Extended Central Composite Designs and Their Statistical Properties[0]

HYUK JOO KIM[1] and SUNG HYUN PARK[2]

Abstract

There are several desirable properties that response surface designs may have. Sometimes we need designs which have more than one desirable property at the same time. In this paper, we have proposed an extended version of central composite design and named it CCD2. We have obtained conditions for orthogonality, rotatability and slope rotatability for the CCD2. CCD2's that have both orthogonality and rotatability, both orthogonality and slope rotatability over axial directions, and both rotatability and uniform precision also have been obtained.

1. Introduction

The central composite design (CCD) is a well-known design widely used for estimating second order response surfaces. It consists of 2^k (k is the number of

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[1]Professor, Division of Mathematics and Informational Statistics and Institute of Basic Natural Sciences, Wonkwang University, Iksan, Jeonbuk 570-749, Korea
E-mail: hjkim@wonkwang.ac.kr

[2]Professor, Department of Statistics, Seoul National University, Seoul 151-742, Korea
E-mail: parksh@plaza.snu.ac.kr

independent variables) or a fraction of 2^k factorial points $(\pm 1, \pm 1, \cdots, \pm 1)$, $2k$ axial points of the form $(\pm\alpha, 0 \cdots, 0)$, $(0, \pm\alpha, \cdots, 0)$, etc., and a center point $(0, 0, \cdots, 0)$. The center point may be replicated n_0 times. Let M denote the total number of experimental runs in the CCD. Then $M = F + 2k + n_0$. Here F is the number of factorial points ($F = 2^k$ if a complete factorial is used).

Since introduced by Box and Wilson (1951), the CCD has been studied and used by many researchers. The CCD has a lot of advantages, one of which is that it enables us to analyze a response surface with a relatively small number of experimental runs.

Among desirable properties that response surface designs may have, there are orthogonality and rotatability, which will be briefly explained in Section 3. The CCD can, of course, have these properties. It is known that the condition for a CCD to be an orthogonal design is that

$$\alpha = \left\{ \frac{\sqrt{F(F + 2k + n_0)} - F}{2} \right\}^{1/2}, \tag{1.1}$$

and the condition for a CCD to be a rotatable design is that

$$\alpha = F^{1/4}. \tag{1.2}$$

Details concerning these matters are given in general response surface methodology books such as Box and Draper (1987), Myers and Montgomery (1995) and Khuri and Cornell (1996).

When we are interested in estimating the slope of a response surface, slope rotatability is a desirable property. This property was proposed by Hader and Park (1978). They showed that a CCD is a slope-rotatable design if the positions of the axial points are given by α which satisfies the following polynomial equation:

$$
\begin{aligned}
&2(F+n_0)\alpha^8 - 4kF\alpha^6 - F\{M(4-k)+kF-8(k-1)\}\alpha^4 \\
&\quad +8(k-1)F^2\alpha^2 - 2(k-1)F^2(M-F) = 0. \qquad (1.3)
\end{aligned}
$$

As we can see from the above, α, the number which indicates the positions of the axial points in the CCD, is very important. A good choice of α can generate CCD's with various desirable properties.

In general, for given k, F and n_0, the values of α satisfying Eqs (1.1), (1.2) and (1.3) are all different. This means that an orthogonal CCD generally can not be either rotatable or slope-rotatable. There may be, however, some cases when we wish to have a design which has both orthogonality and rotatability, or, both orthogonality and slope rotatability, and so on. In this context, we are going to study an extended version of CCD in which the positions of the axial points are determined by two numbers rather than one number. This approach will also make us have flexibility with regard to the positions of the axial points and the number of center points.

2. CCD with two numbers indicating the positions of the axial points

The design matrix of the CCD in which two numbers indicate the positions of the axial points are as follows (in the case of $k = 2$):

$$D = \begin{array}{c} \begin{matrix} x_1 & \quad x_2 \end{matrix} \\ \begin{pmatrix} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ -\alpha_1 & 0 \\ \alpha_1 & 0 \\ 0 & -\alpha_1 \\ 0 & \alpha_1 \\ -\alpha_2 & 0 \\ \alpha_2 & 0 \\ 0 & -\alpha_2 \\ 0 & \alpha_2 \end{pmatrix} \end{array} \tag{2.1}$$

Here the number of center points is n_0, which is a positive integer, and α_1 and α_2, which are numbers indicating the positions of the axial points, are such that $0 < \alpha_1 \leq \alpha_2$.

The design matrix D given in Eq. (2.1) can be easily extended to the cases when $k \geq 3$. For convenience, let us call this kind of design 'CCD2' and call the ordinary central composite design explained in Section 1 'CCD1'. Let N denote the total number of experimental runs in CCD2. Then $N = F + 4k + n_0$, where $F = 2^k$ (or 2^{k-p}; p is a suitable positive integer) is the number of factorial points and n_0 is the number of center points. For the same number of center points, the total number of experimental runs of a CCD2 is larger than that of a CCD1 by $2k$, but is much smaller than that of a 3^k factorial design.

Consider the second order polynomial model

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \beta_{ii} x_{iu}^2 + \sum_{i<j}^{k} \beta_{ij} x_{iu} x_{ju} + \varepsilon_u \quad (u = 1, 2, \cdots, N), \tag{2.2}$$

where ε_u's are uncorrelated random errors with mean zero and variance σ^2. Let us use an alternative model

$$y_u = \beta_0' + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \beta_{ii} (x_{iu}^2 - \overline{x_i^2}) + \sum_{i<j}^{k} \beta_{ij} x_{iu} x_{ju} + \varepsilon_u \ (u = 1, 2, \cdots, N) \tag{2.3}$$

to simplify the calculations. Here $\overline{x_i^2} = \sum_{u=1}^{N} x_{iu}^2 / N$ and $\beta_0' = \beta_0 + \sum_{i=1}^{k} \beta_{ii} \overline{x_i^2}$, and for the CCD2 $\overline{x_i^2} = (F + 2\alpha_1^2 + 2\alpha_2^2)/N$.

Eq. (2.3) can be written in matrix notation as

$$\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon} \quad (\boldsymbol{\varepsilon} \sim (\mathbf{0},\ I\sigma^2)), \tag{2.4}$$

where

$$\mathbf{y} = (y_1,\ y_2,\ \cdots,\ y_n)' \tag{2.5}$$

$$X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{k1} & x_{11}^2 - \overline{x_1^2} & \cdots & x_{k1}^2 - \overline{x_k^2} & x_{11}x_{21} & \cdots & x_{k-1,1}x_{k1} \\ 1 & x_{12} & \cdots & x_{k2} & x_{12}^2 - \overline{x_1^2} & \cdots & x_{k2}^2 - \overline{x_k^2} & x_{12}x_{22} & \cdots & x_{k-1,2}x_{k2} \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 1 & x_{1N} & \cdots & x_{kN} & x_{1N}^2 - \overline{x_1^2} & \cdots & x_{kN}^2 - \overline{x_k^2} & x_{1N}x_{2N} & \cdots & x_{k-1,N}x_{kN} \end{pmatrix} \tag{2.6}$$

$$\boldsymbol{\beta} = (\beta_0',\ \beta_1,\ \cdots,\ \beta_k,\ \beta_{11},\ \cdots,\ \beta_{kk},\ \beta_{12},\ \cdots \beta_{k-1,k})' \tag{2.7}$$

$$\boldsymbol{\varepsilon} = (\varepsilon_1,\ \varepsilon_2,\ \cdots,\ \varepsilon_N)'. \tag{2.8}$$

So for the CCD2, the $X'X$ matrix and $(X'X)^{-1}$ matrix are as follows:

$$X'X = \begin{pmatrix} N & & & & & & & & & \\ & F+2\alpha_1^2+2\alpha_2^2 & & & & & & & & \\ & & \ddots & & & & & & & \\ & & & F+2\alpha_1^2+2\alpha_2^2 & & & & & & \\ & & & & c & d & \cdots & d & & \\ & & & & d & c & \cdots & d & & \\ & & & & \vdots & \vdots & \ddots & \vdots & & \\ & & & & d & d & \cdots & c & & \\ & & & & & & & & FI_{k(k-1)/2} \end{pmatrix} \tag{2.9}$$

$$(X'X)^{-1} = \begin{pmatrix} N^{-1} & & & & & & & & & \\ & (F+2\alpha_1^2+2\alpha_2^2)^{-1} & & & & & & & & \\ & & \ddots & & & & & & & \\ & & & (F+2\alpha_1^2+2\alpha_2^2)^{-1} & & & & & & \\ & & & & e & f & \cdots & f & & \\ & & & & f & e & \cdots & f & & \\ & & & & \vdots & \vdots & \ddots & \vdots & & \\ & & & & f & f & \cdots & e & & \\ & & & & & & & & F^{-1}I_{k(k-1)/2} \end{pmatrix} \tag{2.10}$$

where $I_{k(k-1)/2}$ is an identity matrix of order $k(k-1)/2$, and

$$c = F(1-\overline{x_i^2})^2 + 2(\alpha_1^2-\overline{x_i^2})^2 + 2(\alpha_2^2-\overline{x_i^2})^2 + (4k+n_0-4)(\overline{x_i^2})^2$$
$$= \frac{1}{N}\{F(4k+n_0)-4(\alpha_1^2+\alpha_2^2)(F+\alpha_1^2+\alpha_2^2)+2N(\alpha_1^4+\alpha_2^4)\} \tag{2.11}$$

$$d = F(1-\overline{x_i^2})^2 - 4(\overline{x_i^2})(\alpha_1^2-\overline{x_i^2}) - 4(\overline{x_i^2})(\alpha_2^2-\overline{x_i^2}) + (4k+n_0-8)(\overline{x_i^2})^2$$
$$= \frac{1}{N}\{F(4k+n_0)-4(\alpha_1^2+\alpha_2^2)(F+\alpha_1^2+\alpha_2^2)\} \tag{2.12}$$

$$e = \frac{c+(k-2)d}{(c-d)\{c+(k-1)d\}} = \frac{A_1}{B} \tag{2.13}$$

$$f = \frac{-d}{(c-d)\{c+(k-1)d\}} = \frac{A_2}{B} \tag{2.14}$$

$$A_1 = (k-1)F(4k+n_0)-4(k-1)(\alpha_1^2+\alpha_2^2)(F+\alpha_1^2+\alpha_2^2)+2N(\alpha_1^4+\alpha_2^4) \tag{2.15}$$

$$A_2 = -F(4k+n_0)+4(\alpha_1^2+\alpha_2^2)(F+\alpha_1^2+\alpha_2^2) \tag{2.16}$$

$$B = 2(\alpha_1^4+\alpha_2^4)\{kF(4k+n_0)-4k(\alpha_1^2+\alpha_2^2)(F+\alpha_1^2+\alpha_2^2)+2N(\alpha_1^4+\alpha_2^4)\} \tag{2.17}$$

and the unspecified elements are all zero.

The least squares estimator of β can be obtained by

$$\mathbf{b} = (X'X)^{-1}X'\mathbf{y}, \tag{2.18}$$

and from the fact that the variance-covariance matrix of $\mathbf{b}$ is

$$Var(\mathbf{b}) = \sigma^2(X'X)^{-1}, \tag{2.19}$$

we obtain the following variances and covariances:

$$Var(b_0') = \sigma^2/N \tag{2.20}$$

$$Var(b_i) = \sigma^2/(F+2\alpha_1^2+2\alpha_2^2) \ \ (i = 1, 2, \cdots, k) \tag{2.21}$$

$$Var(b_{ij}) = \sigma^2/F \ \ (i \neq j) \tag{2.22}$$

$$Var(b_{ii}) = \sigma^2 e \ \ (i = 1, 2, \cdots, k) \tag{2.23}$$

$$Cov(b_{ii}, b_{jj}) = \sigma^2 f \ \ (i \neq j) \tag{2.24}$$

All other covariances are zero.

3. Orthogonality, rotatability and slope rotatability

3.1 Orthogonality

As we saw in Section 2, in the CCD2 all the covariances except $Cov(b_{ii}, b_{jj})$ are zero. But if $f = 0$ in the $(X'X)^{-1}$ matrix in Eq. (2.10), the $(X'X)^{-1}$ matrix becomes a diagonal matrix and thus $Cov(b_{ii}, b_{jj})$ becomes zero. This property is called *orthogonality*. As can be seen from Eqs (2.14) and (2.16), in order for $f = 0$, it must hold that

$$\alpha_1^2 + \alpha_2^2 = \frac{\sqrt{F(F+4k+n_0)} - F}{2}. \tag{3.1}$$

Eq.(3.1) is the condition for a CCD2 to be an orthogonal design.

For various values of (k, F) and n_0, the values of $\alpha_1^2 + \alpha_2^2$ that make the CCD2 orthogonal are tabulated in Table 1.

Table 1. Values of $\alpha_1^2 + \alpha_2^2$ for orthogonal CCD2

	(k,F)					
n_0	(2,4)	(3,8)	(4,16)	(5,32)	(5,16)	(6,64)
1	1.606	2.481	3.489	4.591	4.166	5.736
2	1.742	2.633	3.662	4.785	4.329	5.947
3	1.873	2.782	3.832	4.976	4.490	6.158
4	2.000	2.928	4.000	5.166	4.649	6.367
5	2.123	3.071	4.166	5.354	4.806	6.575

	(k,F)					
n_0	(6,32)	(7,128)	(7,64)	(8,256)	(8,128)	(8,64)
1	5.354	6.880	6.575	8.000	7.777	7.395
2	5.541	7.106	6.781	8.235	8.000	7.598
3	5.726	7.330	6.987	8.470	8.222	7.799
4	5.909	7.554	7.192	8.704	8.443	8.000
5	6.091	7.777	7.395	8.938	8.664	8.200

3.2 Rotatability

In the general linear regression model, the variance of the estimated response $\hat{y}$ at the point $\mathbf{x}' = (x_1,\ x_2, \cdots, x_k)$ is

$$Var(\hat{y}) = \mathbf{x_f}'(X'X)^{-1}\mathbf{x_f}\sigma^2, \tag{3.2}$$

where $\mathbf{x_f}' = (1,\ x_1, \cdots, x_k,\ x_1^2, \cdots, x_k^2,\ x_1x_2, \cdots, x_{k-1}x_k)$. This variance depends on the coordinates of the point $\mathbf{x}'$. Here if $Var(\hat{y})$ is a function only of the distance

$$\rho = (x_1^2 + x_2^2 + \cdots + x_k^2)^{1/2} \tag{3.3}$$

from the center point $(0, 0, \cdots, 0)$, we call such a design a *rotatable* design. Box and Hunter (1957) showed that the conditions for a second-order response surface design to be a rotatable design are as follows:

[R1] All odd-order design moments are zero. That is,

$$\sum_{u=1}^{N} {x_{1u}}^{\delta_1} {x_{2u}}^{\delta_2} \cdots {x_{ku}}^{\delta_k} = 0 \tag{3.4}$$

if at least one δ_i is an odd number.

[R2] Pure fourth moments are three times the mixed fourth moments. That is,

$$\sum_{u=1}^{N} x_{iu}^4 = 3 \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 \quad (i \neq j). \tag{3.5}$$

Now we are to find the condition for the CCD2 to be a rotatable design. Let us consider a general case involving k independent variables obtained by extending the design matrix D in Eq. (2.1). We can easily see that all odd-order moments are zero. The fourth-order moments in [R2] are

$$\sum_{u=1}^{N} x_{iu}^4 = F + 2\alpha_1^4 + 2\alpha_2^4 \tag{3.6}$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = F \quad (i \neq j). \tag{3.7}$$

Thus in order to satisfy [R2], it must hold that

$$F + 2\alpha_1^4 + 2\alpha_2^4 = 3F. \tag{3.8}$$

So the condition for the CCD2 to be rotatable is that

$$\alpha_1^4 + \alpha_2^4 = F. \tag{3.9}$$

We note that this value does not depend on n_0, the number of center points.

3.3 Slope rotatability

Since the 1970's, in the design of experiments for response surface analysis, attention has been focused on the estimation of differences in response rather than absolute value of the response variable η (η is the expected value of the variable y in Eq. (2.2)). If differences at points close together in the factor space are involved, estimation of the local slopes (the rates of change) of the response surface is of interest.

When the estimation of the slope of a response surface is of interest, *slope rotatability* is a desirable property. There are two types of slope rotatability: slope rotatability over axial directions and slope rotatability over all directions.

3.3.1 Slope rotatability over axial directions

The regression equation fitted by the least squares method can be represented as

$$\hat{y}(\mathbf{x}) = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{i=1}^{k} b_{ii} x_i^2 + \sum_{i<j}^{k} b_{ij} x_i x_j. \tag{3.10}$$

The first partial derivative of $\hat{y}(\mathbf{x})$ with respect to x_i is

$$\frac{\partial \hat{y}(\mathbf{x})}{\partial x_i} = b_i + 2b_{ii} x_i + \sum_{j=1, j\neq i}^{k} b_{ij} x_j. \tag{3.11}$$

The variance of this derivative is a function of the point $\mathbf{x}$ at which the derivative is estimated and also a function of the design through the relationship

$$Var(\mathbf{b}) = \sigma^2 (X'X)^{-1}. \tag{3.12}$$

Hader and Park (1978) proposed an analog of the Box-Hunter rotatability criterion. This requires the following:

[S1] For each $i = 1, 2, \cdots, k$, the variances of $\partial\hat{y}(\mathbf{x})/\partial x_i$ are equal for all $\mathbf{x}$ that are equidistant from the design center, that is, $Var(\partial\hat{y}(\mathbf{x})/\partial x_i)$ is a function only of $\rho = (\sum_{i=1}^{k} x_i^2)^{1/2}$.

[S2] The variances of $\partial\hat{y}(\mathbf{x})/\partial x_i,\ i = 1, 2, \cdots, k$, are equal, that is,

$$Var\left(\frac{\partial\hat{y}(\mathbf{x})}{\partial x_1}\right) = Var\left(\frac{\partial\hat{y}(\mathbf{x})}{\partial x_2}\right) = \cdots = Var\left(\frac{\partial\hat{y}(\mathbf{x})}{\partial x_k}\right), \tag{3.13}$$

for any point $\mathbf{x}$ in the factor space.

If a design satisfies [S1] and [S2], estimation of the slopes over axial directions will be equally reliable for all points $\mathbf{x}$ equidistant from the design center. Hader and Park (1978) referred to this property as *slope rotatability over axial directions* (SROAXD). They also presented slope-rotatable CCD1's.

Now let us apply the concept of SROAXD to the CCD2. In the CCD2, the following hold:

$$\begin{aligned} c_{i,ii} = c_{i,ij} = c_{ii,ij} = c_{ij,il} = 0 \quad (i \neq j \neq l \neq i), \\ v_1 = v_2 = \cdots = v_k, \\ v_{11} = v_{22} = \cdots = v_{kk}, \\ v_{12} = v_{13} = \cdots = v_{k-1,k}. \end{aligned} \tag{3.14}$$

Here we have used the following notation for the sake of simplicity. This notation will be used hereafter:

$$
\begin{gathered}
v_i = Var(b_i),\ v_{ii} = Var(b_{ii}),\ v_{ij} = Var(b_{ij}), \\
c_{i,ii} = Cov(b_i, b_{ii}),\ c_{i,ij} = Cov(b_i, b_{ij}),\ c_{ii,ij} = Cov(b_{ii}, b_{ij}), \\
c_{ij,il} = Cov(b_{ij}, b_{il}).
\end{gathered} \tag{3.15}
$$

So the variance of the derivative given by Eq. (3.11) becomes

$$
\begin{aligned}
Var\left(\frac{\partial \hat{y}(\mathbf{x})}{\partial x_i}\right) &= v_i + 4x_i^2 v_{ii} + \sum_{j=1, j\neq i}^{k} x_j^2 v_{ij} \\
&= v_1 + 4v_{11}x_i^2 + v_{12}\sum_{j=1, j\neq i}^{k} x_j^2,
\end{aligned} \tag{3.16}
$$

and we can see that the condition for a CCD2 to have SROAXD is that

$$
4v_{11} = v_{12}, \tag{3.17}
$$

which becomes, by Eqs (2.22) and (2.23),

$$
4Fe = 1. \tag{3.18}
$$

Arranging Eq. (3.18), we obtain the following:

$$
\begin{aligned}
&2(F + 2k + n_0)(\alpha_1^8 + \alpha_2^8) - 8k(\alpha_1^6\alpha_2^2 + \alpha_1^2\alpha_2^6) \\
&+ 4(F + 2k + n_0)\alpha_1^4\alpha_2^4 - 4kF(\alpha_1^6 + \alpha_1^4\alpha_2^2 + \alpha_1^2\alpha_2^4 + \alpha_2^6) \\
&- F\{4F - 4k^2 + k(8 - n_0) + 4(2 + n_0)\}(\alpha_1^4 + \alpha_2^4) + 16(k-1)F\alpha_1^2\alpha_2^2 \\
&+ 8(k-1)F^2(\alpha_1^2 + \alpha_2^2) - 2(k-1)F^2(4k + n_0) = 0.
\end{aligned} \tag{3.19}
$$

Eq (3.19) is the condition for a CCD2 to be a slope-rotatable design over axial directions. For given k, F and n_0, there are infinitely many combinations of α_1 and α_2 that satisfy Eq. (3.19). Some of them are tabulated in Table 2 through Table 6.

Table 2. SROAXD CCD2's when $k = 2,\ F = 4$

(a) $n_0 = 1$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.7267
α_2	1.8219	1.8268	1.8348	1.8457	1.8596	1.8760	1.8947	1.9
α_1	0.8	0.9	1.0	1.1	1.1735	1.2	1.3	1.4
α_2	1.9153	1.9374	1.9603	1.9834	2.0	2.0059	2.0266	2.0444
α_1	1.5	1.6	1.7	1.8	1.9	1.9041		
α_2	2.0577	2.0645	2.0618	2.0446	2.0025	2.0		

(b) $n_0 = 2$

α_1	0.1	0.2	0.2550	0.3	0.4	0.5	0.6	0.7
α_2	1.7925	1.7966	1.8	1.8033	1.8125	1.8239	1.8374	1.8524
α_1	0.8	0.9	0.9843	1.0	1.1	1.2	1.3	1.4
α_2	1.8686	1.8856	1.9	1.9027	1.9190	1.9336	1.9452	1.9523
α_1	1.5	1.6	1.7	1.7395	1.8			
α_2	1.9526	1.9427	1.9169	1.9	1.8628			

(A SROAXD CCD2 with α_1 or α_2 equal to 2.0 does not exist.)

Table 3. SROAXD CCD2's when $k = 3,\ F = 8$

(a) $n_0 = 1$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.1144	2.1178	2.1235	2.1314	2.1416	2.1539	2.1683	2.1847
α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.2031	2.2233	2.2449	2.2676	2.2909	2.3141	2.3362	2.3562

α_1	1.7	1.8	1.9	2.0
α_2	2.3730	2.3851	2.3903	2.3861

(b) $n_0 = 2$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.0934	2.0963	2.1012	2.1080	2.1165	2.1268	2.1387	2.1521
α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.1668	2.1828	2.1997	2.2170	2.2343	2.2509	2.2658	2.2777
α_1	1.7	1.8	1.9	2.0				
α_2	2.2852	2.2862	2.2776	2.2547				

Table 4. SROAXD CCD2's when $k = 4,\ F = 16$

(a) $n_0 = 1$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.4877	2.4901	2.4941	2.4997	2.5068	2.5155	2.5257	2.5375
α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.5507	2.5653	2.5813	2.5986	2.6171	2.6363	2.6559	2.6753
α_1	1.7	1.8	1.9	2.0				
α_2	2.6940	2.7110	2.7255	2.7362				

(b) $n_0 = 2$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.4716	2.4738	2.4773	2.4822	2.4884	2.4960	2.5047	2.5147
α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.5257	2.5379	2.5511	2.5652	2.5799	2.5952	2.6104	2.6253

α_1	1.7	1.8	1.9	2.0
α_2	2.6389	2.6506	2.6592	2.6633

Table 5. SROAXD CCD2's when $k = 5,\ F = 32$

(a) $n_0 = 1$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.9439	2.9456	2.9484	2.9523	2.9572	2.9632	2.9703	2.9783
α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.9872	2.9970	3.0076	3.0191	3.0312	3.0438	3.0569	3.0702
α_1	1.7	1.8	1.9	2.0				
α_2	3.0834	3.0961	3.1078	3.1182				

(b) $n_0 = 2$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.9314	2.9329	2.9355	2.9390	2.9435	2.9489	2.9552	2.9623
α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.9702	2.9788	2.9881	2.9979	3.0082	3.0188	3.0297	3.0406
α_1	1.7	1.8	1.9	2.0				
α_2	3.0511	3.0611	3.0699	3.0770				

Table 6. SROAXD CCD2's when $k = 5,\ F = 16$

(a) $n_0 = 1$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.4425	2.4444	2.4476	2.4521	2.4578	2.4648	2.4732	2.4830

α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.4944	2.5075	2.5227	2.5402	2.5603	2.5831	2.6087	2.6365

α_1	1.7	1.8	1.9	2.0
α_2	2.6660	2.6960	2.7253	2.7526

(b) $n_0 = 2$

α_1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
α_2	2.4313	2.4329	2.4357	2.4396	2.4445	2.4504	2.4573	2.4653
α_1	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6
α_2	2.4744	2.4847	2.4963	2.5095	2.5244	2.5413	2.5601	2.5807

α_1	1.7	1.8	1.9	2.0
α_2	2.6025	2.6247	2.6459	2.6648

3.3.2 Slope rotatability over all directions

In slope estimation, it is often of interest to estimate the slope of the response surface at a point $\mathbf{x}$, not only over the axial directions, but also over any specified direction. Let us consider the variance of the slope averaged over all possible directions. This averaged variance is a function of $\mathbf{x}$, the point at which the derivative is being estimated, and also a function of the design. By choice of design it is possible to make the averaged variance constant for all points equidistant from the design center. This property is called *slope rotatability over all directions* (SROALD). Park (1987) proposed SROALD and showed that the necessary and sufficient conditions for a design to be slope-rotatable over all directions are the following:

[C1] $2c_{i,ii} + \sum_{j=1,j\neq i}^{k} c_{j,ij} = 0$ for all i.

[C2] $2(c_{ii,ij} + c_{jj,ij}) + \sum_{l=1,l\neq i,j}^{k} c_{il,jl} = 0$ for any (i,j) when $i \neq j$.

[C3] $4v_{ii} + \sum_{j=1,j\neq i}^{k} v_{ij}$ equal for all i.

Now let us apply SROALD to the CCD2. As stated in the end of Section 2, all the covariances except $c_{ii,jj}$ $(i \neq j)$ are zero, so it is clear that [C1] and [C2] are satisfied. Furthermore, since v_{ii} are equal for all i and v_{ij} are equal for all (i,j) when $i \neq j$, it is apparent that [C3] is also satisfied. So we see the important fact that the CCD2 has SROALD, regardless of the values of α_1 and α_2 and the number of center points, n_0.

4. CCD2's having both orthogonality and rotatability

For given values of k, F and n_0, let us consider Eqs (3.1) and (3.9) simultaneously. The solutions of these simultaneous equations generate CCD2's that have both orthogonality and rotatability. Such CCD2's will henceforth be called *OR CCD2's*. For various values of k, F and n_0 $(n_0 \leq 30)$, the values of α_1 and α_2 that give OR CCD2's have been obtained and tabulated in Table 7.

Table 7. CCD2's having both orthogonality and rotatability

(a) $k = 2,\ F = 4$

n_0	1∼4	5	6	7	8	9	10	11
α_1	X	0.3566	0.5095	0.6318	0.7409	0.8453	0.9533	1.0880
α_2	X	1.4128	1.4082	1.3999	1.3868	1.3667	1.3348	1.2697

n_0	12∼30
α_1	X
α_2	X

(X denotes nonexistence.)

(b) $k = 3, \ F = 8$

n_0	1∼3	4	5	6	7	8	9	10
α_1	X	0.3188	0.5041	0.6426	0.7617	0.8709	0.9760	1.0824
α_2	X	1.6813	1.6784	1.6728	1.6638	1.6507	1.6319	1.6045

n_0	11	12	13∼30
α_1	1.1996	1.4142	X
α_2	1.5605	1.4142	X

(c) $k = 4, \ F = 16$

n_0	1∼4	5	6	7	8	9	10	11
α_1	X	0.4112	0.5862	0.7243	0.8445	0.9547	1.0593	1.1616
α_2	X	1.9991	1.9963	1.9914	1.9839	1.9735	1.9594	1.9405

n_0	12	13	14	15∼30
α_1	1.2652	1.3756	1.5079	X
α_2	1.9146	1.8773	1.8141	X

(d) $k = 5, \ F = 32$

n_0	1∼6	7	8	9	10	11	12	13
α_1	X	0.2629	0.5079	0.6723	0.8074	0.9266	1.0360	1.1391
α_2	X	2.3783	2.3772	2.3746	2.3705	2.3646	2.3567	2.3465

n_0	14	15	16	17	18	19	20	21 ∼30
α_1	1.2382	1.3354	1.4326	1.5324	1.6388	1.7615	2.0000	X
α_2	2.3335	2.3170	2.2960	2.2686	2.2313	2.1749	2.0000	X

(e) $k = 5,\ F = 16$

n_0	1	2	3	4	5	6	7	8
α_1	0.4112	0.5862	0.7243	0.8445	0.9547	1.0593	1.1616	1.2652
α_2	1.9991	1.9963	1.9914	1.9839	1.9735	1.9594	1.9405	1.9146

n_0	9	10	11∼30
α_1	1.3756	1.5079	X
α_2	1.8773	1.8141	X

Table 7 tells us the following facts. First, consider the case when $(k, F) = (2, 4)$. When n_0, the number of center points, is less than or equal to 4 and when $12 \leq n_0 \leq 30$, an OR CCD2 does not exist. When $5 \leq n_0 \leq 11$, however, there exists an OR CCD2, and the value of α_1 increases and that of α_2 decreases gradually as n_0 increases. When $(k, F) = (3, 8), (4, 16), (5, 32)$, similar facts hold, while the range of n_0 for which an OR CCD2 exists changes a little. When $(k, F) = (5, 16)$, in which case we use only a half of the factorial points, an OR CCD2 exists from when $n_0 = 1$ (specifically, for $1 \leq n_0 \leq 10$). When $k = 6, 7, 8$, similar facts have been observed. That is, when we use only a half of the factorial points, the minimum number of center points required for the existence of an OR CCD2 has been found to be less than that when we use all the factorial points, and that when we use only a quarter of the factorial points has been found to be less than that when we use a half of the factorial points.

For reference, let us consider CCD1's which have both orthogonality and rotatability. The condition for a CCD1 to have orthogonality is known to be $\alpha = [\{\sqrt{F(F+2k+n_0)} - F\}/2]^{1/2}$, and that for a CCD1 to have rotatability is known to be $\alpha = F^{1/4}$. Solving these two equations simultaneously gives $n_0 = 4(1+\sqrt{F}) - 2k$. But n_0 is the number of center points, so if the value of n_0 computed from the above formula is not an integer, it means that there does not exist an *OR CCD1* (this means a CCD1 which is both orthogonal and rotatable). Referring to Table 8, we can see that when $(k, F) = (3,8), (5,32), (6,32), (7,128), (8,128)$, an OR CCD1 does not exist because the value of n_0 is not an integer.

Table 8. CCD1's having both orthogonality and rotatability

(k, F)	(2,4)	(3,8)	(4,16)	(5,32)	(5,16)	(6,64)
n_0	8	9.3137	12	16.6274	10	24
Existence	Yes	No	Yes	No	Yes	Yes
α	1.4142		2		2	2.8284

(k, F)	(6,32)	(7,128)	(7,64)	(8,256)	(8,128)	(8,64)
n_0	14.6274	32.2548	22	52	33.2548	20
Existence	No	No	Yes	Yes	No	Yes
α			2.8284	4		2.8284

As we see above, for values of (k, F) for which an OR CCD1 does not exist, an OR CCD2 exists provided that at least a specified number of center points are used. This fact tells us the flexibility and usability of the CCD2. The worth of the CCD2 lies here.

5. CCD2's having both orthogonality and SROAXD

We may want to contrive to simplify the calculation and to obtain uncorrelated estimates of the regression coefficients, and at the same time, we may be interested in estimating the slope of a response surface. In this case, we need a design which has both orthogonality and slope rotatability. Since every CCD2 has SROALD as was shown in Section 3.3.2, only SROAXD between the two types of slope rotatability will be considered from now on.

For given values of k, F and n_0, solving simultaneously Eqs (3.1) and (3.19) gives CCD2's that have both orthogonality and SROAXD. Such CCD2's will be called *OS CCD2's* from now on. After some algebra, it has been found that solving simultaneously Eqs (3.1) and (3.19) is equivalent to solving simultaneously Eq. (3.1) and

$$\alpha_1^4 + \alpha_2^4 = 2F, \tag{5.1}$$

which is of greatly simplified form.

OS CCD2's are presented in Table 9. Among existing response surface designs including CCD1's, none have been found to have both orthogonality and SROAXD. Although more than ten center points are needed, CCD2's are of great value because we can generate CCD2's without limit which have these two properties simultaneously.

Table 9. CCD2's having both orthogonality and SROAXD

(a) $k = 2,\ F = 4$

n_0	1∼11	12	13	14	15	16	17	18
α_1	X	0.2673	0.4209	0.5338	0.6289	0.7137	0.7919	0.8661
α_2	X	1.6815	1.6801	1.6775	1.6735	1.6680	1.6607	1.6514

n_0	19	20	21	22	23	24	25∼30
α_1	0.9379	1.0089	1.0812	1.1577	1.2452	1.4142	X
α_2	1.6396	1.6245	1.6049	1.5782	1.5380	1.4142	X

(b) $k = 3,\ F = 8$

n_0	1∼12	13	14	15	16	17	18	19
α_1	X	0.3550	0.5043	0.6206	0.7205	0.8103	0.8935	0.9721
α_2	X	1.9995	1.6801	1.9954	1.9915	1.9864	1.9798	1.9715

n_0	20	21	22	23	24	25	26	27∼ 30
α_1	1.0478	1.1218	1.1955	1.2702	1.3482	1.4336	1.5387	X
α_2	1.9612	1.9486	1.9329	1.9132	1.8876	1.8525	1.7956	X

(c) $k = 4,\ F = 16$

n_0	1∼14	15	16	17	18	19	20	21
α_1	X	0.2339	0.4508	0.5952	0.7128	0.8156	0.9088	0.9954
α_2	X	2.3784	2.3777	2.3761	2.3736	2.3702	2.3656	2.3600

n_0	22	23	24	25	26	27	28	29
α_1	1.0772	1.1556	1.2317	1.3063	1.3803	1.4547	1.5308	1.6102
α_2	2.3530	2.3446	2.3345	2.3224	2.3079	2.2904	2.2691	2.2422

n_0	30
α_1	1.6965
α_2	2.2068

(d) $k = 5,\ F = 32$

n_0	1∼20	21	22	23	24	25	26	27
α_1	X	0.4097	0.5816	0.7150	0.8290	0.9308	1.0242	1.1116
α_2	X	2.8281	2.8272	2.8255	2.8232	2.8201	2.8162	2.8114

n_0	28	29	30
α_1	1.1943	1.2736	1.3502
α_2	2.8057	2.7989	2.7910

(e) $k = 5,\ F = 16$

n_0	1∼10	11	12	13	14	15	16	17
α_1	X	0.2339	0.4508	0.5952	0.7128	0.8156	0.9088	0.9954
α_2	X	2.3784	2.3777	2.3761	2.3736	2.3702	2.3656	2.3600

n_0	18	19	20	21	22	23	24	25
α_1	1.0772	1.1556	1.2317	1.3063	1.3803	1.4547	1.5308	1.6102
α_2	2.3530	2.3446	2.3345	2.3224	2.3079	2.2904	2.2691	2.2422

n_0	26	27	28	29∼30
α_1	1.6965	1.7977	2.0000	X
α_2	2.2068	2.1548	2.0000	X

Now it is somewhat natural to try to find CCD2's which have both rotatability and SROAXD. This problem corresponds to solving Eqs (3.9) and (3.19) simultaneously. But for $(k, F) = (2, 4), (3, 8), (4, 16), (5, 32), (5, 16), (6, 64), (6, 32), (7, 128), (7, 64), (8, 256), (8, 128), (8, 64)$, it has been found that such designs do not exist for any case of $n_0 = 1, 2, \cdots, 100$.

6. CCD2's having both rotatability and uniform precision

Among response surface designs that have rotatability, a possible and desirable choice is those which have the so-called *uniform precision*. A uniform precision design is a design such that the variance of the estimated response $\hat{y}$ at the design center is equal to the variance of $\hat{y}$ at $\rho = 1$. The uniform precision design is based on the philosophy that in the region for which $\rho < 1$, there should be uniform importance as far as estimation of response is concerned.

The condition for a second order rotatable design to have uniform precision is that $\lambda_4 = N^{-1}\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 \ (i \neq j)$, the mixed fourth moment of the design, has the value presented in Table 10. Here λ_4 is the design moment after scaling the design so that $N^{-1}\sum_{u=1}^{N} x_{iu} \ (i = 1, 2, \cdots, k)$, the first moment of the design, is zero and $N^{-1}\sum_{u=1}^{N} x_{iu}^2 \ (i = 1, 2, \cdots, k)$, the pure second moment, is unity. (See Myers (1976, Chapter 7).)

Table 10. Values of λ_4 for second order rotatable design which result in uniform precision

k	2	3	4	5	6	7	8	9
λ_4	0.7844	0.8385	0.8704	0.8918	0.9070	0.9184	0.9274	0.9346

Source: Box and Hunter (1957)

Let us consider the case of CCD2. The problem of obtaining the CCD2 which has both rotatability and uniform precision (Such CCD2's will henceforth be called *RUP CCD2's*) corresponds to that of solving the following simultaneous equations:

$$\alpha_1^4 + \alpha_2^4 = F \tag{6.1}$$

$$\alpha_1^2 + \alpha_2^2 = \tfrac{1}{2}\left\{\sqrt{\tfrac{F(F+4k+n_0)}{\lambda_4}} - F\right\} \tag{6.2}$$

Table 11 presents RUP CCD2's obtained by solving these simultaneous equations for various values of k, F and n_0. From this table, we see that we can always obtain RUP CCD2's for the cases of $(k, F) = (2,4), (3,8), (4,16), (5,32), (5,16)$. How about CCD1? In many cases, there does not exist a rotatable CCD1 which has uniform precision exactly, so only a near-uniform precision rotatable CCD1 is given. (See Myers (1976, p.153).)

Table 11. CCD2's having both rotatability and uniform precision

(a) $k = 2, F = 4$

n_0	1	2	3	4	5	6	7∼30
α_1	0.2689	0.4889	0.6457	0.7826	0.9169	1.0789	X
α_2	1.4138	1.4091	1.3986	1.3798	1.3471	1.2753	X

(b) $k = 3, F = 8$

n_0	1	2	3	4	5	6	7∼30
α_1	0.5109	0.6722	0.8095	0.9365	1.0623	1.2006	X
α_2	1.6782	1.6710	1.6588	1.6398	1.6105	1.5600	X

(c) $k = 4, F = 16$

n_0	1	2	3	4	5	6	7	8
α_1	0.5730	0.7322	0.8685	0.9929	1.1115	1.2294	1.3534	1.5010
α_2	1.9966	1.9910	1.9820	1.9689	1.9505	1.9244	1.8857	1.8180

n_0	9∼30
α_1	X
α_2	X

(d) $k = 5, F = 32$

n_0	1	2	3	4	5	6	7	8
α_1	0.3870	0.6036	0.7654	0.9031	1.0271	1.1428	1.2537	1.3625
α_2	2.3780	2.3759	2.3720	2.3660	2.3575	2.3461	2.3311	2.3116

n_0	9	10	11	12	13~30
α_1	1.4722	1.5868	1. 7147	1.8934	X
α_2	2.2859	2.2507	2.1984	2.0919	X

(e) $k = 5, F = 16$

n_0	1	2	3	4	5	6~30
α_1	1.0064	1.1218	1.2371	1.3586	1.5039	X
α_2	1.9672	1.9486	1.9224	1.8838	1.8164	X

7. Concluding remarks

There are several desirable properties that response surface designs may have. Among them are orthogonality, rotatability, uniform precision and slope rotatability. In many cases, we may need response surface designs that have more than one desirable property at the same time. In this paper, with this motivation, we have proposed an extended type of central composite design, namely, the CCD2, and studied some properties of the CCD2. We have obtained conditions for orthogonality, rotatability and slope rotatability for the CCD2. We also have obtained CCD2's that have both orthogonality and rotatability, both orthogonality and SROAXD, and both rotatability and uniform precision in Sections 4, 5 and 6, respectively. In Table 12, the ranges of n_0 for which OR, OS and RUP CCD2's exist are given for various values of

(k, F). We considered only $n_0 \leq 30$.

As for existing response surface designs including the CCD1, in many cases there does not exist a design which has two desirable properties at the same time. For the case of CCD2, however, such designs sufficiently exist except in the case of considering rotatability and SROAXD at the same time. From this fact we see that the CCD2 has considerable flexibility and usability. This is an advantage of the CCD2 that other kinds of design do not have.

Table 12. Ranges of n_0 for which OR, OS and RUP CCD2's exist ($n_0 \leq 30$)

(k, F)	OR	OS	RUP
(2,4)	$5 \leq n_0 \leq 11$	$12 \leq n_0 \leq 24$	$1 \leq n_0 \leq 6$
(3,8)	$4 \leq n_0 \leq 12$	$13 \leq n_0 \leq 26$	$1 \leq n_0 \leq 6$
(4,16)	$5 \leq n_0 \leq 14$	$15 \leq n_0 \leq 30$	$1 \leq n_0 \leq 8$
(5,32)	$7 \leq n_0 \leq 20$	$21 \leq n_0 \leq 30$	$1 \leq n_0 \leq 12$
(5,16)	$1 \leq n_0 \leq 10$	$11 \leq n_0 \leq 28$	$1 \leq n_0 \leq 5$
(6,64)	$13 \leq n_0 \leq 29$	$n_0 = 30$	$3 \leq n_0 \leq 18$
(6,32)	$3 \leq n_0 \leq 16$	$17 \leq n_0 \leq 30$	$1 \leq n_0 \leq 9$
(7,128)	$22 \leq n_0 \leq 30$	None	$7 \leq n_0 \leq 27$
(7,64)	$9 \leq n_0 \leq 25$	$26 \leq n_0 \leq 30$	$1 \leq n_0 \leq 15$
(8,256)	None	None	$13 \leq n_0 \leq 30$
(8,128)	$18 \leq n_0 \leq 30$	None	$5 \leq n_0 \leq 25$
(8,64)	$5 \leq n_0 \leq 21$	$22 \leq n_0 \leq 30$	$1 \leq n_0 \leq 12$

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