Slope-Rotatability in Axial Directions for Second Order Response Surface Designs

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Abstract

Hader and Park(1978) suggested the concept of slope-rotatability in axial directions for second order response surface designs. In this paper, the moment conditions for slope-rotatability in axial directions are shown and the measures for evaluating slope-rotatability in axial directions are proposed.

Keywords: rotatability, slope-rotatability in axial directions, slope-rotatability over all directions, slope variance measure.

1. Introduction

There are a number of desirable properties for response surface experimental designs to have. Among these properties, an interesting and important property is that of rotatability. Since the concept of rotatability for response surface designs was first introduced by Box and Hunter(1957), it has become an important criterion. A design is said to be rotatable if the variance of the estimated response is constant at points equidistant from the design origin.

Good estimation of the derivatives of the response may be as important as the estimation of the mean response. Thus, Hader and Park(1978) introduced the concept of slope-rotatability in axial directions. Park(1987) suggested the concept of slope-rotatability over all directions. Slope-rotatability in axial directions require that the variance of the estimated slope in every axial direction be constant at points equidistant from the design origin. Similarly, slope-rotatability over all directions require that the variance of the estimated slope averaged over all directions be constant at points equidistant from the design origin. Park and Kim(1992) proposed a measure of slope-rotatability in axial directions for second order response surface designs and Jang and Park(1993) suggested a graphical method for evaluating slope-rotatability over all directions in response surface designs. Draper and Ying(1994) showed another measure of slope-rotatability over all directions. Ying, Pukelsheim

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and Draper(1995a, b) studied the conditions for slope rotatability over all directions. Kim, Um and Khuri(1996) suggested quantile plots of average slope variance for response surface designs. Jang(2002) proposed a graphical method for evaluating slope-rotatability in axial directions for second order response surface designs.

The purpose of this paper is to investigate the conditions and moment structures for slope-rotatability in axial directions in second order response surface designs and to suggest the measures for evaluating slope-rotatability in axial directions with respect to second order response surface designs.

2. Relations of Rotatability and Slope-Rotatability

It is assumed that the response relationship is adequately approximated by the second-order polynomial model in k design variables, $x' = (x_1, x_2, ..., x_k)$,

$$\eta(\mathbf{x}) = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i \neq j}^k \beta_{ij} x_i x_j, \tag{2.1}$$

which may be written in matrix notation as $\eta(\mathbf{x}) = \mathbf{x}_s' \boldsymbol{\beta}$, in which the $1 \times p$ vector $\mathbf{x}_s' = (1, x_1, x_2, \dots, x_k, x_1^2, \dots, x_k^2, x_1 x_2, \dots, x_{k-1} x_k)$ and $\boldsymbol{\beta}$ is the $p \times 1$ column vector of the corresponding coefficients. Here, \boldsymbol{p} is the number of parameters in the model. By the method of least squares, the fitted equation $\hat{y}(\mathbf{x}) = \mathbf{x}_s' \boldsymbol{b}$ is to be used to estimate $\eta(\mathbf{x})$, where $\boldsymbol{b} = (X'X)^{-1}X' \boldsymbol{y}$ and X is an $N \times p$ model matrix which reflects the experimental design, and \boldsymbol{y} is the observation vector.

Box and Hunter(1957) established the following necessary and sufficient condition for second order rotatability.

- 1. All odd order moments are zeros.
- 2. [iiii] = 3[iijj] for $i \neq j$,

where [iiii] and [iijj] are the pure and mixed fourth order moments, respectively.

Hader and Park(1978) proposed the following concept of slope-rotatability in axial directions, an analogue of the Box-Hunter rotatability criterion.

$$Var(\frac{\partial \widehat{y}(\mathbf{x})}{\partial x_i})$$
 is a function of only $r = (x_1^2 + x_2^2 + \dots + x_k^2)^{1/2}$, (2.2)

where $Var(\frac{\partial \hat{y}(x)}{\partial x_i})$ is the variance of the estimated slope with respect to x_i . $\frac{\partial \hat{y}(x)}{\partial x_i}$

can be as follows:

$$\frac{\partial \widehat{y}(x)}{\partial x_i} = d_i'b, \qquad (2.3)$$

where d_i is the $1 \times p$ vector of which each component is the result of differentiating the each term with respect to x_i in equation (2.1). For example, when k=3, $d_1'=(0,1,0,0,2x_1,0,0,x_2,x_3,0)$. Then,

$$Var(\frac{\partial \widehat{y}(\mathbf{x})}{\partial x_i}) = \mathbf{d}_{i}' Var(b) \mathbf{d}_{i} = \mathbf{d}_{i}' (X'X)^{-1} \mathbf{d}_{i} \sigma^{2}. \tag{2.4}$$

The straightforward form of the variance of the first derivative of $\hat{y}(x)$ with respect to x_i in second order designs is

$$Var(\frac{\partial \hat{y}(\mathbf{x})}{\partial x_{i}}) = Var(b_{i}) + 4x_{i}^{2}Var(b_{ii}) + \sum_{j=1, j\neq i}^{k} x_{j}^{2}Var(b_{ij}) + 4x_{i}Cov(b_{i}, b_{ii}) + 2\sum_{j=1, j\neq i}^{k} x_{j}Cov(b_{i}, b_{ij}) + 4x_{i}\sum_{j=1, j\neq i}^{k} x_{j}Cov(b_{ii}, b_{ij}) + 2\sum_{j=1, j\neq i}^{k$$

Therefore, it can be seen that the necessary and sufficient conditions for slope-rotatability in axial directions(SRIAD) in second order designs are

$$4v_{ii} = v_{ii}(i=1,2,\ldots,k),$$
 (2.6)

$$c_{i,ij} = c_{i,ij} = c_{ii,ij} = c_{ii,ij} = c_{ii,ij} = 0 (i \neq j \neq l \neq i, j \langle l, j, l = 1, 2, \dots, k),$$
(2.7)

where $v_{ii} = Var(b_{ii}), v_{ij} = Var(b_{ij}), c_{i,ii} = Cov(b_{i}, b_{ii}), c_{i,ij} = Cov(b_{i}, b_{ij}),$

 $c_{ii,ij} = Cov(b_{ii}, b_{ij}), c_{ij,il} = Cov(b_{ij}, b_{il})(i \neq j \neq l \neq i).$ We can call this definition as SRIAD(type II).

Park and Kim(1992) added the following condition as the necessary and sufficient conditions for slope-rotatability in axial directions in second order designs with the equation (2.2),

$$Var(\frac{\partial \widehat{y}(\mathbf{x})}{\partial x_1}) = Var(\frac{\partial \widehat{y}(\mathbf{x})}{\partial x_2}) = \dots = Var(\frac{\partial \widehat{y}(\mathbf{x})}{\partial x_k}). \tag{2.8}$$

This definition contains both slope-rotatability and equality in axial directions. We can call this definition as $SRIAD(type\ I)$. This $SRIAD(type\ I)$ have the stronger condition than $SRIAD(type\ I)$.

Park(1987) has proved the following theorem, which gives general conditions for a design to be slope-rotatable over all directions.

Theorem 2.1. For the second order model, the necessary and sufficient conditions for a design to be slope-rotatable over all directions are as the following:

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

2.
$$2[Cov(b_{ii}, b_{ij}) + Cov(b_{jj}, b_{ij})] + \sum_{p=1, p \neq i, j}^{k} Cov(b_{ip}, b_{jp}) = 0$$
 for any (i, j) when $i \neq j$.

3.
$$4 Var(b_{ii}) + \sum_{i=1, i\neq i}^{k} Var(b_{ij})$$
 are equal for all i ,

where b_i and b_{ij} are least squares estimators of the second order polynomial model.

Park(1987) has proved the following corollary.

Corollary 2.2. If the following moment conditions are satisfied, the design is slope-rotatable over all directions.

- 1. All odd order moments are zeros.
- 2. [ii] are equal for all i.
- 3. [iiii] are equal for all i.
- 4. [iiji] are equal for all $i \neq j$,

where [ii] are the pure second order moments.

We can have the following lemma which have relations with corollary 2.2.

Lemma 2.3. If the following moment conditions are satisfied, the design is slope-rotatable in axial directions(type II).

- 1. All odd order moments are zeros.
- 2. [ii] are equal for all i.
- 3. [iiii] are equal for all i.
- 4. [iijj] are equal for all $i \neq j$.

5.
$$\frac{[iiii]}{[iijj]} = 4 \frac{[iiii] + (k-2)[iijj] - (k-1)[ii]^2}{[iiii] + (k-1)[iijj] - k[ii]^2} + 1.$$

(Proof) If the preceding moment condition 1 is satisfied, we can show from the precision matrix $N(X'X)^{-1}$ that the equation (2.7) satisfied. Here, N is the number of design points. If the moment conditions 1 - 4 are satisfied, the form of X'X and $(X'X)^{-1}$ are given by Draper and Smith(1981, pp.392 - 393). It follows that

$$v_{ii} = R$$
 and $v_{ij} = \frac{1}{D}$, $i \neq j$

where $R = \{ N(C + (k-2)D) - (k-1)B^2 \} / A, A = (C-D)\{ N(C + (k-1)D) - kB^2 \},$

$$B = \sum_{u=1}^{N} x_{iu}^{2}, C = \sum_{u=1}^{N} x_{iu}^{4}, D = \sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2}, i \neq j.$$

From the moment condition 5, 4R = 1/D. Hence, the equation (2.6) is satisfied.

Let us denote $\lambda_{ii} = [ii]$, $\lambda_{iiii} = [iiii]$, $\lambda_{iijj} = [iijj]$. Victorbabu and Narasimham(1991) showed that when $\lambda_{ii} = \lambda_2$, $\lambda_{iiii} = c_0 \lambda_4$, and $\lambda_{iijj} = \lambda_4$ in Lemma 2.3, condition 5 changes as $\lambda_4 [(c_0 - 3)^2 - k(5 - c_0)] + \lambda_2^2 [k(5 - c_0) - 4] = 0$. Therefore, we can know that Lemma 2.3 is a generalization of Victorbabu and Narasimham(1991)'s result.

3. Conditions for Slope-Rotatability in Axial Directions

We provided the necessary and sufficient conditions for SRIAD(type II) in equations (2.6) and (2.7). But, it would be much more convenient if we could find the necessary and sufficient conditions for SRIAD(type II) based on the moment matrix rather than the precision matrix. For simplicity, let us assume that all odd order moments are 0. Then, we can provide the necessary and sufficient conditions for SRIAD(type II) in case of k=2 and k=3, respectively.

Case 1. k=2

If all odd order moments are 0, then equation (2.7) is satisfied. Then the moment matrix becomes

$$N^{-1}(X^{'}X) = \left(egin{array}{cccccc} 1 & 0 & 0 & \lambda_{11} & \lambda_{22} & 0 \ 0 & \lambda_{11} & 0 & 0 & 0 & 0 \ 0 & 0 & \lambda_{22} & 0 & 0 & 0 \ \lambda_{11} & 0 & 0 & \lambda_{1111} & \lambda_{1122} & 0 \ \lambda_{22} & 0 & 0 & \lambda_{1122} & \lambda_{2222} & 0 \ 0 & 0 & 0 & 0 & 0 & \lambda_{1122} \end{array}
ight)$$

Then, we can get

$$\begin{split} v_{11} &= \frac{1}{N} \frac{\lambda_{22}^2 - \lambda_{2222}}{\lambda_{2222} \lambda_{11}^2 + \lambda_{1111} \lambda_{22}^2 + \lambda_{1122}^2 - 2\lambda_{11} \lambda_{22} \lambda_{1122} - \lambda_{1111} \lambda_{2222}} \sigma^2 \\ v_{22} &= \frac{1}{N} \frac{\lambda_{11}^2 - \lambda_{1111}}{\lambda_{2222} \lambda_{11}^2 + \lambda_{1111} \lambda_{22}^2 + \lambda_{1122}^2 - 2\lambda_{11} \lambda_{22} \lambda_{1122} - \lambda_{1111} \lambda_{2222}} \sigma^2 \\ v_{12} &= \frac{1}{N} \frac{1}{\lambda_{1122}} \sigma^2 \end{split}$$

Therefore, we can express equation (2.6) by moments as the following:

$$4\lambda_{1122}(\lambda_{11}^2 - \lambda_{1111}) = 4\lambda_{1122}(\lambda_{22}^2 - \lambda_{2222})$$

$$= \lambda_{2222}\lambda_{11}^2 + \lambda_{1111}\lambda_{22}^2 + \lambda_{1122}^2 - 2\lambda_{11}\lambda_{22}\lambda_{1122} - \lambda_{1111}\lambda_{2222}.$$
(3.1)

Example 3.1. Let us consider the design of Box and Draper(1987, Exercise 15.2). The design points are (0,a), (0,-a), (b,c), (b,-c), (-b,c), (-b,-c). Here, a,b,c are all positive and we have (0,0) n_0 times. We can know that all odd order moments are zeros and even moments

$$\lambda_{11} = \frac{4b^2}{6+n_0} \text{, } \lambda_{22} = \frac{2(a^2+2c^2)}{6+n_0} \text{, } \lambda_{1111} = \frac{4b^4}{6+n_0} \text{, } \lambda_{2222} = \frac{2(a^4+2c^4)}{6+n_0} \text{, } \lambda_{1122} = \frac{4b^2c^2}{6+n_0} \text{.}$$

Thus, this design is a unbalanced design. From equation (3.1), we can obtain the following two equations.

$$\frac{(n_0+4)a^4 - 8a^2c^2 + 2(n_0+2)c^4}{4n_0a^4b^4} = \frac{1}{16b^2c^2},$$

$$\frac{n_0+2}{2n_0a^4} = \frac{1}{16b^2c^2}$$

There are infinite solutions. For $n_0 = 1$, one solution is a = 1, b = 0.9375, c = 0.2177.

Case 2. k=3

If all odd order moments are 0, then equation (2.7) is satisfied. Then the moment matrix becomes

Then, we can get

$$\begin{split} v_{11} &= \frac{1}{N} \frac{\lambda_{2222}\lambda_{3333} + 2\lambda_{22}\lambda_{33}\lambda_{2233} - \lambda_{2222}\lambda_{33}^2 - \lambda_{3333}^2\lambda_{22}^2 - \lambda_{2233}^2}{\rho} \sigma^2 \\ v_{22} &= \frac{1}{N} \frac{\lambda_{1111}\lambda_{3333} + 2\lambda_{11}\lambda_{33}\lambda_{1133} - \lambda_{1111}\lambda_{33}^2 - \lambda_{3333}^2\lambda_{11}^2 - \lambda_{1133}^2}{\rho} \sigma^2 \\ v_{33} &= \frac{1}{N} \frac{\lambda_{1111}\lambda_{2222} + 2\lambda_{11}\lambda_{22}\lambda_{1122} - \lambda_{1111}\lambda_{22}^2 - \lambda_{2222}^2\lambda_{11}^2 - \lambda_{1122}^2}{\rho} \sigma^2 \\ v_{12} &= \frac{1}{N} \frac{1}{\lambda_{1122}} \sigma^2 \\ v_{13} &= \frac{1}{N} \frac{1}{\lambda_{1133}} \sigma^2 \\ v_{23} &= \frac{1}{N} \frac{1}{\lambda_{2222}} \sigma^2 \end{split}$$

where $\rho = \lambda_{1111}\lambda_{2222}\lambda_{3333} + \lambda_{11}^2\lambda_{2233}^2 + \lambda_{22}^2\lambda_{1133}^2 + \lambda_{33}^2\lambda_{1122}^2 + 2\lambda_{11}\lambda_{22}\lambda_{1122}\lambda_{3333}$ $+ 2\lambda_{11}\lambda_{33}\lambda_{1133}\lambda_{2222} + 2\lambda_{22}\lambda_{33}\lambda_{2233}\lambda_{1111} + 2\lambda_{1122}\lambda_{1133}\lambda_{2233} - \lambda_{1111}\lambda_{2222}\lambda_{33}^2 - \lambda_{1111}\lambda_{3333}\lambda_{222}^2$ $- \lambda_{2222}\lambda_{3333}\lambda_{11}^2 - \lambda_{1111}\lambda_{2233}^2 - \lambda_{2222}\lambda_{1133}^2 - \lambda_{3333}\lambda_{1122}^2 - 2\lambda_{11}\lambda_{22}\lambda_{1133}\lambda_{2233} - 2\lambda_{11}\lambda_{33}\lambda_{1122}\lambda_{2233}$ $- 2\lambda_{22}\lambda_{33}\lambda_{1122}\lambda_{1133}$.

Therefore, we can express equation (2.6) by moments as the following:

$$\lambda_{1122} = \lambda_{1133} = \lambda_{2233} = \phi, \tag{3.2}$$

$$\begin{split} \lambda_{1111}\lambda_{2222} + 2\lambda_{11}\lambda_{22}\lambda_{1122} - \lambda_{1111}\lambda_{22}^2 - \lambda_{2222}\lambda_{11}^2 - \lambda_{1122}^2 \\ &= \lambda_{1111}\lambda_{3333} + 2\lambda_{11}\lambda_{33}\lambda_{1133} - \lambda_{1111}\lambda_{33}^2 - \lambda_{3333}\lambda_{11}^2 - \lambda_{1133}^2 \\ &= \lambda_{2222}\lambda_{3333} + 2\lambda_{22}\lambda_{33}\lambda_{2233} - \lambda_{2222}\lambda_{33}^2 - \lambda_{3333}\lambda_{22}^2 - \lambda_{2233}^2 = \frac{\rho}{4\phi} \,, \end{split}$$

Example 3.2. Let us consider two equiradial designs, icosahedral design and dodecahedral design. Icosahedral design consists of twelve vertices $(0, \pm a, \pm b)$, $(\pm b, 0, \pm a)$, $(\pm a, \pm b, 0)$ plus $n_0 \ge 1$ center points. This icosahedral design is a balanced design and all odd order moments are zeros. From equation (3.2), we can obtain the following one equation.

$$\frac{(4+n_0)(a^2+b^2)^2-(12+n_0)a^2b^2}{4n_0(a^4-a^2b^2+b^4)(a^2+b^2)^2} = \frac{1}{16a^2b^2}$$

Hence, we can obtain a/b=0.233 or a/b=4.290 for icosahedral design with $n_0=1$. Dodecahedral designs consists of twenty vertices $(0,\pm 1/c,\pm c)$, $(\pm c,0,\pm 1/c)$, $(\pm 1/c,\pm c,0)$, $(\pm 1,\pm 1,\pm 1)$ plus $n_0\geq 1$ center points. This dodecahedral design is also a balanced design and all odd order moments are zeros. From equation (3.2), we can obtain the following one equation.

$$\frac{(20+n_0)(c^4+c^{-4}+5)-8(c+c^{-1})^4}{4(c^4+c^{-4}-1)[(20+n_0)(c^4+c^{-4}+8)-12(c+c^{-1})^4]} = \frac{1}{48}$$

Hence, we can obtain c = 0.416 or c = 2.405 for dodecahedral design with $n_0 = 1$.

4. The Measures for Evaluating Slope-Rotatability

We can suppose slope variance measure Q(D) as the measure for evaluating SRIAD(type II) of balanced designs which satisfy moment condition 1-4 in Lemma 2.3, $\lambda_{ii} = \lambda_2$, $\lambda_{iiii} = c_0 \lambda_4$, and $\lambda_{iiji} = \lambda_4$ as follows:

$$Q(D) = |\lambda_A[(c_0 - 3)^2 - k(5 - c_0)] + \lambda_2^2[k(5 - c_0) - 4]|, \tag{4.1}$$

Q(D) is zero if and only if a design $D(a \text{ balanced design which satisfy moment condition } 1-4 in Lemma 2.3, <math>\lambda_{ii} = \lambda_2$, $\lambda_{iiii} = c_0 \lambda_4$, and $\lambda_{iijj} = \lambda_4$) is slope-rotatable in axial directions(type II). The value of Q(D) becomes larger as design D deviates from a

SRIAD(type II) design. Through the following three examples, we can know that Q(D) is a useful tool for evaluating SRIAD(type II) with respect to balanced designs which satisfy moment condition 1-4 in Lemma 2.3, $\lambda_{ii} = \lambda_2$, $\lambda_{iiii} = c_0 \lambda_4$, and $\lambda_{iijj} = \lambda_4$.

Example 4.1. Let us consider a rotatable central composite design(CCD) (k = 3, $\alpha = 8^{1/4}$) with various n_0 , the number of the central points. Table 4.1 shows the values of Q(D) in cases of various n_0 . We can find that this CCD approaches to a SRIAD(type II) design as the number of center points increases except $n_0 = 2$.

Table 4.1: The values of Q(D) in cases of various n_0

n_0	1	2	3	4	5	6	7	8	9	10
Q(D)	1.542	1.543	1.533	1.515	1.493	1.467	1.440	1.411	1.382	1.352

Example 4.2. Let us consider CCD(k=3, $n_0=1$) with various α . We can find that the value of Q(D) is zero at $\alpha=2.4324$, namely, CCD becomes a SRIAD(type II) design at $\alpha=2.4324$.

Example 4.3. For comparing the conditions for rotatability and slope-rotatability, we can select the CCD, icosahedral design, and dodecahedral design with k = 3 and the number of center points, $n_0 = 1$. Table 4.2 shows the conditions for rotatability and slope-rotatability with respect to three designs.

Table 4.2: The conditions for rotatability and slope-rotatability

design	constant	rotatability	slope-rotatability in axial direction (type II)	slope-rotatability over all direction
CCD	α	1.682	2.432	arbitrary positive
icosahedral design	a/b	1.618	0.233 or 4.290	arbitrary positive
dodecahedral design	c	1.618	0.416 or 2.405	arbitrary positive

We cannot use Q(D) in case of unbalanced designs. And, Q(D) is single-valued ones which describe the nearness to slope-rotatability of the design as a whole and do not give a comprehensive picture of the behavior of the slope variances throughout a region. Thus, we can suggest a graphical method. The quantiles of $\frac{1}{\sigma^2} Var(\frac{\partial \hat{y}(x)}{\partial x_i})$ can be obtained by

randomly selecting a large number of points on the hypersphere of radius r centered at the design origin. We denote pth quantile by $Q_r(p)$. Quantile plots of $Q_r(p)$ versus p can be then obtained for selected values of r within the region. This quantile plots are used to give a comprehensive picture of the behavior of the slope variance throughout a region and hence of the quality of the slope of the predicted response obtained with a particular design. Such plots are used to investigate and compare SRIAD(type II) of certain response surface designs. Through the following example, we can know that quantile plot is a useful tool for evaluating SRIAD(type II) with respect to balanced designs or unbalanced designs.

Example 4.4. Roquemore 311A and 311B designs(Roquemore(1976)) are unbalanced designs and all odd order moments are zeros. Figure 4.1 shows quantile plots of Roquemore 311A and 311B designs with various radii. From these graphs, we can find that Roquemore 311A and 311B designs are not slope-rotatable in axial directions(type II) but that Roquemore 311B design is better than Roquemore 311A design with respect to SRIAD(type II). Roquemore 311B design have the same shape of quantile plot with respect to 3 design variables. On the other hand, in Roquemore 311A design, quantile plot with respect to design variable x_3 is different from quantile plots with respect to design variable x_1 and x_2 .

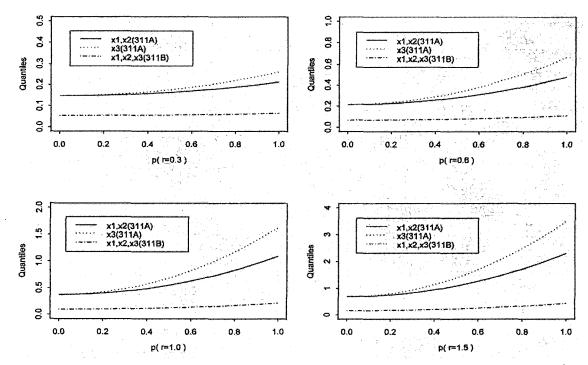


Figure 4.1. Quantile plots for roquemore 311A and 311B designs(r = 0.3, 0.6, 1.0, 1.5)

5. Conclusion

We studied the conditions for slope-rotatability in axial directions and the measures for evaluating slope-rotatability in axial directions. Q(D) and quantile plot can be used as the tools for evaluating slope-rotatability in axial directions(type II) with respect to the given response surface design. Conditions for slope-rotatability in axial directions(type II) in case of $k \ge 4$ based on moment matrix, will be the obvious extension of this study.

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