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Slope-Rotatability over All Directions in Third Order Response Surface Models

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ABSTRACT

In the design of experiments for response surface analysis, sometimes it is of interest to estimate the difference of responses at two points. If differences at points close together are involved, the design that reliably estimates the slope of response surface is important. This idea was conceptualized by slope rotatability by Hader & Park (1978) and Park (1987).

Until now, second order polynomial models were only studied for slope rotatability. In this paper, we will propose the necessary and sufficient conditions for slope rotatability over all directions for the third order polynomial models in two, three and four independent variables. Also practical slope rotatable designs over all directions for two independent variables are suggested.

KEYWORDS: Responce surface model, Rotatability, Slope-rotatability, Third-order model.

1. INTRODUCTION

Response surface analysis is a mathematical and statistical technique used for analysing the several characteristics of response surface where several independent variables influence a dependent variable. So there exists a functional

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relation between the independent variables and a dependent variable. The relation can be expressed by

$$\eta(\boldsymbol{x}) = f(x_1, x_2, \ldots, x_p).$$

But, often the function f is unknown or known but very complicated. Therefore usually the response surface model assumes that a dependent variable can be adequately approximated by a low order polynomial.

Many people took second order polynomial model into account. The second order model with p independent variables may be written by

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

which can be expressed in matrix form as

$$\eta(\boldsymbol{x}) = \boldsymbol{x}'\boldsymbol{\beta},$$

where $\boldsymbol{x}' = (1, x_1, x_2, \ldots, x_p, x_1^2, x_2^2, \ldots, x_p^2, x_1x_2, \ldots, x_{p-1}x_p)$ and $\boldsymbol{\beta}'=(\beta_0,\ \beta_1,\ \ldots,\ \beta_p,\ \beta_1^2,\ \ldots,\ \beta_p^2,\ \beta_{12},\ \ldots\ ,\beta_{p-1p})$. The coefficients in the polynomial are to be estimated, by the least square method, from observations on the response variable, $y_i(\boldsymbol{x}) = \eta(\boldsymbol{x}) + \epsilon_i$,where the $\epsilon's$ are uncorrelated random errors with zero mean and constant variance, σ^2. Then the least squares estimator of $\boldsymbol{\beta}$, is $\boldsymbol{b} = (X'X)^{-1}X'\boldsymbol{y}$, where X is a $n \times p$ matrix of values of the p elements of x taken at n design points and $\boldsymbol{y}$ is $n \times 1$ vector of y observations. The fitted equation

$$\hat{y}(\boldsymbol{x}) = \boldsymbol{x}'\boldsymbol{b}$$

is used to estimate $\eta(\boldsymbol{x})$. It is well known that

$$\text{Var}(\boldsymbol{b}) = (X'X)^{-1}\sigma^2$$

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

Because our attention is focused on the slope of response surface, consider the first derivative of $\hat{y}(\boldsymbol{x})$.

$$\frac{\partial \hat{y}(\boldsymbol{x})}{\partial x_i} = b_i + 2b_{ii}x_i + \sum_{j \neq i} b_{ij}x_j. \tag{1.1}$$

Then the variance of $\frac{\partial \hat{y}(\boldsymbol{x})}{\partial x_i}$ is written as

$$\begin{aligned}
\operatorname{Var}\Big(\frac{\partial \hat{y}(\boldsymbol{x})}{\partial x_i}\Big) =& \operatorname{Var}(b_i) + 4x_i^2 \operatorname{Var}(b_{ii}) + \sum_{j \neq i} x_j^2 \operatorname{Var}(b_{ij}) \\
&+ 4x_i \operatorname{Cov}(b_i, b_{ii}) + 2\sum_{j \neq i} x_j \operatorname{Cov}(b_i, b_{ij}) \\
&+ 4x_i \sum_{j \neq i} x_j \operatorname{Cov}(b_{ii}, b_{ij}) + 2 \sum_{\substack{j<l \\ j,l \neq i}} x_j x_l \operatorname{Cov}(b_{ij}, b_{il}).
\end{aligned} \tag{1.2}$$

In practice, it is often interesting to estimate the slope of the response surface at a point $\boldsymbol{x}$ over any specified directions. For this purpose, we can take the averaged variance of all possible directions into account.
Let the estimated slope vector

$$g(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial \hat{y}(\boldsymbol{x})}{\partial x_1} \\ \frac{\partial \hat{y}(\boldsymbol{x})}{\partial x_i} \\ \vdots \\ \frac{\partial \hat{y}(\boldsymbol{x})}{\partial x_p} \end{pmatrix} = D'\boldsymbol{b}, \tag{1.3}$$

where D is the matrix arising from the differentiation of $\boldsymbol{x}'\boldsymbol{b}$ with respect to each of the p independent variables. The estimated derivative at any point $\boldsymbol{x}$ in the direction specified by the $p \times 1$ vector of direction cosines $\boldsymbol{k}' = (k_1, k_2, \ldots, k_p)$ is $\boldsymbol{k}'g(\boldsymbol{x})$, where $\sum_{i=1}^{p} k_i^2 = 1$. The variance of this slope is

$$V(\boldsymbol{x}) = \operatorname{Var}(\boldsymbol{k}'g(\boldsymbol{x})) = \boldsymbol{k}'D(X'X)^{-1}D'\boldsymbol{k}\sigma^2. \tag{1.4}$$

Park (1987) showed that the average of $V(\boldsymbol{x})$ over all possible directions was

$$\bar{V}(\boldsymbol{x}) = \frac{\sigma^2}{p} \operatorname{tr}(D(X'X)^{-1}D'). \tag{1.5}$$

In that paper he assumed that the distribution over all directions was uniform. $\bar{V}(\boldsymbol{x})$ is a function of $\boldsymbol{x}$, the point at which the derivative is being estimated, and also a function of the design. By a well chosen design, we can make this variance $\bar{V}(\boldsymbol{x})$ equal for all points which are at the same distance from the design center. This property has been called slope rotatability over all directions.

Park(1987) showed that the equivalent conditions for a design to be slope rotatable over all directions are the following.

Park (1987) suggested a class of slope rotatable designs over all directions. Later, Kim (1993) introduced a measure of slope rotatability over all directions for second order response surface experimental designs. Also, Jang and Park (1993) studied a measure and a graphical method for evaluating slope rotatability.

2. CONDITIONS FOR SLOPE-ROTATABLE DESIGN OVER ALL DIRECTIONS

In this section, we will show the equivalent conditions for slope rotatability over all directions with 2, 3, 4 independent variables respectively in third order polynomial models.

The third order model with p independent variables may be written by

$$\begin{aligned}\eta(\boldsymbol{x}) =& \beta_0 + \sum_{i=1}^{p}\beta_i x_i + \sum_{i=1}^{p}\beta_{ii}x_i^2 + \sum_{i<j}^{p}\beta_{ij}x_i x_j + \sum_{i=1}^{p}\beta_{iii}x_i^3 \\ &+ \sum_{i=1}^{p}\sum_{j\neq i}\beta_{iij}x_i^2 x_j + \sum_{i<j<k}\beta_{ijk}x_i x_j x_k\end{aligned} \tag{2.1}$$

which can be expressed in matrix form as

$$\eta(\boldsymbol{x}) = \boldsymbol{x}'\boldsymbol{\beta},$$

where $\boldsymbol{x}' = (1, x_1, \ldots, x_p, x_1^2, \ldots, x_p^2, x_1x_2, \ldots, x_{p-1}x_p, x_1^3, \ldots, x_p^3, x_1^2x_2, \ldots, x_p^2x_{p-1}, x_1x_2x_3, \ldots, x_{p-2}x_{p-1}x_p)$, $\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_p, \beta_{11}, \ldots, \beta_{pp}, \beta_{12}, \ldots, \beta_{p-1p}, \beta_{111}, \ldots, \beta_{ppp}, \beta_{112}, \ldots, \beta_{ppp-1}, \beta_{123}, \ldots, \beta_{p-2p-1p})'$. Note that the equations (1.3) to (1.5) are not changed for the third order model.

First consider the third order response surface model with **two** variables. The partial derivative of $\hat{y}(\boldsymbol{x})$ is

$$
\begin{aligned}
\frac{\partial \hat{\boldsymbol{y}}}{\partial x_1} &= b_1 + 2b_{11}x_1 + b_{12}x_2 + 3b_{111}x_1^2 + 2b_{112}x_1x_2 + b_{122}x_2^2, \\
\frac{\partial \hat{\boldsymbol{y}}}{\partial x_2} &= b_2 + 2b_{22}x_2 + b_{12}x_1 + 3b_{222}x_2^2 + 2b_{122}x_1x_2 + b_{112}x_1^2.
\end{aligned} \tag{2.2}
$$

Then,

$$
g(\boldsymbol{x}) = D\boldsymbol{b}, \tag{2.3}
$$

where $\boldsymbol{b} = (b_0, b_1, b_2, b_{11}, b_{22}, b_{12}, b_{111}, b_{222}, b_{112}, b_{122})'$ and

$$
D = \begin{pmatrix} 0 & 1 & 0 & 2x_1 & 0 & x_2 & 3x_1^2 & 0 & 2x_1x_2 & x_2^2 \\ 0 & 0 & 1 & 0 & 2x_2 & x_1 & 0 & 3x_2^2 & x_1^2 & 2x_1x_2 \end{pmatrix}
$$

$$
D'D = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & 1 & 0 & 2x_1 & 0 & x_2 & 3x_1^2 & 0 & 2x_1x_2 & x_2^2 \\
 & & 1 & 0 & 2x_2 & x_1 & 0 & 3x_2^2 & x_1^2 & 2x_1x_2 \\
 & & & 4x_1^2 & 0 & 2x_1x_2 & 6x_1^3 & 0 & 4x_1^2x_2 & 2x_1x_2^2 \\
 & & & & 4x_2^2 & 2x_1x_2 & 0 & 6x_2^3 & 2x_1^2x_2 & 4x_1x_2^2 \\
 & & & & & x_1^2+x_2^2 & 3x_1^2x_2 & 3x_1x_2^2 & x_1^3+2x_1x_2^2 & x_2^3+2x_1^2x_2 \\
 & & & & & & 9x_1^4 & 0 & 6x_1^3x_2 & 3x_1^2x_2^2 \\
 & & & \text{(symmetric)} & & & & 9x_2^4 & 3x_1^2x_2^2 & 6x_1x_2^3 \\
 & & & & & & & & x_1^4+4x_1^2x_2^2 & 2x_1x_2^3+2x_1^3x_2 \\
 & & & & & & & & & x_2^4+4x_1^2x_2^2
\end{pmatrix}.
$$

Then,

$$
\begin{aligned}
\bar{V}(\boldsymbol{x}) &= \frac{\sigma^2}{p}\mathrm{tr}[D(XX)^{-1}D'] \\
&= \frac{\sigma^2}{p}\mathrm{tr}[(XX)^{-1}D'D] \\
&= \frac{1}{p}\Big[v_1 + v_2 + x_1(4c_{1,11} + 2c_{2,12}) + x_2(4c_{2,22} + 2c_{1,12}) \\
&\quad + x_1^2(4v_{11} + v_{12} + 6c_{1,111} + 2c_{2,112}) \\
&\quad + x_2^2(4v_{22} + v_{12} + 6c_{2,222} + 2c_{1,122}) \\
&\quad + x_1x_2(4c_{1,112} + 4c_{2,122} + 4c_{11,12} + 4c_{22,12}) \\
&\quad + x_1^3(12c_{11,111} + 2c_{12,112}) + x_2^3(12c_{22,222} + 2c_{12,122})
\end{aligned} \tag{2.4}
$$

$$+x_1^2x_2(8c_{11,112}+4c_{22,112}+6c_{12,111}+4c_{12,122})$$
$$+x_1x_2^2(8c_{22,122}+4c_{11,122}+6c_{12,222}+4c_{12,112})$$
$$+x_1^4(9v_{111}+v_{112})+x_2^4(9v_{222}+v_{122})$$
$$+x_1^3x_2(12c_{111,112}+4c_{112,122})+x_1x_2^3(12c_{222,122}+4c_{112,122})$$
$$\left.+x_1^2x_2^2(4v_{112}+4v_{122}+6c_{111,122}+6c_{222,112})\right].$$

Note that $v_{ijk}=\mathrm{Var}(b_{ijk})$, $c_{i,jkl}=\mathrm{Cov}(b_i, b_{jkl})$, $c_{ij,klm}=\mathrm{Cov}(b_{ij}, b_{klm})$, and so on.

Theorem 1.1. The necessary and sufficient conditions for slope rotatability over all directions for the third order polynomial model with two independent variables are the following.

$$\begin{aligned}
&1.\ 4v_{11}+6c_{1,111}+2c_{2,112}=4v_{22}+6c_{2,222}+2c_{1,122}\\
&2.\ 9v_{111}+v_{112}=9v_{222}+v_{122}=\frac{1}{2}(4v_{112}+4v_{122}+6c_{111,122}+6c_{222,112})\\
&3.\ 2c_{1,11}+c_{2,12}=2c_{2,22}+c_{1,12}=0\\
&4.\ c_{1,112}+c_{2,122}+c_{11,12}+c_{22,12}=0 \qquad\qquad (2.5)\\
&5.\ 6c_{11,111}+c_{12,112}=6c_{22,222}+c_{12,122}=0\\
&6.\ 4c_{11,112}+2c_{22,112}+3c_{12,111}+2c_{12,122}\\
&\qquad =4c_{22,122}+2c_{11,122}+3c_{12,222}+2c_{12,112}=0\\
&7.\ 3c_{111,112}+c_{112,122}=3c_{222,122}+c_{112,122}=0.
\end{aligned}$$

Proof.
Sufficiency : If the conditions (2.5) are satisfied, non-zero terms in the equation (2.4) are the constant term and the terms containing x_1^2, x_2^2, x_1^4, x_2^4, $x_1^2x_2^2$. Also the coefficients of x_1^2 and x_2^2 are equal, and the coefficients of x_1^4 and x_2^4 are a half of that of $x_1^2x_2^2$. Then,

$$\bar{V}(\boldsymbol{x})=\frac{1}{p}(v_1+v_2)+\frac{1}{p}\{4v_{11}+v_{12}+6c_{1,111}+2c_{2,112}\}\rho^2+\frac{1}{p}\{9v_{111}+v_{112}\}\rho^4.$$

So, $\bar{V}(\boldsymbol{x})$ is a function of only ρ, where $\rho = (x_1^2 + x_2^2)^{\frac{1}{2}}$.
Necessicity : If any of the conditions are not satisfied, then $\bar{V}(\boldsymbol{x})$ may be written as

$$\begin{aligned}\bar{V}(\boldsymbol{x}) =& C_0 + C_1x_1 + C_2x_2 + C_{11}x_1^2 + C_{22}x_2^2 + C_{12}x_1x_2 \\ &+ C_{111}x_1^3 + C_{222}x_2^3 + C_{112}x_1^2x_2 + C_{122}x_1x_2^2 + C_{1111}x_1^4 \\ &+ C_{2222}x_2^4 + C_{1112}x_1^3x_2 + C_{1222}x_1x_2^3 + C_{1122}x_1^2x_2^2,\end{aligned}$$

where C_0, C_1, C_2, C_{11}, C_{22}, C_{12}, C_{111}, C_{222}, C_{112}, C_{122}, C_{1111}, C_{2222}, C_{1112}, C_{1222}, C_{1122} are arbitrary constants which are not satisfying the conditions. Then for given constants we can choose infinitely many points which are at the same distance from the center but yield the different values of $\bar{V}(\boldsymbol{x})$. So, $\bar{V}(\boldsymbol{x})$ is not a function of ρ.

For the case of two independent variables, the following theorem is useful to find slope rotatable designs over all directions. We will use the usual moment notations, $[ii] = \sum_{k=1}^{N} x_{ik}^2/N, [iijj] = \sum_{k=1}^{N} x_{ik}^2 x_{jk}^2$ and so on.

Theorem 1.2. When the number of independent variables is equal to 2, if the following moment conditions are satisfied for the third order model, then the design is slope rotatable over all directions.

1. All odd order moments are zero.
2. $N[11] = N[22] = \lambda_0, N[1111] = N[2222] = \lambda_1,$
   $N[111111] = N[222222] = \lambda_3, N[111122] = N[112222] = \lambda_4.$
3. $3(\lambda_0\lambda_4 - \lambda_2^2) = (\lambda_0\lambda_3 - \lambda_1^2) + 2(\lambda_1\lambda_2 - \lambda_0\lambda_4),$

where N is the number of design points and

$$\lambda_0 = \sum_{k=1}^{N} x_{1k}^2 = \sum_{k=1}^{N} x_{2k}^2,$$

$$\lambda_1 = \sum_{k=1}^{N} x_{1k}^4 = \sum_{k=1}^{N} x_{2k}^4, \qquad \lambda_2 = \sum_{k=1}^{N} x_{1k}^2 x_{2k}^2,$$

$$\lambda_3 = \sum_{k=1}^{N} x_{1k}^6 = \sum_{k=1}^{N} x_{2k}^6, \qquad \lambda_4 = \sum_{k=1}^{N} x_{1k}^4 x_{2k}^2 = \sum_{k=1}^{N} x_{1k}^2 x_{2k}^4.$$

Proof. If the first and second conditions of Thoerem 1.2 are satisfied, then the moment matrix, $X'X$ is

$$X'X = \begin{array}{cc} & \begin{array}{cccccccccc} x_0 & x_1^2 & x_2^2 & x_1x_2 & x_1 & x_1^3 & x_1x_2^2 & x_2 & x_2^3 & x_1^2x_2 \end{array} \\ \begin{array}{c} x_0 \\ x_1^2 \\ x_2^2 \\ x_1x_2 \\ x_1 \\ x_1^3 \\ x_1x_2^2 \\ x_2 \\ x_2^3 \\ x_1^2x_2 \end{array} & \begin{pmatrix} N & \lambda_0 & \lambda_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & \lambda_1 & \lambda_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & \lambda_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & & \lambda_0 & \lambda_1 & \lambda_2 & 0 & 0 & 0 \\ & & & & & \lambda_3 & \lambda_4 & 0 & 0 & 0 \\ & & & & & & \lambda_4 & 0 & 0 & 0 \\ & & & & & & & \lambda_0 & \lambda_1 & \lambda_2 \\ & & & & & & & & \lambda_3 & \lambda_4 \\ & & & & & & & & & \lambda_4 \end{pmatrix} \end{array}. \tag{2.6}$$

Then, the inverse matrix of $X'X$ is

$$(X'X)^{-1} = \begin{pmatrix} P^{-1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \lambda_2^{-1} & \mathbf{0} & \mathbf{0} \\ & & Q^{-1} & \mathbf{0} \\ & & & Q^{-1} \end{pmatrix}, \tag{2.7}$$

where

$$P^{-1} = \frac{1}{\det 1} \begin{pmatrix} \lambda_1^2 - \lambda_2^2 & \lambda_0(\lambda_2 - \lambda_1) & \lambda_0(\lambda_2 - \lambda_1) \\ & \lambda_1 N - \lambda_0^2 & \lambda_0^2 - \lambda_2 N \\ & & \lambda_1 N - \lambda_0^2 \end{pmatrix},$$

$$Q^{-1} = \frac{1}{\det 2} \begin{pmatrix} \lambda_3\lambda_4 - \lambda_4^2 & \lambda_2\lambda_4 - \lambda_1\lambda_4 & \lambda_1\lambda_4 - \lambda_2\lambda_3 \\ & \lambda_0\lambda_4 - \lambda_2^2 & \lambda_1\lambda_2 - \lambda_0\lambda_4 \\ & & \lambda_0\lambda_3 - \lambda_1^2 \end{pmatrix},$$

where

$$\det 1 = N(\lambda_1^2 - \lambda_2^2) + 2\lambda_0^2(\lambda_2 - \lambda_1),$$

$$\det 2 = \lambda_0\lambda_3\lambda_4 + 2\lambda_1\lambda_2\lambda_4 - \lambda_2^2\lambda_3 - \lambda_1^2\lambda_4 - \lambda_0\lambda_4^2.$$

Hence the conditions of Theorem 1.2 are reduced to

$$9v_{111} + v_{112} = 4v_{112} + 6c_{111,122}. \tag{2.8}$$

If we substitute variances and covariances in the equations (2.8) with their moments, then

$$\begin{aligned}
&\text{equation (2.8)}\\
\Leftrightarrow\ & \frac{3(\lambda_0\lambda_4-\lambda_2^2)}{\det 2} = \frac{\lambda_0\lambda_3-\lambda_1^2}{\det 2} + \frac{2(\lambda_1\lambda_2-\lambda_0\lambda_4)}{\det 2} = 0\\
\Leftrightarrow\ & 3(\lambda_0\lambda_4-\lambda_2^2) = (\lambda_0\lambda_3-\lambda_1^2) + 2(\lambda_1\lambda_2-\lambda_0\lambda_4).
\end{aligned}$$

Let's consider the third order response surface model with **three** variables. The partial derivative of $\hat{y}(\boldsymbol{x})$ is

$$\begin{aligned}
\frac{\partial \hat{\boldsymbol{y}}}{\partial x_1} =& b_1 + 2b_{11}x_1 + b_{12}x_2 + b_{13}x_3 + 3b_{111}x_1^2\\
&+ 2b_{112}x_1x_2 + 2b_{113}x_1x_3 + b_{122}x_2^2 + b_{133}x_3^2 + b_{123}x_2x_3\\
\frac{\partial \hat{\boldsymbol{y}}}{\partial x_2} =& b_2 + 2b_{22}x_2 + b_{12}x_1 + b_{23}x_3 + 3b_{222}x_2^2\\
&+ b_{112}x_1^2 + 2b_{122}x_1x_2 + 2b_{223}x_2x_3 + b_{233}x_3^2 + b_{123}x_1x_3\\
\frac{\partial \hat{\boldsymbol{y}}}{\partial x_3} =& b_3 + 2b_{33}x_3 + b_{13}x_1 + b_{23}x_2 + 3b_{333}x_3^2\\
&+ b_{113}x_1^2 + b_{223}x_2^2 + 2b_{133}x_1x_3 + 2b_{233}x_2x_3 + b_{123}x_1x_2.
\end{aligned} \tag{2.9}$$

Then,

$$g(\boldsymbol{x}) = D\boldsymbol{b}, \tag{2.10}$$

where $\boldsymbol{b}=(b_0, b_1, b_2, b_3, b_{11}, b_{22}, b_{33}, b_{12}, b_{13}, b_{23}, b_{111}, b_{222}, b_{333}, b_{112}, b_{113}, b_{122}, b_{223}, b_{133}, b_{233}, b_{123})'$ and $D = [\underline{0}; I_3; M1; M2; M3; M4; M5]$, where

$$\begin{aligned}
M1 &= \operatorname{diag}(2x_1, 2x_2, 2x_3),\\
M2 &= \begin{pmatrix} x_2 & x_3 & 0\\ x_1 & 0 & x_3\\ 0 & x_1 & x_2 \end{pmatrix},\\
M3 &= \operatorname{diag}(3x_1^2, 3x_2^2, 3x_3^2),
\end{aligned}$$

$$M4 = \begin{pmatrix} 2x_1x_2 & 2x_1x_3 & x_2^2 & 0 & x_3^2 & 0 \\ x_1^2 & 0 & 2x_1x_2 & 2x_2x_3 & 0 & x_3^2 \\ 0 & x_1^2 & 0 & x_2^2 & 2x_1x_3 & 2x_2x_3 \end{pmatrix},$$

$$M5 = \begin{pmatrix} x_2x_3 \\ x_1x_3 \\ x_1x_2 \end{pmatrix}.$$

By straightforward algebra, it may be shown that

$$\begin{aligned}
\bar{V}(\boldsymbol{x}) &= \frac{\sigma^2}{p}\mathrm{tr}[D(XX)^{-1}D'] \\
&= \frac{1}{p}\Big[v_1 + v_2 + v_3 + x_1(4c_{1,11} + 2c_{2,12} + 2c_{3,13}) \\
&\quad + x_2(4c_{2,22} + 2c_{1,12} + 2c_{3,23}) + x_3(4c_{3,33} + 2c_{1,13} + 2c_{2,23}) \\
&\quad + x_1^2(4v_{11} + v_{12} + v_{13} + 6c_{1,111} + 2c_{2,112} + 2c_{3,113}) \\
&\quad + x_2^2(4v_{22} + v_{12} + v_{23} + 6c_{2,222} + 2c_{1,122} + 2c_{3,223}) \\
&\quad + x_3^2(4v_{33} + v_{13} + v_{23} + 6c_{3,333} + 2c_{1,133} + 2c_{2,233}) \\
&\quad + x_1x_2(4c_{1,112} + 4c_{2,122} + 4c_{11,12} + 4c_{22,12} + 2c_{3,123} + 2c_{13,23}) \\
&\quad + x_1x_3(4c_{1,113} + 4c_{3,133} + 4c_{11,13} + 4c_{33,13} + 2c_{2,123} + 2c_{12,23}) \\
&\quad + x_2x_3(4c_{2,223} + 4c_{3,233} + 4c_{22,23} + 4c_{33,23} + 2c_{1,123} + 2c_{12,13}) \\
&\quad + x_1^3(12c_{11,111} + 2c_{12,112} + 2c_{13,113}) \\
&\quad + x_2^3(12c_{22,222} + 2c_{12,122} + 2c_{23,223}) \\
&\quad + x_3^3(12c_{33,333} + 2c_{13,133} + 2c_{23,233}) \\
&\quad + x_1^2x_2(8c_{11,112} + 4c_{22,112} + 6c_{12,111} + 4c_{12,122} + 2c_{23,113} + 2c_{13,123}) \\
&\quad + x_1^2x_3(8c_{11,113} + 4c_{33,113} + 6c_{13,111} + 4c_{13,133} + 2c_{23,112} + 2c_{12,123}) \\
&\quad + x_2^2x_1(8c_{22,122} + 4c_{11,122} + 6c_{12,222} + 4c_{12,112} + 2c_{13,223} + 2c_{23,123}) \\
&\quad + x_2^2x_3(8c_{22,223} + 4c_{33,223} + 6c_{23,222} + 4c_{23,233} + 2c_{13,122} + 2c_{12,123})
\end{aligned}$$

$$
\begin{aligned}
&+x_3^2x_1(8c_{33,133}+4c_{11,133}+6c_{13,333}+4c_{13,113}+2c_{12,233}+2c_{23,123})\\
&+x_3^2x_2(8c_{33,233}+4c_{22,233}+6c_{23,333}+4c_{23,223}+2c_{12,133}+2c_{13,123})\\
&+4x_1x_2x_3\{c_{11,123}+c_{22,123}+c_{33,123}+c_{12,113}+c_{12,223}\\
&\quad+c_{13,112}+c_{13,233}+c_{23,122}+c_{23,133}\}+x_1^4(9v_{111}+v_{112}+v_{113})\\
&+x_2^4(9v_{222}+v_{122}+v_{223})+x_3^4(9v_{333}+v_{133}+v_{233})\\
&+x_1^2x_2^2(4v_{112}+4v_{122}+v_{123}+6c_{111,122}+6c_{222,112}+2c_{113,223})\\
&+x_1^2x_3^2(4v_{113}+4v_{133}+v_{123}+6c_{111,133}+6c_{333,113}+2c_{112,233})\\
&+x_2^2x_3^2(4v_{223}+4v_{233}+v_{123}+6c_{222,233}+6c_{333,223}+2c_{122,133})\\
&+x_1^3x_2(12c_{111,112}+4c_{112,122}+2c_{113,123})\\
&+x_1^3x_3(12c_{111,113}+4c_{113,133}+2c_{112,123})\\
&+x_2^3x_1(12c_{222,122}+4c_{112,122}+2c_{223,123})\\
&+x_2^3x_3(12c_{222,223}+4c_{223,233}+2c_{122,123})\\
&+x_3^3x_1(12c_{333,133}+4c_{113,133}+2c_{233,123})\\
&+x_3^3x_2(12c_{333,233}+4c_{223,233}+2c_{133,123})\\
&+x_1^2x_2x_3(6c_{111,123}+8c_{112,113}+4c_{112,223}\\
&\qquad\qquad+4c_{113,233}+4c_{122,123}+4c_{133,123})\\
&+x_1x_2^2x_3(6c_{222,123}+8c_{122,223}\\
&\qquad\qquad+4c_{113,122}+4c_{223,133}+4c_{112,123}+4c_{233,123})\\
&+x_1x_2x_3^2(6c_{333,123}+8c_{133,233}\\
&\qquad\qquad+4c_{112,133}+4c_{122,233}+4c_{113,123}+4c_{223,123})\Big].
\end{aligned}
\tag{2.11}
$$

Theorem 1.3. The necessary and sufficient conditions for slope rotatability over all directions for the third order polynomial model with three independent variables are the following.

1. $4v_{11} + v_{12} + v_{13} + 6c_{1,111} + 2c_{2,112} + 2c_{3,113}$
$= 4v_{22} + v_{12} + v_{23} + 6c_{2,222} + 2c_{1,122} + 2c_{3,223}$
$= 4v_{33} + v_{13} + v_{23} + 6c_{3,333} + 2c_{1,133} + 2c_{2,233}$

2. $18v_{111} + 2v_{112} + 2v_{113}$
$= 18v_{222} + 2v_{122} + 2v_{223}$
$= 18v_{333} + 2v_{133} + 2v_{233}$ (2.12)
$= 4v_{112} + 4v_{122} + v_{123} + 6c_{111,122} + 6c_{222,112} + 2c_{113,223}$
$= 4v_{113} + 4v_{133} + v_{123} + 6c_{111,133} + 6c_{333,113} + 2c_{112,233}$
$= 4v_{223} + 4v_{233} + v_{123} + 6c_{222,233} + 6c_{333,223} + 2c_{122,133}$

3. All coefficients of the terms, except for constant, $x_1^2, x_2^2, x_3^2, x_1^4, x_2^4, x_3^4, x_1^2x_2^2, x_1^2x_3^2, x_2^2x_3^2$, equal zero.

We can prove Theorem 1.2 in the similar way to Theorem 1.1.

Finally consider the response surface model with **four** variables.

$$g(\boldsymbol{x}) = D\boldsymbol{b}, \tag{2.13}$$

where $D = [\underline{0}; I_4; M1; M2; M3; M4_1; M4_2; M5]$

$$\begin{aligned}
M1 &= \text{diagonal}(2x_1, 2x_2, 2x_3, 2x_4), \\
M2 &= \begin{pmatrix} x_2 & x_3 & x_4 & 0 & 0 & 0 \\ x_1 & 0 & 0 & x_3 & x_4 & 0 \\ 0 & x_1 & 0 & x_2 & 0 & x_4 \\ 0 & 0 & x_1 & 0 & x_2 & x_3 \end{pmatrix}, \\
M3 &= \text{diagonal}(3x_1^2, 3x_2^2, 3x_3^2, 3x_4^2), \\
M4_1 &= \begin{pmatrix} 2x_1x_2 & 2x_1x_3 & 2x_1x_4 & x_2^2 & 0 & 0 \\ x_1^2 & 0 & 0 & 2x_1x_2 & 2x_2x_3 & 2x_2x_4 \\ 0 & x_1^2 & 0 & 0 & x_2^2 & 0 \\ 0 & 0 & x_1^2 & 0 & 0 & x_2^2 \end{pmatrix}, \\
M4_2 &= \begin{pmatrix} x_3^2 & 0 & 0 & x_4^2 & 0 & 0 \\ 0 & x_3^2 & 0 & 0 & x_4^2 & 0 \\ 2x_1x_3 & 2x_2x_3 & 2x_3x_4 & 0 & 0 & x_4^2 \\ 0 & 0 & x_3^2 & 2x_1x_4 & 2x_2x_4 & 2x_3x_4 \end{pmatrix},
\end{aligned}$$

$$M5 \;=\; \begin{pmatrix} x_2x_3 & x_2x_4 & x_3x_4 & 0 \\ x_1x_3 & x_1x_4 & 0 & x_3x_4 \\ x_1x_2 & 0 & x_1x_4 & x_2x_4 \\ 0 & x_1x_2 & x_1x_3 & x_2x_3 \end{pmatrix}.$$

By straightforward algebra, it may be shown that

$$\begin{aligned}
\bar{V}(\boldsymbol{x}) &= \frac{\sigma^2}{p}\mathrm{tr}[D(XX)^{-1}D'] \\
&= \frac{\sigma^2}{p}\mathrm{tr}[(XX)^{-1}D'D] \\
&= \frac{1}{p}\Big[\sum_{i=1}^{4} v_i + \sum_{i=1}^{4} x_i^2\{4v_{ii} + 6c_{i,iii} + \sum_{j\neq i}(v_{ij} + 2c_{j,iij})\} \\
&\quad + \sum_{i=1}^{4} x_i\{4c_{i,ii} + 2\sum_{j\neq i} c_{j,ij}\} + \sum_{i=1}^{4} x_i^4(9v_{iii} + \sum_{j\neq i} v_{iij}) \\
&\quad + \sum_{i=1}^{4} x_i^3\{12c_{ii,iii} + 2\sum_{j\neq i} c_{ij,iij}\} \\
&\quad + \sum_{i<j} x_i^2x_j^2\{4v_{iij} + 4v_{jji} + \sum_{k\neq i,j}(v_{ijk} + 2c_{iik,jjk}) + 6c_{jjj,iij} + 6c_{iii,jji}\} \\
&\quad + \sum_{i<j} x_ix_j\{4c_{i,iij} + 4c_{j,jji} + 4c_{ii,ij} + 4c_{jj,ij} + \sum_{k\neq i,j}(2c_{k,ijk} + 2c_{ki,kj})\} \\
&\quad + \sum_{i}\sum_{j\neq i} x_i^2x_j\{8c_{ii,iij} + 4c_{jj,iij} + 6c_{ij,iii} + 4c_{ij,jji} + 2\sum_{k\neq i,j}(c_{jk,iik} + c_{ik,ijk})\} \\
&\quad + \sum_{i<j<k} x_ix_jx_k\{4c_{ii,ijk} + 4c_{jj,ijk} + 4c_{kk,ijk} + 4c_{ij,iik} + 4c_{ik,iij} + 4c_{ji,jjk} \\
&\qquad\qquad + 4c_{jk,jji} + 4c_{ki,kkj} + 4c_{kj,kki} + 2\sum_{l\neq i,j,k}(c_{il,jkl} + c_{jl,ikl} + c_{kl,ijl})\} \\
&\quad + \sum_{i}\sum_{j\neq i} x_i^3x_j\{12c_{iii,iij} + 4c_{iij,jji} + 2\sum_{k\neq i,j} c_{iik,ijk}\} \qquad\qquad (2.14)\\
&\quad + \sum_{i}\sum_{\substack{j<k\\ j,k\neq i}} x_i^2x_jx_k\{6c_{iii,ijk} + 8c_{iij,iik} + 4c_{iij,jjk} + 4c_{iik,kkj}
\end{aligned}$$

$$+4c_{ijj,ijk} + 4c_{ikk,ijk} + 2 \sum_{l\neq i,j,k} (c_{iil,jkl} + c_{ijl,ikl})\}$$

$$+4x_1x_2x_3x_4 \sum_{i<j<k} \sum_{l\neq i,j,k} (c_{iil,ijk} + c_{jjl,ijk} + c_{kkl,ijk})\Big].$$

Theorem 1.4. The equivalent conditions for slope rotatability over all directions for the third order polynomial model with four independent variables are the following.

1. $4v_{ii} + 6c_{i,iii} + \sum_{j\neq i}(v_{ij} + 2c_{j,iij})$ equals for all $i = 1, 2, 3, 4$.

2. $9v_{iii} + \sum_{j\neq i} v_{iij}$ equals for all $i = 1, 2, 3, 4$, (2.15)
   $4v_{iij} + 4v_{jji} + \sum_{k\neq i,j}(v_{ijk} + 2c_{iik,jjk}) + 6c_{jjj,iij} + 6c_{iii,jji}$ equals for all $i < j$ and the value of the second equation is two times of that of the first equation.

3. All coefficients of the terms, except for constant, $x_1^2, x_2^2, x_3^2, x_4^2, x_1^4, x_2^4, x_3^4, x_4^4, x_1^2x_2^2, x_1^2x_3^2, x_1^2x_4^2, x_2^2x_3^2, x_2^2x_4^2, x_3^2x_4^2$, equal zero.

We can prove Theorem 1.4 by the same way as Theorem 1.1.

3. EXAMPLES OF SLOPE-ROTATABLE DESIGN IN TWO INDEPENDENT VARIABLES

In this chapter, we will show some examples which are slope rotatable over all directions in the third order models. Because the design with two independent variables is useful for a practical experiment in the third order models, we will only consider the case of two variables.

For a slope rotatable design, first the equiradial design with two concentric circles is considered. If we arrange equally spaced n_1 points on a circle of radius ρ_1, and equally spaced n_2 points on a circle of radius ρ_2, then the design matrix is

$$
D = \begin{array}{c}
\begin{array}{cc} \quad x_1 & \quad\quad x_2 \end{array} \\
\begin{pmatrix}
\rho_1 \cos\left(\frac{2\pi}{n_1} + \theta_1\right) & \rho_1 \sin\left(\frac{2\pi}{n_1} + \theta_1\right) \\
\rho_1 \cos\left(\frac{4\pi}{n_1} + \theta_1\right) & \rho_1 \sin\left(\frac{4\pi}{n_1} + \theta_1\right) \\
\vdots & \vdots \\
\rho_1 \cos\left(\frac{2n_1\pi}{n_1} + \theta_1\right) & \rho_1 \sin\left(\frac{2n_1\pi}{n_1} + \theta_1\right) \\
\rho_2 \cos\left(\frac{2\pi}{n_2} + \theta_2\right) & \rho_2 \sin\left(\frac{2\pi}{n_2} + \theta_2\right) \\
\rho_2 \cos\left(\frac{4\pi}{n_2} + \theta_2\right) & \rho_2 \sin\left(\frac{4\pi}{n_2} + \theta_2\right) \\
\vdots & \vdots \\
\rho_2 \cos\left(\frac{2n_2\pi}{n_2} + \theta_2\right) & \rho_2 \sin\left(\frac{2n_2\pi}{n_2} + \theta_2\right) \\
0 & 0 \\
0 & 0
\end{pmatrix}
\end{array}.
$$

Gadiner (1956) showed that the necessary and sufficient conditions for all moments of order p of n points equally spaced on a circle to be invariant under rotation is that n be greater than p. Hence if $n \geq 7$, then

$$
\begin{aligned}
&\sum_{k=0}^{n-1} \left[\cos\left(\frac{2k\pi}{n} + \theta\right)\right]^{p-q} \left[\sin\left(\frac{2k\pi}{n} + \theta\right)\right]^{q} \\
&= \sum_{k=0}^{n-1} \left[\cos\left(\frac{2k\pi}{n}\right)\right]^{p-q} \left[\sin\left(\frac{2k\pi}{n}\right)\right]^{q}, \quad q = 0, 1, \ldots, p.
\end{aligned}
$$

Let's check the conditions in Theorem 1.2 for the above design. By algebra of trigonometric, we know that

$$
\begin{aligned}
\sum_{k=0}^{n-1} \left[\cos\left(\frac{2k\pi}{n}\right)\right]^{2} &= \sum_{k=0}^{n-1} \left[\sin\left(\frac{2k\pi}{n}\right)\right]^{2} = \frac{n}{2}, \\
\sum_{k=0}^{n-1} \left[\cos\left(\frac{2k\pi}{n}\right)\right]^{4} &= \sum_{k=0}^{n-1} \left[\sin\left(\frac{2k\pi}{n}\right)\right]^{4} = \frac{3n}{8}, \\
\sum_{k=0}^{n-1} \left[\cos\left(\frac{2k\pi}{n}\right)\right]^{6} &= \sum_{k=0}^{n-1} \left[\sin\left(\frac{2k\pi}{n}\right)\right]^{6} = \frac{5n}{16}.
\end{aligned}
$$

So,

$$\begin{aligned}
\sum_{k=0}^{n-1}\Big[\cos\Big(\frac{2k\pi}{n}\Big)\Big]^2\Big[\sin\Big(\frac{2k\pi}{n}\Big)\Big]^2 &= \sum_{k=0}^{n-1}\Big[\cos\Big(\frac{2k\pi}{n}\Big)\Big]^2-\sum\Big[\cos\Big(\frac{2k\pi}{n}\Big)\Big]^4=\frac{n}{8},\\
\sum_{k=0}^{n-1}\Big[\cos\Big(\frac{2k\pi}{n}\Big)\Big]^4\Big[\sin\Big(\frac{2k\pi}{n}\Big)\Big]^2 &= \sum_{k=0}^{n-1}\Big[\cos\Big(\frac{2k\pi}{n}\Big)\Big]^4-\sum\Big[\cos\Big(\frac{2k\pi}{n}\Big)\Big]^6=\frac{n}{16},\\
\sum_{k=0}^{n-1}\Big[\cos\Big(\frac{2k\pi}{n}\Big)\Big]^2\Big[\sin\Big(\frac{2k\pi}{n}\Big)\Big]^4 &= \sum_{k=0}^{n-1}\Big[\sin\Big(\frac{2k\pi}{n}\Big)\Big]^4-\sum\Big[\sin\Big(\frac{2k\pi}{n}\Big)\Big]^6=\frac{n}{16}.
\end{aligned}$$

Hence the second condition in Theorem 1.2 is satisfied and all odd order moments are zero. Then for the above design,

$$\begin{aligned}
\lambda_0 &= \sum_{k=0}^{n_1-1}\rho_1^2\Big[\cos\Big(\frac{2k\pi}{n_1}\Big)\Big]^2+\sum_{k=0}^{n_2-1}\rho_2^2\Big[\cos\Big(\frac{2k\pi}{n_2}\Big)\Big]^2=\frac{1}{2}(n_1\rho_1^2+n_2\rho_2^2)\\
\lambda_1 &= \sum_{k=0}^{n_1-1}\rho_1^4\Big[\cos\Big(\frac{2k\pi}{n_1}\Big)\Big]^4+\sum_{k=0}^{n_2-1}\rho_2^4\Big[\cos\Big(\frac{2k\pi}{n_2}\Big)\Big]^4=\frac{3}{8}(n_1\rho_1^4+n_2\rho_2^4)\\
\lambda_2 &= \sum_{k=0}^{n_1-1}\rho_1^4\Big[\cos\Big(\frac{2k\pi}{n_1}\Big)\Big]^2\Big[\sin\Big(\frac{2k\pi}{n_1}\Big)\Big]^2+\sum_{k=0}^{n_2-1}\rho_2^4\Big[\cos\Big(\frac{2k\pi}{n_2}\Big)\Big]^2\Big[\sin\Big(\frac{2k\pi}{n_1}\Big)\Big]^2\\
&= \frac{1}{8}(n_1\rho_1^4+n_2\rho_2^4)\\
\lambda_3 &= \sum_{k=0}^{n_1-1}\rho_1^6\Big[\cos\Big(\frac{2k\pi}{n_1}\Big)\Big]^6+\sum_{k=0}^{n_2-1}\rho_2^6\Big[\cos\Big(\frac{2k\pi}{n_2}\Big)\Big]^6=\frac{5}{16}(n_1\rho_1^6+n_2\rho_2^6)\\
\lambda_4 &= \sum_{k=0}^{n_1-1}\rho_1^6\Big[\cos\Big(\frac{2k\pi}{n_1}\Big)\Big]^4\Big[\sin\Big(\frac{2k\pi}{n_1}\Big)\Big]^2+\sum_{k=0}^{n_2-1}\rho_2^6\Big[\cos\Big(\frac{2k\pi}{n_2}\Big)\Big]^4\Big[\sin\Big(\frac{2k\pi}{n_1}\Big)\Big]^2\\
&= \frac{1}{16}(n_1\rho_1^6+n_2\rho_2^6).
\end{aligned}$$

Note that

$$\lambda_1=3\lambda_2,\lambda_3=5\lambda_4. \tag{3.1}$$

Because the equation (3.1) holds, the third condition in the Theorem 1.2 is always satisfied. Hence, if $n_1\geq 7$ and $n_2\geq 7$ and $\rho_1\neq\rho_2$, then the above equiradial design is slope rotatable design over all directions. For instance, when $n_1 = 7$, $n_2 = 7$, $\rho_1 = 1.0$, $\rho_2 = 0.5$ and the number of center points is two, $\bar{V}(\boldsymbol{x}) = \frac{1}{p}(4.127 - 13.611\rho^2 + 30.461\rho^4)$.

More generally combinations of equiradial designs such as $s(s \geq 2)$ sets of equiradial points on concentric circles, the wth containing $n_w(n_w \geq 7)$ points and having radius ρ_w are slope rotatable over all directions.

Let's consider the following extended central composite design. The design matrix is

$$D = \begin{array}{c} \begin{array}{cc} x_1 & x_2 \end{array} \\ \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & -1 \\ 0 & -1 \\ \alpha & 0 \\ -\alpha & 0 \\ 0 & \alpha \\ 0 & -\alpha \end{pmatrix} \end{array}.$$

For the above design, $\lambda_0 = 6 + 2\alpha^2$, $\lambda_1 = 6 + 2\alpha^4$, $\lambda_2 = \lambda_4 = 4$, $\lambda_3 = 6 + 2\alpha^6$. Then the third conditions in Theorem 1.2 can be rewritten as

$$3\alpha^6 - 2\alpha^4 - 7\alpha^2 - 6 = 0.$$

Therefore when α is 1.472491, the above design is slope rotatable over all directions.

4. CONCLUDING REMARKS

In this paper, we have considered the slope rotatability over all directions for the third order model. The necessary and sufficient conditions for slope rotatablility over all directions in two, three and four independent variables were derived.

For further study, it will be of interest to extend the equivalent conditions for slope rotatability over all directions to the case with k independent variables. Also a measure of slope rotatability for the third order polynomial model is desired to be developed.

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