\rho)$ where $V_{\max}(\rho) = \max_{x\in U_\rho}\frac{\overline{V}(x)}{\sigma^2}$ and $V_{\min}(\rho) = \min_{x\in U_\rho}\frac{\overline{V}(x)}{\sigma^2}$. Note that $RV(\rho)$ is zero if and only if a design is slope rotatable over all directions. $RV(\rho)$ becomes larger as a design deviates from a slope rotatable design.

3. Slope Rotatable Design with Equal Maximum Directional Variance with Correlated Errors

For the formulation of the maximum and minimum of $V_p(x)$, let $\lambda_{\max}(x) = \max_{p:p'p=1} V_p(x)$ and $\lambda_{\min}(x) = \min_{p:p'p=1} V_p(x)$ where x is a point in the region of interest. Let us call $\lambda_{\max}(x)$ and $\lambda_{\min}(x)$ as the maximum directional variance and the minimum directional variance at a given point x, respectively. Let $M=D(X'V^{-1}X)^{-1}D'$. The eigenvalues of the matrix M are the roots of the characteristic equation for the matrix M. When the number of independent variables is 2, the matrix M at a point $x'=(x_1,x_2)$ in the design space is 2×2 and can be written as

$$M=D(X'V^{-1}X)^{-1}D' = \begin{pmatrix} m_{1.1} & m_{1.2} \\ m_{2.1} & m_{2.2} \end{pmatrix} = D\begin{pmatrix} v^{00} & v^{0.11} & v^{0.22} & v^{0.1} & v^{0.2} & v^{0.12} \\ v^{11.0} & v^{11.11} & v^{11.22} & v^{11.1} & v^{11.2} & v^{11.12} \\ v^{22.0} & v^{22.11} & v^{22.22} & v^{22.1} & v^{22.2} & v^{22.12} \\ v^{1.0} & v^{1.11} & v^{1.22} & v^{1.1} & v^{1.2} & v^{1.12} \\ v^{2.0} & v^{2.11} & v^{2.22} & v^{2.1} & v^{2.2} & v^{2.12} \\ v^{12.0} & v^{12.11} & v^{12.22} & v^{12.1} & v^{12.2} & v^{12.12} \end{pmatrix} D'.$$

The two roots of the characteristic equation are given by $\lambda = \dfrac{(m_{1.1}+m_{2.2}) \pm \sqrt{(m_{1.1}-m_{2.2})^2+4m_{1.2}^2}}{2}$. Therefore, if and only if the larger value of the two roots $\dfrac{(m_{1.1}+m_{2.2}) + \sqrt{(m_{1.1}-m_{2.2})^2+4m_{1.2}^2}}{2}$ is a function of $\rho^2 = x_1^2+x_2^2$, then the maximum directional variances are equal at all points x equidistant from the origin of a design.

Theorem 3.1 The necessary and sufficient conditions for a design to have the slope rotatability with equal maximum directional variances for the second order response model with correlated errors in two independent variables are as follows:

[1] $v^{i.j} = v^{i.ii} = v^{i.ij} = v^{i.jj} = v^{ii.ij} = 0, \quad (i \neq j, i,j=1,2)$, [2] $v^{1.1} = v^{2.2}$, [3] $v^{11.11} = v^{22.22}$,

[4] $2(v^{11.11})^2 - v^{11.11}v^{12.12} - 2(v^{11.22})^2 - v^{11.22}v^{12.12} = 0$.

Corollary 3.1 In case of k=2, the conditions for a design to be rotatable with correlated errors are sufficient for a design to be slope rotatable with equal maximum directional variance with correlated error structures.

Proof. From the conditions for rotatability 2, the first three conditions of Theorem 3.1 are easily confirmed. Recall that the conditions for rotatability with correlated errors. When the conditions for rotatability are satisfied, the fourth condition is $2(v^{11.11})^2 - v^{11.11}v^{12.12} - 2(v^{11.22})^2 - v^{11.22}v^{12.12} = 2(\frac{c}{2}+d_1)^2 - (\frac{c}{2}+d_1)^2c - d_1^2 - d_1c = 0$

4. Summary

In this article, we have considered design problems associated with estimation of derivatives of second order polynomial response surface model assuming correlated errors. The variance of the derivative $V_p(x)$ at any point x is a function of direction and a function of design. Then the averaged variance $\overline{V}(x)$ is only a function of the point x and the design and the parameters involved in the dispersion matrix of errors.

In case of k=2, the conditions for a rotatable design with correlated errors are sufficient for a slope rotatable second order response surface design with equal maximum directional variance assuming errors are correlated by analog with case of uncorrelated errors. That is, we can also obtain a slope rotatable design over all directions and with equal maximum directional variance if we can find a rotatable design when errors are correlated.

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