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SLOPE ROTATABILITY OF ICOSAHEDRON AND DODECAHEDRON DESIGNS†

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ABSTRACT

Icosahedron and dodecahedron designs are experimental designs which can be used for response surface analysis for the case when three independent variables are involved. When we are interested in estimating the slope of a response surface, slope rotatability is a desirable property. In this paper, we derive conditions for icosahedron and dodecahedron designs to have slope rotatability, and actually obtain some slope-rotatable icosahedron and dodecahedron designs. We also apply Park and Kim (1992)'s measure of slope rotatability to icosahedron and dodecahedron designs, and observe resultant facts.

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1. INTRODUCTION

Icosahedron and dodecahedron designs are response surface designs which can be used for the case when three independent variables are under consideration. One of the advantages of these types of design is that they conveniently afford rotatable designs and orthogonal designs. They also provide uniform precision designs and designs which are both rotatable and orthogonal or near-orthogonal if the numbers of center points are suitably determined.

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When we are interested in estimating the slope of a response surface, slope rotatability is a desirable property. There are two types of slope rotatability: slope rotatability over axial directions (Hader and Park, 1978) and slope rotatability over all directions (Park, 1987). It was found that every icosahedron design and every dodecahedron design have slope rotatability over all directions. So, from now on, slope rotatability means slope rotatability over axial directions.

This problem, estimation of slopes, occurs frequently in practical situations. For instance, there are cases in which one wants to estimate rates of reaction in chemical experiments, rates of change in the yield of a crop to various fertilizers, rates of disintegration of radioactive material in an animal, and so forth (see Park, 1987).

In this paper, we will derive conditions for icosahedron and dodecahedron designs to be slope-rotatable designs, and actually obtain some slope-rotatable icosahedron and dodecahedron designs. We will also apply the measure of slope rotatability proposed by Park and Kim (1992) to icosahedron and dodecahedron designs, and observe some resultant facts.

2. A MEASURE OF SLOPE ROTATABILITY

We consider the second order polynomial regression model

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \beta_{ii} x_{iu}^2 + \sum_{i<j}^{k} \beta_{ij} x_{iu} x_{ju} + \varepsilon_u, \ u = 1, 2, \ldots, N,$$

where x_{iu} denotes the level of the i^{th} factor in the u^{th} run of the experiment and y_u is the observed value of the response variable in the u^{th} run. β_0, β_i, β_{ii} and β_{ij} are unknown regression coefficients and ε_u's are uncorrelated random errors with mean zero and variance σ^2. The fitted equation by the least squares method can be written as

$$\hat{y} = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{i=1}^{k} b_{ii} x_i^2 + \sum_{i<j}^{k} b_{ij} x_i x_j,$$

where b_0, b_i, b_{ii} and b_{ij} are the least squares estimates of $\beta_0, \beta_i, \beta_{ii}$ and β_{ij} respectively.

Let us consider a particular class of response surface designs that satisfy the following conditions:

$$\begin{aligned}
&\mathrm{Cov}(b_i, b_{ii}) = \mathrm{Cov}(b_i, b_{ij}) = \mathrm{Cov}(b_{ii}, b_{ij}) = \mathrm{Cov}(b_{ij}, b_{il}) = 0, \quad i \neq j \neq l \neq i, \\
&\mathrm{Var}(b_i) \text{ are equal for all } i, \\
&\mathrm{Var}(b_{ii}) \text{ are equal for all } i \text{ and} \\
&\mathrm{Var}(b_{ij}) \text{ are equal for all } (i,j) \text{ where } i \neq j. \qquad (2.1)
\end{aligned}$$

Icosahedron and dodecahedron designs belong to this class.

Park and Kim (1992) proposed a measure of slope rotatability for second order response surface designs. The measure generally has a very complicated form, but for the class of designs satisfying (2.1) it has a much simpler form as follows:

$$\begin{aligned}
Q_k(D) &= \frac{1}{\sigma^4}\{4\mathrm{Var}^{(a)}(b_{11}) - \mathrm{Var}^{(a)}(b_{12})\}^2 \\
&= \frac{[ii]^4}{\sigma^4}\{4\mathrm{Var}^{(b)}(b_{11}) - \mathrm{Var}^{(b)}(b_{12})\}^2, \qquad (2.2)
\end{aligned}$$

where $^{(a)}$ and $^{(b)}$ represent 'after scaling' and 'before scaling' respectively, and $[ii] = \sum_{u=1}^{N} x_{iu}^2/N$ (before scaling). Here scaling means letting the designs have the following first and pure second design moments so that fair comparisons can be made (see Myers, 1976, p. 135; Khuri and Cornell, 1996, p. 108)

$$\begin{aligned}
[i] &= \frac{1}{N}\sum_{u=1}^{N} x_{iu} = 0 \quad \text{and} \\
[ii] &= \frac{1}{N}\sum_{u=1}^{N} x_{iu}^2 = 1.
\end{aligned}$$

The design D is slope-rotatable if and only if the value of $Q_k(D)$ is zero, and D becomes further from a slope-rotatable design as $Q_k(D)$ becomes larger.

3. ICOSAHEDRON DESIGN

This type of design is for the case of three independent variables. It consists of twelve vertices of the icosahedron, plus $n_0 \geq 1$ center points. The design matrix D is given by

x_1	x_2	x_3
0	$-a_1$	$-a_2$
0	$-a_1$	a_2
0	a_1	$-a_2$
0	a_1	a_2
$-a_2$	0	$-a_1$
a_2	0	$-a_1$
$-a_2$	0	a_1
a_2	0	a_1
$-a_1$	$-a_2$	0
$-a_1$	a_2	0
a_1	$-a_2$	0
a_1	a_2	0
0	0	0
⋮	⋮	⋮
0	0	0 .

Here a_1 and a_2 are positive numbers such that $a_1 \geq a_2$. Note that if $a_1 = a_2$, then the icosahedron design is the same as the Box-Behnken design (Box and Behnken, 1960). The moments of this configuration are given by

$$[ii] = \frac{4(a_1^2 + a_2^2)}{12 + n_0} \text{ for all } i,$$

$$[iiii] = \sum_{u=1}^{N} \frac{x_{iu}^4}{N} = \frac{4(a_1^4 + a_2^4)}{12 + n_0} \text{ for all } i,$$

$$[iijj] = \sum_{u=1}^{N} \frac{x_{iu}^2 x_{ju}^2}{N} = \frac{4a_1^2 a_2^2}{12 + n_0} \text{ for any } (i, j) \text{ where } i \neq j,$$

and all odd moments $= 0$. $a_1/a_2 = (\sqrt{5} + 1)/2 = 1.6180$ gives an icosahedron design which is rotatable in the Box-Hunter (1957) sense.

The variances of the quadratic coefficients are found to be

$$\text{Var}^{(b)}(b_{12}) = \frac{\sigma^2}{4a_1^2 a_2^2} \text{ and}$$

$$\text{Var}^{(b)}(b_{11}) = \left\{ \frac{(4 + n_0)(a_1^2 + a_2^2)^2 - (12 + n_0)a_1^2 a_2^2}{4n_0(a_1^4 - a_1^2 a_2^2 + a_2^4)(a_1^2 + a_2^2)^2} \right\} \sigma^2.$$

Therefore, we have by (2.2)

$$Q_3(D) = \left\{\frac{4(t^2+1)}{12+n_0}\right\}^4 \left\{\frac{(4+n_0)t^4+(n_0-4)t^2+(4+n_0)}{n_0(t^4-t^2+1)(t^2+1)^2} - \frac{1}{4t^2}\right\}^2,$$

where $t = a_1/a_2$. $Q_3(D)$ depends on a_1 and a_2 only through a_1/a_2. Setting $Q_3(D) = 0$ leads to a fourth degree polynomial equation in t^2:

$$n_0t^8 - (16+3n_0)t^6 + (16-4n_0)t^4 - (16+3n_0)t^2 + n_0 = 0.$$

The solution of this equation gives the value of t which makes the icosahedron design slope-rotatable. These values of t for various n_0 are given in Table 3.1. From Table 3.1, we note that the value of t that makes the icosahedron design slope-rotatable decreases as n_0 increases.

TABLE 3.1 *Values of $t = a_1/a_2$ for slope-rotatable icosahedron designs*

n_0	t	n_0	t
1	4.2900	6	2.4573
2	3.2744	7	2.3957
3	2.8796	8	2.3496
4	2.6711	9	2.3137
5	2.5433	10	2.2850

For example, when $n_0 = 1$, an icosahedron design with $t = 4.29$ is a slope-rotatable design. Such a design is obtained if we use $(a_1, a_2) = (4.29, 1), (8.58, 2)$ or (12.87, 3), *etc.* Suppose we use $a_1 = 4.29$ and $a_2 = 1$. Then the levels used for each independent variable are −4.29, −1, 0, 1 and 4.29. Let us illustrate this in terms of natural variables. Suppose one of the factors is temperature. If the central level of temperature is 250°C and the difference between the levels represented by 0 and 1 (in coded variables) is 20°C, then the five levels of temperature (in °C) will be 164.2, 230, 250, 270 and 335.8.

On the other hand, Table A.1 in Appendix gives the values of $Q_3(D)$ for the icosahedron designs for various values of t and n_0. It is observed from Table A.1 that for a given n_0, as t increases ($t \geq 1.0$), the value of $Q_3(D)$ decreases to zero and increases thereafter. The results in Table A.1 are displayed in Figure 3.1.

4. DODECAHEDRON DESIGN

This type of design is also for the case of three independent variables. It consists of twenty vertices of the dodecahedron, plus $n_0 \geq 1$ center points, where

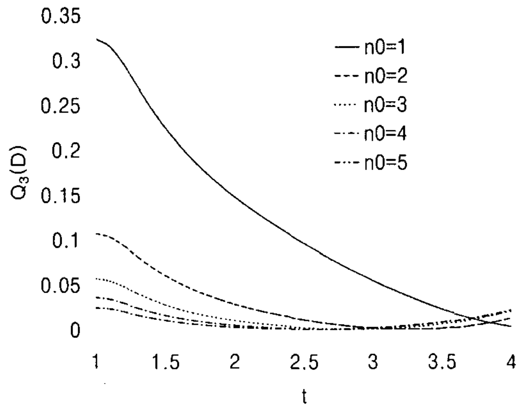

FIGURE 3.1 *Plot of $Q_3(D)$ against $t = a_1/a_2$ for icosahedron designs*

$c \geq 1$. The design matrix D is given by

x_1	x_2	x_3
0	$-c^{-1}$	$-c$
0	$-c^{-1}$	c
0	c^{-1}	$-c$
0	c^{-1}	c
$-c$	0	$-c^{-1}$
c	0	$-c^{-1}$
$-c$	0	c^{-1}
c	0	c^{-1}
$-c^{-1}$	$-c$	0
$-c^{-1}$	c	0
c^{-1}	$-c$	0
c^{-1}	c	0
-1	-1	-1
-1	-1	1
-1	1	-1
-1	1	1
1	-1	-1

(*continued*)

x_1	x_2	x_3
1	−1	1
1	1	−1
1	1	1
0	0	0
⋮	⋮	⋮
0	0	0 .

The moments of this configuration are

$$[ii] = \frac{4(c+c^{-1})^2}{20+n_0} \text{ for all } i,$$

$$[iiii] = \frac{4(c^2+c^{-2})^2}{20+n_0} \text{ for all } i \text{ and}$$

$$[iijj] = \frac{12}{20+n_0} \text{ for any } (i,j) \text{ where } i \neq j,$$

and all odd moments = 0. $c = (\sqrt{5}+1)/2 = 1.6180$ gives a dodecahedron design which is rotatable in the Box-Hunter (1957) sense.

The variances of the quadratic coefficients are found to be

$$\mathrm{Var}^{(b)}(b_{12}) = \frac{1}{12}\sigma^2,$$

$$\mathrm{Var}^{(b)}(b_{11}) = \left[\frac{(20+n_0)c^4(c^8+5c^4+1) - 8c^4(c^2+1)^4}{4(c^8-c^4+1)\{(20+n_0)(c^8+8c^4+1) - 12(c^2+1)^4\}}\right]\sigma^2.$$

Hence by (2.2) it is obtained that

$$Q_3(D) = \frac{\{2(c+c^{-1})\}^8}{(20+n_0)^4} \times \left[\frac{(20+n_0)c^4(c^8+5c^4+1) - 8c^4(c^2+1)^4}{(c^8-c^4+1)\{(20+n_0)(c^8+8c^4+1) - 12(c^2+1)^4\}} - \frac{1}{12}\right]^2.$$

Setting $Q_3(D) = 0$ leads to an eighth degree polynomial equation in c^2:

$$(8+n_0)c^{16} - 48c^{14} - (64+5n_0)c^{12} + 384c^{10} - (696+66n_0)c^8 + 384c^6 - (64+5n_0)c^4 - 48c^2 + (8+n_0) = 0.$$

The solution of this equation gives the value of c which makes the dodecahedron design slope-rotatable. Table 4.1 shows these values of c for various n_0. It is noted from Table 4.1 that the value of c that makes the dodecahedron design slope-rotatable decreases as n_0 increases. For example, when $n_0 = 1$, a dodecahedron design with $c = 2.4050$ is a slope-rotatable design. For this design, the levels used for each independent variable are -2.4050, -1, -0.4158, 0, 0.4158, 1 and 2.4050. Suppose again that one of the factors is temperature. If the central level of temperature is 250°C and the difference between the levels represented by 0 and 1 (in coded variables) is 20°C, then the seven levels of temperature (in °C) will be 201.90, 230, 241.68, 250, 258.32, 270 and 298.10.

The values of $Q_3(D)$ for the dodecahedron designs are given in Table A.2 in Appendix for various values of c and n_0. From Table A.2, we observe that when $n_0 \geq 2$, as c increases ($c \geq 1.0$), the value of $Q_3(D)$ decreases to zero and increases thereafter, but when $n_0 = 1$, $Q_3(D)$ has a local minimum and a local maximum before it becomes zero ($Q_3(D) = 0.2017$ and 0.2098 when $c = 1.4$ and 1.5, respectively), and decreases to zero and increases thereafter. The results in Table A.2 are displayed in Figure 4.1.

TABLE 4.1 *Values of c for slope-rotatable dodecahedron designs*

n_0	c	n_0	c
1	2.4050	6	2.0948
2	2.3103	7	2.0648
3	2.2362	8	2.0403
4	2.1779	9	2.0199
5	2.1317	10	2.0028

5. CONCLUDING REMARKS

One of the advantages of icosahedron and dodecahedron designs is that they require relatively small number of experimental runs as compared with designs of other types. Table 5.1 shows the numbers of experimental runs required for 3^3 factorial, central composite, icosahedron and dodecahedron designs. As we see in this table, in particular, the number of experimental runs for the icosahedron design is less than that for the central composite design if the number of center points is the same. Another advantage of icosahedron and dodecahedron designs is that they enable us to conveniently obtain designs having various desirable properties by handling the values of the design parameters (a_1/a_2 for the icosahedron design and c for the dodecahedron design). This is just like that we can

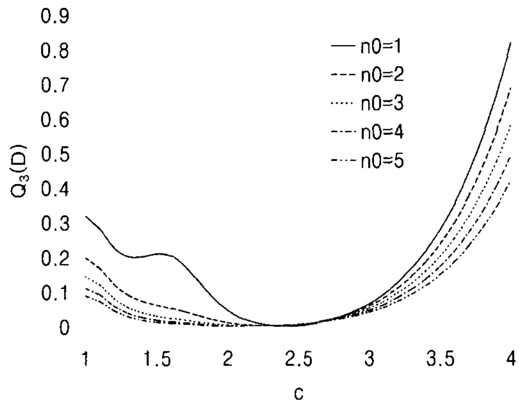

FIGURE 4.1 *Plot of $Q_3(D)$ against c for dodecahedron designs.*

TABLE 5.1 *Numbers of experimental runs for some kinds of design*

n_0	1	2	3	4	5
3^3 factorial	27	28	29	30	31
central composite	15	16	17	18	19
icosahedron	13	14	15	16	17
dodecahedron	21	22	23	24	25

obtain central composite designs with desirable properties by handling the value of α, which is the number determining the positions of the axial points.

When we are interested in the estimation of the slope of a response surface, slope rotatability is an important property. In this paper, we studied slope rotatability of icosahedron and dodecahedron designs. Specifically, we derived conditions that icosahedron and dodecahedron designs be slope-rotatable designs, and we actually obtained slope-rotatable icosahedron and dodecahedron designs for which the numbers of center points are from one to ten. We also computed the values of the measure of slope rotatability proposed by Park and Kim (1992) for various icosahedron and dodecahedron designs. In addition, for visual comprehension, we displayed plottings of the slope rotatability measure for various icosahedron and dodecahedron designs.

APPENDIX

TABLE A.1 *Values of $Q_3(D)$ for icosahedron designs*

t \ n_0	1	2	3	4	5	6	7
1.0	0.3227	0.1066	0.0562	0.0352	0.0240	0.0173	0.0130
1.1	0.3142	0.1024	0.0535	0.0333	0.0227	0.0163	0.0122
1.2	0.2942	0.0927	0.0474	0.0291	0.0196	0.0140	0.0104
1.3	0.2702	0.0812	0.0403	0.0242	0.0161	0.0113	0.0083
1.4	0.2464	0.0701	0.0336	0.0197	0.0128	0.0089	0.0065
1.5	0.2247	0.0602	0.0277	0.0157	0.0100	0.0068	0.0049
1.6	0.2055	0.0518	0.0228	0.0125	0.0077	0.0052	0.0036
1.7	0.1885	0.0445	0.0186	0.0098	0.0059	0.0038	0.0026
1.8	0.1733	0.0383	0.0152	0.0076	0.0044	0.0028	0.0018
1.9	0.1597	0.0329	0.0122	0.0058	0.0032	0.0019	0.0012
2.0	0.1472	0.0281	0.0097	0.0043	0.0022	0.0013	0.0008
2.1	0.1357	0.0238	0.0076	0.0031	0.0015	0.0008	0.0004
2.2	0.1249	0.0200	0.0057	0.0021	0.0009	0.0004	0.0002
2.3	0.1147	0.0166	0.0042	0.0013	0.0004	0.0001	0.0000
2.4	0.1050	0.0135	0.0029	0.0007	0.0002	0.0000	0.0000
2.5	0.0957	0.0107	0.0018	0.0003	0.0000	0.0000	0.0001
2.6	0.0868	0.0082	0.0010	0.0000	0.0000	0.0001	0.0002
2.7	0.0782	0.0061	0.0004	0.0000	0.0002	0.0004	0.0004
2.8	0.0700	0.0042	0.0001	0.0002	0.0005	0.0007	0.0008
2.9	0.0622	0.0027	0.0000	0.0005	0.0010	0.0012	0.0012
3.0	0.0546	0.0015	0.0002	0.0011	0.0016	0.0018	0.0018
3.1	0.0475	0.0006	0.0007	0.0019	0.0025	0.0026	0.0025
3.2	0.0407	0.0001	0.0015	0.0030	0.0035	0.0035	0.0033
3.3	0.0343	0.0000	0.0026	0.0043	0.0048	0.0046	0.0043
3.4	0.0283	0.0003	0.0040	0.0059	0.0062	0.0059	0.0054
3.5	0.0228	0.0011	0.0058	0.0077	0.0079	0.0074	0.0066
3.6	0.0177	0.0023	0.0080	0.0099	0.0099	0.0091	0.0080
3.7	0.0133	0.0041	0.0106	0.0124	0.0121	0.0109	0.0096
3.8	0.0093	0.0064	0.0137	0.0153	0.0146	0.0130	0.0114
3.9	0.0060	0.0093	0.0172	0.0185	0.0174	0.0154	0.0134
4.0	0.0034	0.0127	0.0212	0.0222	0.0205	0.0180	0.0155

TABLE A.2 *Values of $Q_3(D)$ for dodecahedron designs*

c \ n_0	1	2	3	4	5	6	7
1.0	0.3185	0.1999	0.1443	0.1111	0.0887	0.0725	0.0602
1.1	0.2806	0.1686	0.1191	0.0904	0.0715	0.0580	0.0480
1.2	0.2269	0.1211	0.0805	0.0589	0.0454	0.0362	0.0295
1.3	0.2018	0.0901	0.0547	0.0379	0.0281	0.0218	0.0174
1.4	0.2017	0.0729	0.0399	0.0258	0.0183	0.0137	0.0106
1.5	0.2098	0.0621	0.0306	0.0185	0.0124	0.0089	0.0067
1.6	0.2047	0.0525	0.0236	0.0133	0.0085	0.0058	0.0042
1.7	0.1742	0.0418	0.0175	0.0093	0.0056	0.0037	0.0025
1.8	0.1274	0.0304	0.0121	0.0060	0.0034	0.0021	0.0013
1.9	0.0816	0.0198	0.0074	0.0033	0.0017	0.0009	0.0005
2.0	0.0466	0.0112	0.0037	0.0014	0.0006	0.0002	0.0001
2.1	0.0234	0.0050	0.0012	0.0003	0.0000	0.0000	0.0000
2.2	0.0095	0.0013	0.0001	0.0000	0.0002	0.0003	0.0004
2.3	0.0023	0.0000	0.0003	0.0007	0.0010	0.0012	0.0012
2.4	0.0000	0.0009	0.0019	0.0025	0.0027	0.0028	0.0027
2.5	0.0017	0.0039	0.0050	0.0054	0.0054	0.0051	0.0048
2.6	0.0068	0.0092	0.0099	0.0097	0.0092	0.0084	0.0077
2.7	0.0154	0.0169	0.0167	0.0156	0.0143	0.0129	0.0116
2.8	0.0276	0.0275	0.0258	0.0234	0.0210	0.0187	0.0166
2.9	0.0440	0.0414	0.0376	0.0335	0.0297	0.0262	0.0231
3.0	0.0651	0.0592	0.0527	0.0464	0.0407	0.0356	0.0313
3.1	0.0918	0.0816	0.0716	0.0624	0.0544	0.0474	0.0414
3.2	0.1251	0.1094	0.0950	0.0823	0.0713	0.0620	0.0540
3.3	0.1661	0.1437	0.1239	0.1067	0.0922	0.0798	0.0694
3.4	0.2164	0.1856	0.1591	0.1366	0.1176	0.1016	0.0882
3.5	0.2774	0.2365	0.2018	0.1727	0.1484	0.1280	0.1109
3.6	0.3509	0.2978	0.2533	0.2163	0.1855	0.1598	0.1383
3.7	0.4393	0.3714	0.3151	0.2685	0.2299	0.1978	0.1710
3.8	0.5447	0.4592	0.3888	0.3308	0.2829	0.2432	0.2101
3.9	0.6700	0.5635	0.4763	0.4048	0.3458	0.2971	0.2565
4.0	0.8183	0.6869	0.5798	0.4922	0.4202	0.3607	0.3113

REFERENCES

BOX, G. E. P. AND BEHNKEN, D. W. (1960). "Some new three level designs for the study of quantitative variables", *Technometrics*, **2**, 455–475.

BOX, G. E. P. AND HUNTER, J. S. (1957). "Multi-factor experimental designs for exploring response surfaces", *Annals of Mathematical Statistics*, **28**, 195–241.

HADER, R. J. AND PARK, S. H. (1978). "Slope-rotatable central composite designs", *Technometrics*, **20**, 413–417.

KHURI, A. I. AND CORNELL, J. A. (1996). *Response Surfaces. Designs and Analyses*, 2nd ed., Marcel Dekker, New York.

MYERS, R. H. (1976). *Response Surface Methodology*, Blacksburg, VA:Author (distributed by Edwards Brothers, Ann Arbor, MI).

PARK, S. H. (1987). "A class of multifactor designs for estimating the slope of response surfaces", *Technometrics*, **29**, 449–453.

PARK, S. H. AND KIM, H. J. (1992). "A measure of slope-rotatability for second order response surface experimental designs", *Journal of Applied Statistics*, **19**, 391–404.