Mathematical Theory and Modeling
ISSN 2224-5804 (Paper) ISSN 2225-0522 (Online)
Vol.6, No.7, 2016

D-optimal Rotatable Central Composite Designs Constructed through Resolutions

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Abstract

Response surface methodology is widely used for developing, improving, and optimizing processes in various fields. A design is of resolution R if no p factors effect is confounded with any other effect containing less than $R-p$ factors. In this study, a method for constructing second order rotatable designs based on resolution R, in particular resolution III and IV for three and four factors respectively, argumented with star points is presented. Attention is given to the moment matrices and the related information surfaces based on the parameter subsystem of interest on the second-order Kronecker model and their corresponding rotatable Central Composite Designs (CCDs). Weighted Central Composite Designs (WCCDs) are derived by assigning different weights to two portions of the CCD namely the cube and star portion. The derived designs achieve the property of rotatability and high efficiency and are shown to be D-optimal. Experimental runs are reduced hence economical and the resulting designs are improved in terms of optimality and estimation efficiency. The results show that the cube portion is of great importance in D-optimal resolution III design while the two portions are of equall importance in resolution IV design.

Key Words: Resolution R, Kronecker model, Optimality Criterion, Weighted Central Composite Designs, Second – Order designs, Moment matrices, Information matrices

1.0. Introduction

In the Design of experiments for estimating statistical models, optimal designs allow parameters to be estimated without bias and with minimum-variance. Response Surface Designs is one of the experimental designs for optimization used for the study of response surface methodology (RSM). RSM is a collection of mathematical and statistical techniques useful for modeling and analysis of problems in which a response of interest is influenced by several variables and the objective is to optimize this response (Montgomery, 2005).

In this field, the main objective of the experimenter is usually to estimate the absolute response or the parameters of a model providing a functional relationship between the response and the factors. If the response Y is represented as a suitable function f of the levels $x_{1u}, x_{2u}, \dots, x_{mu}$ of the m factors and, θ the set of parameters then a typical model may be of the form:

$$y_u = f(x_{1u}, x_{2u}, \dots, x_{mu}; \theta + e_u)' \tag{1}$$

where $u = 1, 2, \dots, N$ represents the N observations with x_{iu} representing the level of the ith factor $(i = 1, 2, \dots, m)$ in the uth observation. This particular function is called the response surface (Pukelsheim, 1993). The objective of the study now becomes the estimated response surface whose statistical properties are determined by the moment matrix

$$M(\xi) = \int f(x) f(x)' d\xi \tag{2}$$

The information that a design with moment matrix M contains for the model response surface $f(x)'\theta$ is represented by the information surface given by

$$i_M(x) = \begin{cases} \frac{1}{f(x)'M^{-1}f(x)} & for\ f(x) \in range\ M \\ 0 & otherwise \end{cases}$$

In terms of information matrices $C_K(M(\xi))$, we have

$$i_M(x) = C_{f(x)}(M(\xi)) \tag{3}$$

Definition 1

In an $m-way$ second - degree model $m \geq 2$, we take the regression function to be

$$f(x) = \begin{pmatrix} 1 \\ x \\ x \otimes x \end{pmatrix} : \mathrm{T}_{\sqrt{m}} \to \mathbb{R}^k \quad (4)$$

with $\mathrm{T}_{\sqrt{m}}$ the ball of radius $\sqrt{m}$ in $\mathbb{R}^k$ and $k = 1 + m + m^2$. The moment matrix of a design $\tau \in T$ is denoted by (1.2) above. The portion $x \otimes x$ which is an $m^2 \times 1$ matrix represents the mixed products for $i \neq j$ twice, as $x_i x_j$ and as $x_j x_i$.

The second-degree Kronecker model is

$$E(Y_x) = f(x)'\theta = \theta_0 + \sum_{i=1}^{m} \theta_i x_i + \sum_{i=1}^{m} \theta_{ii} x_i^2 + \sum_{i,j=1}^{m} (\theta_{ij} + \theta_{ji}) x_i x_j \quad (5)$$

Where Y_x the observed response under the experimental conditions $x \in T$, is taken to be a scalar random variable and

$$\Theta = (\theta_0, \theta_1, \dots, \theta_{11}, \theta_{22}, \dots, \theta_{mm})' \in \mathbb{R}^{m^2} \text{ is an unknown parameter.} \quad (6)$$

The second – degree Kronecker model (5) has $(1 + m + m^2)$ parameters and is expressed as follows:

(a) $m = 3$

$$\eta(\theta, x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_{11} x_1^2 + \theta_{12} x_1 x_2 + \theta_{13} x_1 x_3 + \theta_{21} x_2 x_1 + \theta_{22} x_2^2 + \theta_{23} x_2 x_3 + \theta_{31} x_3 x_1 + \theta_{32} x_3 x_2 + \theta_{33} x_3^2$$

(b) $m = 4$

$$\eta(\theta, t) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4 + \theta_{11} x_1^2 + \theta_{12} x_1 x_2 + \theta_{13} x_1 x_3 + \theta_{14} t_1 t_4 + \theta_{21} x_2 x_1 + \theta_{22} x_2^2 + \theta_{23} x_2 x_3 + \theta_{24} x_2 x_4 + \theta_{31} x_3 x_1 + \theta_{32} x_3 x_2 + \theta_{33} x_3^2 + \theta_{34} x_3 x_4 + \theta_{41} x_4 x_1 + \theta_{42} x_4 x_2 + \theta_{43} x_4 x_3 + \theta_{44} x_4^2 \quad (7)$$

The Kronecker representation has several advantages such as offering attractive symmetry, more compact notations, more convenient invariance properties, and the homogeneity of the regression terms (Draper and Pukelsheim, 1998 and Prescott, et al, 2002).

In this study, information matrices based on the parameter subsystem of interest and their corresponding rotatable CCDs for fitting second - degree Kronecker model as suggested by Draper and Pukelsheim (1998) and as cited by Koech et.al. (2014) are investigated.

The CCD is one of the main types of response surface designs. The CCDs comprise of three portions: a 2^m factorial (or fractional factorial) design and center points (used for fitting first order model) and $2m$ axial points at a distance α from the origin (added when the second-order terms are further incorporated). Hence a CCD is extremely useful and powerful in sequential experimentations.

Yin-Jie Huang (2007) constructed minimal-point designs for second-order response surface using a two-stage method to find the minimal-point composite designs formulated as:

$$\xi = \frac{n_1 + 1}{p} \xi_1 + \left(1 - \frac{n_1 + 1}{p}\right) \xi_2$$

where ξ_1 is the design of the first-order portion and one center point, n_1 is the number of the support points of the first-order design, and ξ_2 is the equal-weight design with the $(p - n_1 - 1)$ distinct added support points. A comparison was made with CCDs, other small composite designs and minimal-point designs by relative efficiencies and the proposed composite designs performed well in general. Ray-Bing et al. (2008) constructed small composite designs for a second-order response surface which they referred to as Conditionally Optimal Small Composite Designs. The designs considered were represented as

$$\xi = \frac{nc}{n} \xi_c + \frac{n_1}{n} \xi_1 + \frac{n_2}{n} \xi_2$$

where ξ_c is the one-point design at center point, 0, with n_c replications; ξ_1 is the selected first-order design and n_1 is the number of supports of this first-order design; ξ_2 is the equal-weight design for n_2 added points, and $n = n_1 + n_c + n_2$. Chuan-Pin and Mong-Na (2011) investigated D-optimal designs for different models showed that, at each qualitative level, the corresponding D-optimal design also consists of three portions as central composite design, i.e. the cube design, the axial design and center points, but with different weights.

2.0. Design Problem

In this study, the design problem is to obtain second order optimal rotatable designs constructed through resolution III and IV to explore and optimize response surfaces based on the Central Composite Design.

Optimality will be accomplished through the application of D-optimality criterion which follows from the General Equivalent Theorem (Pukelsheim, 1993).

2.1. Constructed Rotatable CCD Through Resolutions

A $Resolution\ R$ design of an m-factor design in n runs is constructed in this section.

Let X be the $n\ by\ m$ design matrix, with high and low levels of a factor denoted by +1 and -1 respectively. To construct one-half fraction, we write down a full 2^{m-1} factorial design, then add the mth factor by identifying its plus and minus levels with the signs of $ABC\ldots(M-1)$. Then

$M = ABC\ldots(M-1) \Rightarrow I = ABC\ldots M$ where $A,B,C,\ldots,M = x_1,x_2,x_3,\ldots,x_m$ respectively. When additional factors are added to the interactions, generators are created. The set of distinct words formed by all possible products of any subsets of the factors involving p generators gives the defining relation which contains 2^p terms including the identity term $\boldsymbol{I}$. For a set of generators $W = \{W_1, W_2, \ldots, W_p\}$, we have $IW = WI = W$ and $W^2 = I$. Another way is to partition the runs into two blocks with the highest-order interaction $ABC\ldots M$ confounded

To create a resolution III design, we assign the additional factors to the generators. For $m = 3$ factors, a resolution III design will be such that $x_{3=}x_1x_2$ and hence the defining relation is given by $\mathrm{I} = x_1x_2x_3$ and this is a resolution III^* design. For $m = 4$ factors, a resolution IV design is such that $x_4 = x_1x_2x_3$ and hence the defining relation is given by $\mathrm{I} = \mathrm{x}_1\mathrm{x}_2\mathrm{x}_3\mathrm{x}_4$ denoted as 2_{IV}^{4-1} design. Further, for $m = 5$ factors, a resolution V design is such that $x_5 = x_1\mathrm{x}_2\mathrm{x}_3\mathrm{x}_4$ and hence the defining relation is given by $\mathrm{I} = \mathrm{x}_1\mathrm{x}_2\mathrm{x}_3\mathrm{x}_4\mathrm{x}_5$ denoted as 2_V^{5-1}design.

In this article, the CCD is a resolution R design with the levels of each factor coded to the usual $-1, +1$, augmented by the following points: $(\pm\alpha, 0, \ldots, 0), (0, \pm\alpha, \ldots, 0)$ and $(0, 0, \ldots, \pm\alpha)$.

Generally, the design matrix for a CCD experiment involving m factors is derived from a matrix $\boldsymbol{d}$ which is a vertical concatenation and is of the form

$$d = \begin{bmatrix} R \\ E \end{bmatrix} \tag{8}$$

containing the following three different parts corresponding to the two types of experimental runs:

1. The matrix $\boldsymbol{R}$ obtained from the fractional factorial (Resolution R) experiment (Tables 1, 2 and 3 above).
2. A matrix $\boldsymbol{E}$ from the axial points, with $2m$ rows.

We select the value of α according to the rotatability restrictions $\alpha = 2^{\frac{m-p}{4}} = \sqrt[4]{F}$, where F is the number of experimental runs in the fractional factorial portion.. In order to show how these restrictions are made in choosing α, attention was paid to the expanded design matrix, X and the information matrix, $X'X$, for the general CCD. In fitting the second-degree Kronecker model (8) (Draper and Pukelsheim, 1998), the design matrix X is the horizontal concatenation of a column of $1's$ (intercept) and all element products of a pair of columns of d.

Thus using matrix d the design matrix X takes the form:

$$X = [1\ \ d\ \ d(1)^2\ d(1)\times d(2) \ldots d(1)\times d(m)\quad d(2)\times d(1)\ \ldots\ d(m-1)\times d(m)\ \ldots\ d(m)\times d(m-1)\ \ d(m)^2] \tag{9}$$

2.2. Optimality Criteria and General Equivalence Theorem (Pukelsheim, 1993)

Most often, all the available criteria in literature may be classified into four types; information-based criteria, distance-based criteria, compound criteria and other types criteria; according to their definitions. In this study, we focus on information-based criteria which are related to the information matrix X^TX for the design. This matrix is important because it is proportional to the inverse of the variance-covariance matrix for the least-squares estimates of the linear parameters of the model of interest (El-Monsef, M. M. E. A., Rady, E. A., and Seyam, M. M. (2009). The ultimate purpose of any optimality criterion is to measure the largeness of a nonnegative definite $s \times s$ information matrix C. The D-optimality criterion is in the family of matrix means discussed in detail by Pukelsheim (1993) and is defined as:

$$\emptyset_p(C) = \left\{ (\det C)^{\frac{1}{s}} \qquad for\ p = 0 \right. \tag{10}$$

The CCD $\eta(\xi)$ is $D-optimal$ for θ if and only if

$$trace\ \ C_i\, C^{p-1} \begin{cases} = traceC^p & for\ \ i = 1,2 \\ < traceC^p & otherwise \end{cases} \qquad p = 0 \tag{11}$$

2.3. Subsystem of Interest of the Mean Parameters

In this article, we study s out of the total k components, where $s \le k$ and the linear parameter subsystem is of the form $K'\theta$ of the parameter vector $\theta \in \mathcal{R}^k$ for some $k \times s$ matrix $K \in \mathcal{R}^{k\times(m+1)}$ assumed to have full column rank. K is called the coefficient matrix of the maximum parameter subsystem $K'\theta$. We consider the Euclidean unit vectors in $\mathbb{R}^m$ denoted by $e_{1,}\, e_2, \dots, e_m$ and the sets

$e_{ii} = e_i \otimes e_i$, $e_{ij} = e_i \otimes e_j$, $for\ i < j < k,\ \ i,j,k = \{1,2,\dots,m\}$.

We let the $k \times s$ coefficient matrix K be such that:

$$K = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & K_1 & K_2 \end{pmatrix} \in \mathbb{R}^{(m^2+m+1)\times s} \ \text{ for } m \ge 3 \tag{12}$$

Where

$K_1 = \sum_{i=1}^{m} e_{ii}e_i'$, an $(m^2 \times m)$ matrix

and

$$K_2 = \begin{cases} \frac{1}{2}\left(\sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{ij} + e_{ji}) E_r' \right) & for\ \ m = 3 \\ \frac{1}{4}\left(\sum_{\substack{i,j=1 \\ i<j \\ k<l}}^{m} (e_{ij} + e_{ji} + e_{kl} + e_{lk}) E_r' \right) & for\ \ m = 4 \\ & r = 1, \dots, (s-(m+1)) \end{cases} \qquad K_2 \text{ is an } m^2 \times (s-(m+1)) \text{ matrix.}$$

where r is the number of times each column corresponding to the interaction factors is repeated in the design matrix X of the respective CCD.

Thus

$$K'(\theta) = \begin{cases} \left.\begin{cases} \theta_0 & \\ \theta_{ii} & for\ \ 1 \le i \le m \\ \frac{1}{2}\{(\theta_{ij} + \theta_{ji})\} & for\ i = 1, \dots, m \\ & i < j \le m \end{cases}\right\} \text{for } m = 3 \text{ factors} \\ \left.\begin{cases} \theta_0 & \\ \theta_{ii} & for\ \ 1 \le i \le m \\ \frac{1}{4}\{(\theta_{ij} + \theta_{ji} + \theta_{kl} + \theta_{lk})\} & for\ i,j,k,l = 1, \dots, m \\ & i \ne j \ne\ k \ne l \\ & i < j, \end{cases}\right\} \text{for } m = 4 \text{ factors} \end{cases} \tag{13}$$

The information matrix for $K'\theta$ with $k \times s$ coefficient matrix K of column rank s, is defined to be $C_k(M)$ when the mapping $C_k: NND(k) \to sym(s)$ is given by all $A\ \in\ NND(k)$ with minimum taken relative to the loewner ordering over all left inverses L of K where M is the moment matrix (2) Pukelsheim (1993). The amount of information which the design ξ contains on the parameter subsystem $K'\theta$ is captured by the information matrix (3) now defined as, $C_k(\xi) = \min\{LM(\xi)L'\}; L \in \mathbb{R}^{S\times(m^2+m+1)}$ and this is the precision matrix of the best linear unbiased estimator for $K'\theta$ under design τ, Pukelsheim (1993), Koske et. al.(2011) and Cherutich (2012).

The information matrices for $K'\theta$ are linear transformations of moment matrices and takes the following form:

$$C_k(M(\xi)) \ = \ LM(\xi)L' \tag{14}$$

where L is left inverse of K defined as $L = (K'K)^{-1}K'$

3.0. Optimum Rotatable Weighted Central Composite Design

A CCD is a mixture of three building blocks: cubes, stars and center points. In this thesis the CCD is separated into a factorial (cube) block and an axial (star) point block. A convex combination

$\xi_{WCCD}(w) = \sum_{i=1}^{p} w_i \xi_i$ with $w = (w_1, w_2, \dots, w_p)' \in \mathrm{T}_p$ is called a WCCD with weight vector with $\sum_{i=1}^{p} w_i = 1$.

From the linearity of the information matrix mapping C_K, we obtain for every $w \in \mathrm{T}_p$,

$$C_K\left(M\big(\xi(w)\big)\right) = \sum_{i=1}^{p} w_i C_K\big(M(\xi_i)\big) \qquad i = 1,2 \tag{15}$$

The rotatable WCCD ($\alpha^4 = 2^{m-p}$) is expressed as follows:

$$\xi_{WCCD} = w_1 \xi_F + w_2 \xi_s \tag{16}$$

Where

a) w_i , $i = 1,2$ satisfies the conditions $\sum_{i=1}^{2} w_i = 1$ and $w_1, w_2 \geq 0$

b) ξ_F is the design with support points n_F determined by combining the first order design obtained from half- fraction factorial design (either Resolution III, IV) and ξ_s is the design with $2m$ distinct supports ($2m$ is the star portion) and hence total design points will be $n = n_F + 2m$.

3.1. Moment Matrix $M(\xi)$ for m-Factors

Generally, for m −factors, with the cube portion constructed through resolution R, the second – order kronecker model moment matrix of a rotatable CCD may be expressed as follows:

Let d be a vertical concatenation of the form $d = \begin{bmatrix} R \\ E \end{bmatrix}$ given in equation (11), then for m −factors and N experimental runs, the design matrix X takes the form given in equation (9),

By definition, the moment matrix for a second-order kronecker model is given by:

$$M(\xi) = \frac{X^T X}{N}$$

$$= \frac{1}{N}[1 \;\; d \;\; d(1)^2 \; d(1) \times d(2) \dots d(1) \times d(m) \quad d(2) \times d(1) \;\dots\; d(m-1) \times d(m) \;\dots\; d(m) \times d(m-1) \;\; d(m)^2]^T \; [1 \;\; d \;\; d(1)^2 \; d(1) \times d(2) \dots d(1) \times d(m) \quad d(2) \times d(1) \;\dots\; d(m-1) \times d(m) \;\dots\; d(m) \times d(m-1) \;\; d(m)^2]$$

$$= \begin{cases} \dfrac{1}{N}\begin{pmatrix} N & \emptyset' & (F+2\alpha^2)(vec\, I_m)' \\ \emptyset & (F+2\alpha^2) I_m & F\big(E_{ijk}\big)' \\ (F+2\alpha^2) vec\, I_m & F E_{ijk} & H_m \end{pmatrix} \in \mathbb{R}^{(1+m+m^2)\times(1+m+m^2)} \; for\ m \geq 3\ Resolution\ III \\ \dfrac{1}{N}\begin{pmatrix} N & \emptyset_1' & (F+2\alpha^2)(vec\, I_m)' \\ \emptyset_1 & (F+2\alpha^2) I_m & \emptyset_2' \\ (F+2\alpha^2) vec\, I_m & \emptyset_2 & H_m \end{pmatrix} \in \mathbb{R}^{(1+m+m^2)\times(1+m+m^2)} for\ m \geq 4\ Resolution\ R \geq IV \end{cases} \tag{17}$$

where

N is the total number of experimental runs

$\alpha = 2^{\frac{m-p}{4}}$ and this satisfies the condition for second-order rotatable designs, m is number of factors,

$I_m \in \mathbb{R}^{m\times m}$ denotes the identity matrix and $vec\ I_m = I_m \otimes I_m$

F is the number of runs in the cube portion.

$E_{ijk} = \sum_{i\neq j\neq k=1}^{m} \big(e_i \otimes e_j\big)\, e_k^T$, e_i's are the Euclidean unit vectors in $\mathbb{R}^m$ denoted by $e_1, e_2, \dots, e_m$

H_m denotes an $m^2 \times m^2$ matrix whose entries are given by $(F + 2\alpha^4)V_1 + FV_2$

$V_1 = \sum_{i=1}^{m} E_{ii}$ with $E_{ii} = (e_i e_i^T) \otimes (e_i e_i^T)$

$$V_2 = \begin{cases} \sum_{i \neq j = 1}^{m} \left(E_{ij} + E_{ij'} + E_{ji}\right) & \text{for } m \geq 3 \text{ Resolution } III \\ \sum_{i \neq j = 1}^{m} \left(E_{ij} + E_{ij'} + E_{ji}\right) + \sum_{i \neq j \neq k \neq l = 1}^{m} E_{ijkl} & \text{for } m \geq 4 \text{ Resolution } R \geq IV \end{cases}$$

with $E_{ij} = (e_i e_i^T) \otimes \left(e_j e_j^T\right)$;

$$E_{ij'} = \left(e_i e_j^T\right) \otimes \left(e_i e_j^T\right) \qquad E_{ji} = \left(e_i e_j^T\right) \otimes \left(e_j e_i^T\right)$$

$$E_{ijk} = \left(e_i e_j^T\right) \otimes (e_i e_k^T) \qquad E_{ijkl} = \left(e_i e_j^T\right) \otimes (e_k e_l^T)$$

3.2. Information Matrix $C_K\big(M(\xi)\big)$ for m-Factors

The information matrix for $K'\theta$ with $k \times s$ coefficient matrix K of column rank s, is defined to be $C_k(M)$ (Koske et. al.,2011 and Cherutich, 2012) where M is the moment matrix. Defining L every left inverse of K as $L = (K'K)^{-1}K'$, then

$C_k(M(\xi)) = LM(\xi)L'$. thus we obtain:

$$C_K\big(M(\xi)\big) = \frac{1}{N}\begin{pmatrix} N & (F + 2\alpha^2)(1_m)^T & \emptyset_1^T \\ (F + 2\alpha^2)1_m & G_m & \emptyset_2^T \\ \emptyset_1 & \emptyset_2 & 2(F + \alpha^4)I_c \end{pmatrix} \tag{18}$$

Where

$1_m = (1, \ldots, 1)^T \in \mathbb{R}^m$ denotes the vector with all elements equal to 1,

G_m denotes an $m \times m$ circulant matrix with diagonal and off-diagonal elements a and b respectively and entries in a and b are given by $(F + 2\alpha^4)$ and F. Thus

$G_m = (F + 2\alpha^4)I_m + F\sum_{i \neq j = 1}^{m} e_i e_j^T$, where e_i's and e_j's are the Euclidean unit vectors in $\mathbb{R}^m$ denoted by $e_1, e_2, \ldots, e_m$ and $I_m \in \mathbb{R}^{m \times m}$ denotes an identity matrix.

$I_c \in \mathbb{R}^{c \times c}$ denotes an identity matrix where c is the number of parameters resulting from averaging the interaction factors.

$\emptyset_1$ is a $c \times 1$ vector with all elements zeros

$\emptyset_2$ is a $\boldsymbol{c} \times m$ matrix with all elements zeros

Thus the information matrix $C_K\big(M(\xi)\big)$ is of order $(1 + m + c) \times (1 + m + c)$.

4.0. $D - optimal$ Rotatable Weighted Central Composite Design

Let s be the number of parameters in the subsystem of interest vector $K'(\theta)$. Further let a rotatable CCD of m factors comprise of elementary designs ξ_F and ξ_s i.e. the fractional factorial portion constructed through resolution R and the star portion respectively. Then $D - optimal$ Rotatable Weighted Central Composite Design (ξ_{WCCD})is given by:

$$\xi_{WCCD} = \frac{s-m}{s}\xi_F + \frac{m}{s}\xi_s \tag{19}$$

Where $w_1 = \frac{s-m}{s}$ and $w_2 = \frac{m}{s}$ are the weights assigned to each of the design portions, factorial and star respectively.

Further, the determinant of the information matrix can be obtained by using the formula for computing determinant of a partitioned symmetric matrix.

By definition, if $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix}$, then the determinant of A is given by:

$|A| = |A_{22}||A_{11} - A_{12}A_{22}^{-1}A_{12}^T| = |A_{11}||A_{22} - A_{12}^T A_{11}^{-1} A_{12}|$. (Kaare B. P. and Michael S.P., 2012)

Partition the general information matrix (17) such that

$$C_k\big(M(\xi)\big) = \begin{bmatrix} U & \emptyset^T \\ \emptyset & V \end{bmatrix}$$

where $U = \begin{bmatrix} 1 & \frac{1}{N}(F + 2\alpha^2)(1_m)^T \\ \frac{1}{N}(F + 2\alpha^2)1_m & \frac{1}{N}G_m \end{bmatrix}$ and $V = \frac{2}{N}(F + \alpha^4)I_c$.

Then the determinant is:

$|C_k(M(\xi))| = |V||U - \emptyset^T V \emptyset^T| = |V||U|$

Now V is a $c \times c$ diagonal matrix (c is the number of parameters resulting from averaging the interaction factors)

Hence $|V| = \left(\frac{2}{N}(F+\alpha^4)\right)^c$

Next $|U| = |U_{11}||U_{22} - U_{12}^T U_{11}^{-1} U_{12}|$

$= \left|\frac{1}{N} G_m - \frac{1}{N^2}(F+2\alpha^2)^2(1_m)(1_m)^T\right|$

Substituting G_m from (20),

$$|U| = \left|\frac{1}{N}\{(F+2\alpha^4)I_m + F\textstyle\sum_{i\neq j=1}^m e_i e_j^T\} - \frac{1}{N^2}(F+2\alpha^2)^2(1_m)(1_m)^T\right|$$

Thus

$$|C_k(M(\xi))| = \left(\frac{2}{N}(F+\alpha^4)\right)^c \times \left|\frac{1}{N^2}\{N(F+2\alpha^4)I_m + NF\textstyle\sum_{i\neq j=1}^m e_i e_j^T - (F+2\alpha^2)^2 J_m\}\right| \tag{20}$$

where I_m is an $m \times m$ identity matrix, J_m is an $m \times m$ matrix of ones and $e_i's$ are the Euclidean unit vectors in $\mathbb{R}^m$ denoted by $e_1, e_2, \dots, e_m$

Consequently, using formula (10) the D-optimal value is

$$\boldsymbol{V}(\emptyset_0) = \left[\left(\frac{2}{N}(F+\alpha^4)\right)^c \times \left|\frac{1}{N^2}\{N(F+2\alpha^4)I_m + NF\textstyle\sum_{i\neq j=1}^m e_i e_j^T - (F+2\alpha^2)^2 J_m\}\right|\right]^{\frac{1}{s}} \tag{21}$$

4.1. D-Optimal Rotatable WCCD

In this section the constructed rotatable CCD for m=3 and m=4 are investigated and the corresponding optimal rotatable WCCDs are derived. Results obtained in sections 2.2, 3.0 and 3.1 are used in this section.

4.1.1. Three Factors

D-optimal rotatable WCCD for three factors is derived. Using (14), (15), (16) and (17) the following matrices are obtained.

$$L = \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&1&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0&1\\ 0&0&0&0&0&1&0&1&0&0&0&0&0\\ 0&0&0&0&0&0&1&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&0&0&1&0&1&0 \end{bmatrix}$$

the information matrices for the two portions of the CCD are:

$$C_k(M_{\xi_F}) = \begin{bmatrix} 1&1&1&1&0&0&0\\ 1&1&1&1&0&0&0\\ 1&1&1&1&0&0&0\\ 1&1&1&1&0&0&0\\ 0&0&0&0&4&0&0\\ 0&0&0&0&0&4&0\\ 0&0&0&0&0&0&4 \end{bmatrix} \quad \text{and} \quad C_k(M_{\xi_s}) = \begin{bmatrix} 1&\frac{2}{3}&\frac{2}{3}&\frac{2}{3}&0&0&0\\ \frac{2}{3}&\frac{4}{3}&0&0&0&0&0\\ \frac{2}{3}&0&\frac{4}{3}&0&0&0&0\\ \frac{2}{3}&0&0&\frac{4}{3}&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0 \end{bmatrix} \tag{22}$$

The information matrix for the WCCD is:

$C_k(M(\xi)) = w_1 C_k(M_{\xi_F}) + w_2 C_k(M_{\xi_s})$

$$= \begin{bmatrix} w_1 + w_2 & \frac{3w_1+2w_2}{3} & \frac{3w_1+2w_2}{3} & \frac{3w_1+2w_2}{3} & 0 & 0 & 0 \\ \frac{3w_1+2w_2}{3} & \frac{3w_1+4w_2}{3} & w_1 & w_1 & 0 & 0 & 0 \\ \frac{3w_1+2w_2}{3} & w_1 & \frac{3w_1+4w_2}{3} & w_1 & 0 & 0 & 0 \\ \frac{3w_1+2w_2}{3} & w_1 & w_1 & \frac{3w_1+4w_2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4w_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4w_1 \end{bmatrix} \tag{23}$$

To obtain $D - optimal$ Rotatable WCCD, matrices (22) and (23) are used in the relation (13) and this results in relation (19) such that

$$w_1 = \frac{4}{7} \text{ and } w_2 = 1 - w_1 = \frac{3}{7} \tag{24}$$

Hence the $D - optimal$ WCCD is

$$\xi_{WCCD} = w_1\xi_F + w_2\xi_s = \frac{4}{7}\xi_F + \frac{3}{7}\xi_s \tag{25}$$

Using (24) in (23) and working out (21) the D-optimal value is obtained as:

$$V(\emptyset_0) = 0.849 \tag{26}$$

4.1.2. Four Factors

D-optimal rotatable WCCD for four factors is derived. Using (14), (15), (16) and (17) the following matrices are obtained.

$$L = \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1 \\ 0&0&0&0&0&0&1&0&0&1&0&0&0&0&0&0&1&0&0&1&0 \\ 0&0&0&0&0&0&0&1&0&0&0&0&1&1&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0&1&0&0&1&0&0&1&0&0&1&0&0&0 \end{bmatrix} \tag{27}$$

Information matrices for the two portions of the CCD are:

$$C_k(M_{\xi_F}) = \begin{bmatrix} 1&1&1&1&1&0&0&0 \\ 1&1&1&1&1&0&0&0 \\ 1&1&1&1&1&0&0&0 \\ 1&1&1&1&1&0&0&0 \\ 1&1&1&1&1&0&0&0 \\ 0&0&0&0&0&16&0&0 \\ 0&0&0&0&0&0&16&0 \\ 0&0&0&0&0&0&0&16 \end{bmatrix} \text{ and}$$

$$C_k(M_{\xi_s}) = \begin{bmatrix} 1&0.7071&0.7071&0.7071&0.7071&0&0&0 \\ 0.7071&2&0&0&0&0&0&0 \\ 0.7071&0&2&0&0&0&0&0 \\ 0.7071&0&0&2&0&0&0&0 \\ 0.7071&0&0&0&2&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \end{bmatrix} \tag{28}$$

The information matrix for the WCCD is:

$$C_k(M(\xi)) = w_1C_k(M_{\xi_F}) + w_2C_k(M_{\xi_s}) =$$

$$\begin{bmatrix} w_1+w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1+2w_2 & w_1 & w_1 & w_1 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1 & w_1+2w_2 & w_1 & w_1 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1 & w_1 & w_1+2w_2 & w_1 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1 & w_1 & w_1 & w_1+2w_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 16w_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 16w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16w_1 \end{bmatrix} \quad (29)$$

To obtain $D-optimal$ Rotatable WCCD, matrices (28) and (29) are used in the relation (13) and this results in relation (19) such that

$$w_1 = 0.4999861 \cong 0.5 \quad \Longrightarrow \quad w_2 = 0.5000139 \cong 0.5 \quad (30)$$

Hence the $D-optimal$ WCCD is

$$\xi_{WCCD} = 0.50\boldsymbol{\xi_F} + 0.50\boldsymbol{\xi_s} \quad (31)$$

Using (30) in (29) and working out (21) the D-optimal value is obtained as:

$$V(\emptyset_0) = (de\,t\,C)^{\frac{1}{8}} = 1.605 \quad (32)$$

5.0. Results and conclusion

The theoretical results obtained in this study are given in the table below and a discussion is done.

Table 5.1 D-optimal Rotatable Designs

m-Factors	Resolution R	Uniform weighted CCD	WCCD	Efficiency	Weights	
3	III	0.8	0.84	1.061	$w_1 = \frac{4}{7}$	$w_2 = \frac{3}{7}$
4	IV	1.66	1.60	0.969	$w_1 = \frac{1}{2}$	$w_2 = \frac{1}{2}$
5	V	1.53	1.54	1.0114	$w_1 = \frac{11}{16}$	$w_2 = \frac{5}{16}$

D-optimal rotatable weighted central composite designs have been derived for three and four factors constructed through resolution III and IV. Optimal values and weights for the weighted central composite designs were numerically obtained using both R and wxMaxima softwares. A generalized form of the moment matrix $M(\xi)$, coefficient matrix K, the information matrix $C_K(M(\xi))$, D-optimal rotatable WCCD for m-factors were also obtained. A comparison is done on the optimal values for the uniform weighted rotatable CCDs and the derived optimal rotatable WCCDs as well as the weights assigned to each of the two portions of the D-optimal rotatable WCCD.

Resolution III and V weighted central composite design is better than the uniformly weighted CCD in terms of the D- optimality criterion since the D-optimal value is larger. Resolution IV uniformly weighted CCD is better than the weighted central composite design since the D- optimal value is greater

The mass assigned to the cube portion is greater than the one assigned to the star portion for resolution III and V designs indicating that the cube portion plays a greater role in D-optimal resolution III and V designs. But equal weight is assigned to the two portions of the design constructed through resolution IV indicating that the two portions are of equal importance in D-optimal resolution IV designs.

Recommendation

From the results of this study it would be interesting to compare the same designs investigated under the A-, E- and I-optimality criteria as well the practicability of the theoretical results.

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