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ON THE DESIGN POINTS FOR A ROTATABLE ORTHOGONAL CENTRAL COMPOSITE DESIGN

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Abstract:

- The aim of this paper is to adjust the existing believe on the condition that a Rotatable Orthogonal Central Composite Design can be created from an Orthogonal Central Composite Design. Therefore the appropriate introduction is discussed concerning the Rotatable Orthogonal Central Composite Design. Then, the main result is presented, i.e. The necessary and sufficient conditions in order an Orthogonal Central Composite Design to be Rotatable.

Key-Words:

- *rotatable design; orthogonal design; central design; composite design.*

AMS Subject Classification:

- 62K20, 62K10, 62K15.

1. INTRODUCTION

When we are constructing designs to explore the overall response surface, rather than the response to individual factors, the main request is for optimum position, i.e. the combination of factor levels for which the expected response is maximized. In principle, the design of an experiment to explore the response surface will cover — eventually — only a region of the unknown surface, for which a rather known center exists. Therefore observations at the center are important. Moreover, blocking and replication are always important, as for any experiment. Therefore, the Response Surface Method (RSM) is based on this framework. As an example, there is a nice experiment to investigate the effect of the levels of two additives on the quality of a cake production process in [7]. In addition to the factorial experiment portion as well as to the number of observations at the center, additional points are added to the design of each factor or, equivalently, to each axis, known as axial (or star).

Therefore, a Central Composite Design (CCD) is: an experimental fractional design which is supplemented by additional experimental points such as center points and star points. In principle, we need the main effects to be separately estimated. That is why the sense of Orthogonal design is essential: a design in which the given variables (or a linear combination of them) are regarded as statistical independent. In RSM it is important to choose the "path" towards the optimum. Thus, the steepest accent method is applied from the Numerical Analysis (see [5] among others), while the sequential principle of design is adopted. Therefore, the Rotatable design is a real need to be defined, as the one which has equal predictive power (predictiveness) in all directions from the center point and from the points that are at equidistant from the center.

The aim of this paper is to discuss, and eventually adjust, the necessary and sufficient conditions, for the number of design points, to be satisfied so that to estimate the design points for an Orthogonal Central Composite Design (OCCD) to be rotatable (ROCCD). The problem has been discussed extensively by [3], [7], [6], [8], where the conditions for a Central Composite Design (CCD) to be OCCD and ROCCD are reviewed and examined. We shall refer and extend/adjust the condition for a ROCCD, as appeared in [6, p. 304] and [7, p. 550]. The improvement is that the imposed already condition is now used for obtaining real solutions, when positive integer solution is actually needed. To to the best of our knowledge, we have not see any attempts trying to adjust this conclusion. This adjustment is our contribution, so that the experimenter can work to Response Surface Methods, with a number of up to 14 input variables, as we are providing the appropriate calculations, based on the developed theory. For a compact form of the obtained calculations see Table 1. Through out this paper the standard notation for the Response Surface Methods is adopted; see [6] and [8].

2. CONDITIONS FOR A ROCCD

The Central Composite Design (CCD) appears an aesthetic appeal within the class of the second order response surface design. It was introduced in the pioneering paper of [4]. In principle the Central Composite Design (CCD) can always be constructed as a two block Orthogonal (OCCD). This is based in two blocks: the factorial portion and the star portion. The first block is based on N_{F} factorial points and N_{CF} center points. The second block is based on N_{A} axial points and N_{CA} center points for the star portion. It has been traditionally denoted by (a) the distance of the star points from the center of the design. For a factorial or fractional factorial experiment $N_{\mathrm{F}} = 2^q$ or 2^{k-q} observations are needed. Consider $N_{\mathrm{A}} = 2k$ points with k being the number of input variables and q such that $0 < k < q$.

For Orthogonal blocking, in two blocks in a CCD, the fractional of the total sum of squares, of each input variable contributed by every block, has to be equal to the fraction of the total observations allotted to the block. It is, for each block,

$$\frac{N_{\mathrm{F}}}{N_{\mathrm{F}} + 2a^2} = \frac{N_{\mathrm{F}} + N_{\mathrm{CF}}}{N} \quad \text{and} \tag{2.1a}$$

$$\frac{2a^2}{N_{\mathrm{F}} + 2a^2} = \frac{N_{\mathrm{A}} + N_{\mathrm{CA}}}{N}\,, \tag{2.1b}$$

respectively. The total number of observation is then $N = N_{\mathrm{F}} + N_{\mathrm{A}} + N_{\mathrm{C}}$, with N_{C} the number of central points i.e. $N_{\mathrm{C}} = N_{\mathrm{CF}} + N_{CA}$. Then from (2.1a) and (2.1b) it is

$$a^2 = \frac{N_{\mathrm{F}}\big(2k + N_{\mathrm{CA}}\big)}{2\big(N_{\mathrm{F}} + N_{\mathrm{CF}}\big)}\,. \tag{2.2}$$

When the design is required to be also a rotatable one, then [6, p. 304],

$$a^2 = N_{\mathrm{F}}^{1/2}\,. \tag{2.3}$$

From (2.2) and (2.3) the second degree equation

$$2N_{\mathrm{F}} - N_{\mathrm{F}}^{1/2}\big(2k + N_{\mathrm{CA}}\big) + 2N_{\mathrm{CF}} \;=\; 0\,, \tag{2.4}$$

has to be satisfied, see also [7, p. 550]. Both [7] and [6] note that is not always possible to find a design that satisfies (2.4). Moreover, in [6] is provided as a necessary condition for the satisfaction of equation (2.4) the relation

$$D \;=\; \big(2k + N_{\mathrm{CA}}\big)^2 - 16N_{\mathrm{CF}} \;\geq\; 0\,, \tag{2.5}$$

But the discriminant D positive means that (2.4) has real roots. And we are looking for positive integers as solution of (2.4). This is the crucial point. The necessary and sufficient conditions, so that the number of the design points N_{F} for a ROCCD needs more investigation and we are providing this investigation in section 3.

3. INTEGER SOLUTION FOR A ROCCD

Trivially the coefficient of the second order equation (2.4) are asked to be positive integers and not just real numbers. We state and prove in Appendix A the following Theorem which shall help us to develop the line of though tackling the problem, see Theorem 3.1 and Proposition 3.1.

Theorem 3.1. *Consider the second order equation*

$$Ax^2 + Bx + C = 0\,, \tag{3.1}$$

with A, B and C integers. Then the roots of (3.1) *are integers if and only if*

1. *A divides B, i.e.* $A \big| B$,
2. *A divides C, i.e.* $A \big| C$, *and*
3. *The discriminant D of* (3.1) *is a square, i.e.* $D = \mu^2 \in \mathbb{Z}$.

Now, consider (2.4). The following theorem holds.

Theorem 3.2. *The necessary and sufficient conditions in order the equation*

$$2N_{\rm F} - N_{\rm F}^{1/2}\big(2k + N_{\rm CA}\big) + 2N_{\rm CF} \;=\; 0\,, \tag{3.2}$$

to have positive integer solutions are:

$$2\big|N_{\rm CA}\,, \quad \text{i.e. 2 divides } N_{\rm CA}\,, \quad \text{i.e. is even}\,, \tag{3.3a}$$

$$D = \big(2k + N_{\rm CA}\big)^2 - 16N_{\rm CF} \;=\; \mu^2\,, \qquad \mu \in \mathbb{Z}\,. \tag{3.3b}$$

Proof: Trivially, if we let $x = N_{\rm F}^{1/2}$, (3.2) is then reduced to (3.1) with $A = 2$, $B = -\big(2k + N_{\rm CA}\big)$, $C = 2N_{\rm CF}$. Therefore condition (1) of Theorem 3.1 is reduced to (3.3a), (2) holds, and (3) is reduced to (3.3b). Thus, the roots are integer numbers. Moreover the sum of roots of (3.2) is $(2k + N_{\rm CA}) > 0$ and the product of roots is $2N_{CF} > 0$. Therefore, the integer roots are positive. Eventually the conditions (3.3a) and (3.3b) are necessarily and sufficient to have positive integer roots. □

Practically the factorial portion consists from a 2^k design. Usually k is not greater than 6, otherwise a portion 2^{k-p} is used. We investigate next the cases of k up to 14 in the following Proposition.

Proposition 3.1. *Consider (3.2) and the case that $N_{\rm F} = 2^k$. Then, an integer solution exists for k even. Moreover, for*

$$k = 2, 4, 6, 8, 10, 12, 14\,, \tag{3.4}$$

the relation between $N_{\rm CF}$ and $N_{\rm CA}$ should be of the form

$$N_{\rm CF} = 2^v\big(N_{\rm CA} - K\big)\,, \qquad v = \tfrac{1}{2}k - 1\,, \tag{3.5}$$

and $K = K(k)$

$$K = 0, 0, 4, 16, 44, 104, 228\,, \tag{3.6}$$

respectively.

Proof: Trivially k has to be an even integer otherwise there is no integer solution. Thus, $2^{k/2}$ has to be integer. Now, from (3.2), we obtain:

For $k = 2$: $2^3 - 2\big(4 + N_{\rm CA}\big) + 2N_{\rm CF} = 0$, i.e. $N_{\rm CF} = N_{\rm CA} = 2^0(N_{\rm CA} - 0)$.

For $k = 4$: $N_{\rm CF} = 2N_{\rm CA} = 2^1\big(N_{\rm CA} - 0\big)$.

For $k = 6$: $N_{\rm CF} = 4N_{\rm CA} - 16 = 2^2\big(N_{\rm CA} - 4\big)$.

In order that both $N_{\rm CF}$ and $N_{\rm CA}$ be positive integers, it is required to be $N_{\rm CF} = 4p$, $p \in \mathbb{Z}^+$ as

$$\tfrac{1}{4}N_{\rm CF} + 4 = N_{\rm CA}.$$

Therefore for $k = 6$,

$$N_{\rm CF} = 4p\,, \qquad N_{\rm CA} = p + 4\,.$$

For $k = 8$ it is from (3.2)

$$\begin{aligned} 2^8 - 2^3\big(16 + N_{\rm CA}\big) + N_{\rm CF} &= 0, \quad \text{i.e.} \\ N_{\rm CF} &= 8N_{\rm CA} - 128 = 2^3\big(N_{\rm CA} - 16\big)\,. \end{aligned}$$

Now, in order that both $N_{\rm CA}$ and $N_{\rm CF}$ are positive integers, $N_{\rm CA}$ should be an integer greater than 16, so $\frac{1}{8}N_{\rm CF} + 16 = N_{\rm CA}$ and therefore, $N_{\rm CF} = 8p$, $N_{\rm CA} = 8(p + 2)$. Thus the case $k = 8$ can rarely be of practical use.

For $k = 10$ it is from (3.2)

$$\begin{aligned} 1024 - 320 - 16N_{\rm CA} + N_{\rm CF} &= 0, \quad \text{i.e.} \\ N_{\rm CF} &= 2^4 N_{\rm CA} - 2^4 44 = 2^4\big(N_{\rm CA} - 44\big)\,. \end{aligned}$$

There is no practical use for the case $k = 10$ as well as in order $N_{\rm CF}$ to be positive $N_{\rm CA}$ has to be greater than 44 i.e.

$$N_{\rm CF} = 2^4 p\,, \qquad N_{\rm CA} = p + 44\,.$$

Similar, for $k = 12$, it is

$$N_{\rm CF} = 32N_{\rm CA} - 3328 = 2^5\big(N_{\rm CA} - 104\big)\,,$$
$$N_{\rm CF} = 2^5 p\,, \qquad N_{\rm CA} = p + 104\,.$$

For $k = 14$ it is then

$$N_{\rm CF} = 64N_{\rm CS} - 14592 = 2^6\big(N_{\rm CA} - 228\big), \quad \text{i.e.}$$
$$N_{\rm CF} = 2^6 p\,, \qquad N_{CA} = p + 228\,. \qquad \square$$

There is no practical use to investigate grater values, as the number of observations turns to be very large in such a case. From the above discussion it is easy to see that the following holds.

Corollary 3.1. *In principle,*

$$N_{\rm CF} = 2^{k/2-1}\Big[N_{\rm CA} - \big(2^{k/2-1} - 2k\big)\Big]\,, \qquad k = 2, 4, 6, \ldots \tag{3.7}$$

Corollary 3.2. *The general form of required samples are:*

$$N_{\rm CF} = 2^{k/2-1}p\,, \qquad N_{\rm CA} = p + 2^{k/2+1} - 2k\,, \qquad p \in \mathbb{Z}^+\,. \tag{3.8}$$

Proposition 3.2. *For the equation* (3.2) *as in Theorem 3.2, considering* $k = 2(2)14$ *the corresponding pair of values* $(N_{\rm CA}, N_{\rm CF})$ *for a double root* $x = N_{\rm F}^{1/2} = 2^{k/2}$, *are*

$$(4, 4), (8, 16), (20, 64), (48, 256), (108, 1024), (232, 4096), (484, 16384)\,.$$

Proof: The proof is based on (3.3b) with $\nu = 0$ and on the results obtained in Proposition 3.1. Namely for:

- $k = 2,\ D = (4 - N_{\rm CA})^2$, hence $N_{\rm CA} = 4 = N_{\rm CF}$;
- $k = 4,\ D = (8 + N_{\rm CA})^2 - 32N_{\rm CA} = (8 - N_{\rm CA})^2$, hence $N_{\rm CA} = 8$, $N_{\rm CF} = 16$;
- $k = 6,\ D = (12 + N_{\rm CA})^2 - 16(4N_{\rm CA} - 16) = (20 - N_{\rm CA})^2$, so $N_{\rm CA} = 20$, $N_{\rm CF} = 64$;
- $k = 8,\ D = (16 + N_{\rm CA})^2 - 16(8N_{\rm CA} - 128) = (48 - N_{\rm CA})^2$, so $N_{\rm CA} = 48$, $N_{\rm CF} = 256$;
- $k = 10,\ D = (20 + N_{\rm CA})^2 - 16(16N_{\rm CA} - 704) = (108 - N_{\rm CA})^2$, so $N_{\rm CA} = 108$, $N_{\rm CF} = 1024$;
- $k = 12,\ D = (24 + N_{\rm CA})^2 - 16(32N_{\rm CA} - 3328) = (232 - N_{\rm CA})^2$, so $N_{\rm CA} = 232$, $N_{\rm CF} = 4096$;
- $k = 14,\ D = (28 + N_{\rm CA})^2 - 16(64N_{\rm CA} - 14592) = (484 - N_{\rm CA})^2$, so $N_{\rm CA} = 484$, $N_{\rm CF} = 16384$. $\square$

It is clear that for k greater than 8 there is no practical use, as we have already comment, as the required observations are too many and it is not practical use of an experiment 2^8.

4. DISCUSSION

The above provided analysis proves that the restriction $D \geq 0$ is not the appropriate one for an OCCD to be ROCCD. In Table 1 we summarize, for practical use values of k and the appropriate values of design points, according to the above-mentioned calculations. The appropriate necessary and sufficient condition was stated and proved, adjusting an old wrong result, with a rather "simple" approach. Some experimenters decide in advance, rather from experience or depending on how easy is to perform the experiment, the needed size of the experiment. But the investigation needs a deeper approach, we believe, with not such a difficult mathematical approach for the experimenter. We worked towards this direction: to keep it simple. Table 1 summarizes the results from the above discussion. In a future attempt, it would be interesting to construct, mainly from a theoretical point of view, the appropriate calculations with k larger than 14, in order to see the behavior of the discussed "system" for "large" values. It is also clear that the researcher working at EVOP designs (see the pioneering paper in [2]) can adopt the calculations performed here, for the initial design, as EVOP is based, briefly speaking, on a "factorial + centre" design. Therefore, despite its theoretical framework and background, the above proposed integer solution can be very helpful in practice as well.

Table 1: Design points needed for a ROCCD with $k = 2(2)8$, for a double root $x = N_{\mathrm{F}}^{1/2}$.

k	N_{F}	N_{A}	N_{CF}	N_{CA}	N_{C}	N
4	4	4	2	2	4	12
			3	3	6	14
			4	4	8	16
4	16	8	4	2	6	30
			6	3	9	33
			8	4	12	36
			16	8	24	48
6	64	12	4	5	9	85
			8	6	14	90
			12	7	19	95
			64	20	84	160
6	256	16	8	17	25	297
			16	18	34	306
			24	19	34	306
			256	48	304	576

APPENDIX A

Proposition A.1. *Let $x^2 + px + q$, $p, q \in \mathbb{Z}$. Then its roots $x_1, x_2 \in \mathbb{Z}$ if and only if the discriminant $D = \mu^2$, $\mu \in \mathbb{Z}$, or $\mu = 0$.*

Proof: If $x_1,\ x_2 \in \mathbb{Z}$: $x^2 + px + q \Leftrightarrow x^2 - (x_1 + x_2)x + x_1x_2 = 0$.

Let $D = (x_1 + x_2)^2 - 4x_1x_2 = (x_1 - x_2)^2 = \mu^2$, with $\mu = x_1 - x_2 \in \mathbb{Z}$ as $x_1, x_2 \in \mathbb{Z}$. Now, let $D = p^2 - 4q = \mu^2$, $\mu \in \mathbb{Z}$. Then

$$x_1, x_2 = \frac{-p \pm \mu}{2} = -\frac{p \mp \mu}{2}\,.$$

But: $p^2 - 4q = \mu^2 \Rightarrow p^2 - \mu^2 = 4q \Leftrightarrow (p - \mu)(p + \mu) = 4q \Rightarrow p + \mu\ = 2n_1$, $n_1 \in \mathbb{Z}$ and $p - \mu = 2n_2$, $n_2 \in \mathbb{Z}$. Therefore $x_1 = n_1$ and $x_2 = -n_2$, i.e. x_1 and x_2 are integers. □

Proof of Theorem 3.1: If $A\big|B$ and $A\big|C$ then:

$$Ax^2 + Bx + C = 0 \ \Leftrightarrow\ x^2 + \tfrac{B}{A}x + \tfrac{C}{A} = 0 \ \Leftrightarrow\ x^2 + px + q = 0\,, \quad p, q \in \mathbb{Z}\,.$$

It is also: $D_1 = p^2 - 4q = \mu_1^2,\ \ \mu_1^2 \in \mathbb{Z} \ \Leftrightarrow$

$$\frac{B^2}{A^2} - 4\frac{C}{A} = \mu_1^2 \ \Leftrightarrow\ \frac{B^2 - 4AC}{A^2} = \mu_1^2 \ \Rightarrow\ D = B^2 - 4Ac = (\mu_1 A)^2 = \mu_1^2, \quad \mu \in \mathbb{Z}\,.$$

So $x^2 + px + q = 0$ has integer roots and so does $Ax^2 + Bx + C = 0$.

The inverse: Let $x_1, x_2 \in \mathbb{Z}$ be the roots of $Ax^2 + Bx + C = 0$. Then: $x_1 + x_2 = -\frac{B}{A}$ and $x_1x_2 = \frac{C}{A}$. Thus $x_1 + x_2 \in \mathbb{Z} \Rightarrow A\big|B$ and $x_1x_2 \in \mathbb{Z} \Rightarrow A\big|C$. Moreover:

$$Ax^2 + Bx + C = 0 \ \Rightarrow\ x^2 + \tfrac{B}{A}x + \tfrac{C}{A} = 0 \ \Rightarrow\ x^2 + px + q = 0\,,$$

has integer roots (Proposition A.1).

Let $D_1 = p^2 - 4q = \mu_1^2$, $\mu_1 \in \mathbb{Z}$, i.e.

$$\frac{B^2}{A^2} - 4\frac{C}{A} = \mu_1^2 \ \Rightarrow\ \frac{B^2 - 4AC}{A^2} = \mu_1^2 \ \Rightarrow\ D = B^2 - 4AC = (A\mu_1)^2 = \mu^2, \quad \mu \in \mathbb{Z}.$$

□

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