

I-optimal Rotatable Central Composite Designs

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Abstract: *Optimal designs are those that are constructed on the basis of a certain optimality criterion. The proper meaning of 'optimal' depends on the situation, and can include: most effective, minimum variance, minimum bias, etc. This paper investigates Central Composite Designs whose cube portion is constructed through resolution III and IV. I-optimal rotatable Weighted Central Composite Designs (WCCDs) are derived by assigning different weights to two portions of the CCD namely the cube and star portion. The results showed that a greater weight is assigned to the star portion than the cube portion in both resolution III and IV designs and each WCCD has an I-- efficiency of near one for both designs relative to the uniformly weighted CCD.*

1. Introduction

In recent years, the use of optimal designs in industrial experimentation has grown rapidly. These designs are used for the study of response surface methodology (RSM) which is useful for developing, improving, and optimizing products and processes. It's application to design optimization aims at reducing the cost of expensive analysis methods and their associated numerical noise. The optimization process involves three major steps: performing the statistically designed experiments, estimating the coefficients in mathematical model and predicting the response and checking the adequacy of the model [7].

Designing an experiment to fit a response surface model involves selecting designs among several candidate designs. Optimal designs are those that are constructed on the basis of a certain optimality criterion that pertains to the 'closeness' of the predicted response, $\hat{y}(x)$, to the mean response, $\mu(x)$, over a certain region of interest denoted by R . There are often many competing criteria that could be considered in selecting the design [5]. The design criteria that address the minimization of the variance associated with the estimation of model unknown parameters are called variance-related criteria. The

most prominent of such criteria is the D-optimality criterion that maximizes the determinant of the matrix $X'X$. I-optimality criterion is prediction based and aims at minimizing the average variance of prediction over the region of experimentation. The General Equivalence Theorem for I-Optimality was used by [3] to investigate V-optimal mixture designs for the q th degree model using the simplex centroid design.

Designs discussed in this paper are based on the central composite design with the cube portion constructed through resolutions III and IV. Optimal rotatable Weighted Central Composite Designs are derived for three and four factors and optimality is accomplished through the application of I-optimality criterion which follows from the General Equivalence Theorem [2]

2. Design Problem and the Model

In this paper, the design problem is to obtain second – order I - optimal rotatable weighted central composite design with the cube portion constructed through resolution III and IV. An $m – way$ second – degree Kronecker model for $m \geq 2$ of the K-regression function f is fitted. This involves the Kronecker product whose powerful properties make f superior to any other form of parametrizing the second - degree model [6]. The model has $(1 + m + m^2)$ parameters and is expressed as:

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

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

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

3.1. The Central Composite Design (CCD)

A CCD uses cube points, extreme (corner) points and either face points (requires three levels) or extended points (requires five levels). For a rotatable CCD:

$$\mu_4 = 3\mu_{22} \quad \text{giving} \quad \alpha = 2^{\frac{m-p}{4}} = \sqrt[4]{F} \quad \text{where} \\ F = 2^{m-p}$$

Resulting from the relations

$$\mu_4 = 2^{m-p} + 2\alpha^4 \quad \text{and} \quad \mu_{22} = 2^{m-p}$$

Rotatability also includes singularity condition

$$\frac{\mu_4}{(\mu_{22})^2} > \frac{m}{m+2}$$

The rotatable design ξ (where $\alpha^4 = 2^{m-p}$) may be formed by combining a fractional factorial design (cube portion ξ_F replicated n_c times) obtained from resolution R (R= III and IV) for sample size $2^{m-p}n_c$, a star portion (ξ_s replicated n_s times) for sample size $2mn_s$ plus a centre point portion (ξ_0 replicated n_0 times). The design $\xi = n_c\xi_F + n_s\xi_s + n_0\xi_0$ has sample size $n = 2^{m-p}n_c + 2mn_s + n_0$.

In this paper the number of replicates chosen are $n_c = 1$, $n_s = 1$ and $n_0 = 0$ to obtain a central composite design $\xi = \xi_F + \xi_s$ such that the sample size is $n = 2^{m-p} + 2m$ and $p = 1$.

(Resolution III and IV factorial designs and the corresponding CCDs are in the appendix).

Further in this paper information matrices for three and four factors based on the parameter subsystem of interest and their corresponding rotatable CCDs for fitting second - degree Kronecker model derived by [4] are used.

3.2. I-optimality Criterion

Popular implementations of the I- optimality criterion (also known as V- optimality criterion) are based on a grid of points covering the experimental region. Continuous I - optimality designs involve a set of distinct design points and a relative frequency or weight for each of these points. These weights w_1, w_2, \dots, w_m of the different types of points in that design satisfy the constraint:

$$\sum_{i=1}^m \eta_i w_i = qw_1 + \binom{m}{2} w_2 + \dots + \binom{m}{m-1} w_{m-1} \\ + w_m = 1$$

The weight of each design point indicates the proportion of the experimental runs to be performed at that point [3].

I - optimality criterion seeks designs that minimize the average variance of prediction over the experimental region χ [3]. By definition

Average variance

$$\frac{\int_{\chi} f(x)M^{-1}f'(x)dx}{\int_{\chi} dx} = \frac{\int_{\chi} f(x)(X'X)^{-1}f'(x)dx}{\int_{\chi} dx} \quad (2)$$

and can be calculated exactly for simplex shaped experimental regions as

$$\frac{1}{\Gamma q} \left[\text{tr}(X'X)^{-1} \left[\int_{\chi} f(x)f'(x)dx \right] \right]$$

moment matrix

The numerator in (2) may be expressed as

$$\int_{\chi} f(x)M^{-1}f'(x)dx = \text{tr} \left[M^{-1} \int_{\chi} f(x)f'(x)dx \right]$$

Define $B = \int_{\chi} f(x)f'(x)dx$

Then

$$I - \text{optimality} = \frac{\text{tr}[M^{-1}B]}{\int_{\chi} dx} \quad (3)$$

Assuming that the experimental region χ is the full $(m - 1)$ -dimensional simplex s_{q-1} , the elements of B can be obtained using the formula:

$$B = \int_{s_{q-1}} x_1^{p_1} x_2^{p_2} \dots x_m^{p_m} dx_1 dx_2 \dots dx_m \\ = \frac{\prod_{i=1}^{q-1} (p_i + 1)}{\left(m + \sum_{i=1}^m p_i \right)} = \frac{\prod_{i=1}^m p_i!}{\left(m - 1 + \sum_{i=1}^m p_i \right)!} \quad (4)$$

where p is the power of the factors and m is the number of factors. And

$$\int_{\chi} dx = \int_{s_{m-1}} dx = \frac{1}{m}$$

Define

$$L = \Gamma(m) \times B \quad \text{where} \quad \Gamma(m) = (m - 1)!$$

Thus from (3)

$$I - \text{optimality} = \text{tr}[M^{-1}L] \quad (5)$$

3.3. m - Factors Rotatable CCD I-Optimal Value

The I - optimal value for m - factors is a linear function of order four moments. Generally

$$I - \text{optimality} = \text{tr} \left[\left(C_K(M(\xi)) \right)^{-1} L_m \right] \quad (6)$$

for $C_K(M(\xi))$ (see [4] for general form of $C_K(M(\xi))$) equal to the information matrix,

$$L_m = \Gamma(m) \times B, \quad (7)$$

$$B = \int_{S_{q-1}} x_1^{p_1} x_2^{p_2} \dots x_m^{p_m} dx_1 dx_2 \dots dx_m = \frac{\prod_{i=1}^m p_i!}{\left(m-1 + \sum_{i=1}^m p_i \right)!}$$

p is the power of the factors and m is the number of factors.

Therefore (6) results to

I - optimality

$$= \beta_0 - \frac{\beta_1}{3m-1} \mu_2 + \frac{\beta_2}{3m-1} \mu_4 + \frac{\beta_3}{3m-1} \mu_{22} + \beta_4 (\text{sum of cross products second moment})$$

Where β_i is a multiple of \sqrt{m} and $i = 1, 2, \dots, m$.

Further using (5), *I - efficiency* of the design ξ is defined as

$$I(\xi) = \frac{\text{tr}[M^{-1}L(\xi^*)]}{\text{tr}[M^{-1}L(\xi)]} \quad (9)$$

where ξ^* is *I - optimal*

An I-efficiency less than one indicate that Design ξ^* is better than Design ξ in terms of the average prediction variance [2].

4.0. I-Optimal Value for the Rotatable CCDs

In this section, *I - optimal values* are computed based on the parameter subsystem of interest for three and four factors CCD where the cube portion is constructed through resolution III and IV.

4.1. I-Optimal Value for Three Factors

For $m = 3$

$$f(x) = [1 \quad x_1^2 \quad x_2^2 \quad x_3^2 \quad x_1x_2 \quad x_1x_3 \quad x_2x_3]'$$

Thus

$$C_K(M(\xi)) = f(x)f'(x)$$

gives

$$C_K(M(\xi)) =$$

$$\begin{bmatrix} 1 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3 \\ x_1^2 & x_1^4 & x_1^2x_2^2 & x_1^2x_3^2 & x_1^3x_2 & x_1^3x_3 & x_1^2x_2x_3 \\ x_2^2 & x_1^2x_2^2 & x_2^4 & x_2^2x_3^2 & x_1x_2^3 & x_1x_2^2x_3 & x_2^3x_3 \\ x_3^2 & x_1^2x_3^2 & x_2^2x_3^2 & x_3^4 & x_1x_2x_3^2 & x_1x_3^3 & x_2x_3^3 \\ x_1x_2 & x_1^3x_2 & x_1x_2^3 & x_1x_2x_3^2 & x_1^2x_2^2 & x_1^2x_2x_3 & x_1x_2^2x_3 \\ x_1x_3 & x_1^3x_3 & x_1x_2^2x_3 & x_1x_3^3 & x_1^2x_2x_3 & x_1^2x_3^2 & x_1x_2x_3^2 \\ x_2x_3 & x_1^2x_2x_3 & x_2^3x_3 & x_2x_3^3 & x_1x_2^2x_3 & x_1x_2x_3^2 & x_2^2x_3^2 \end{bmatrix} \quad (10)$$

From (7)

$$L_3 = \sqrt{3} \times B$$

where

$$B = \int_{S_{3-1}} x_1^{p_1} x_2^{p_2} x_3^{p_3} dx_1 dx_2 dx_3 = \frac{\prod_{i=1}^3 (p_i + 1)}{\left(3 + \sum_{i=1}^3 p_i \right)} = \frac{\prod_{i=1}^3 p_i!}{\left(3 - 1 + \sum_{i=1}^3 p_i \right)!} \quad (11)$$

p is the power of the factors and

$$\int_x dx = \frac{1}{\sqrt{3}}$$

Thus

$$L_3 = \begin{bmatrix} 1 & v & v & v & g & g & g \\ v & w & h & h & n & n & a \\ v & h & w & h & n & a & n \\ v & h & h & w & a & n & n \\ g & n & n & a & h & a & a \\ g & n & a & n & a & h & a \\ g & a & n & n & a & a & h \end{bmatrix} \quad (12)$$

with

$$v = \sqrt{3} \int x_i^2 dx, \quad i = 1, 2, 3,$$

$$h = \sqrt{3} \int x_1^2 x_2^2 dx, \quad w = \sqrt{3} \int x_i^4 dx,$$

$$a = \sqrt{3} \int x_i^2 x_j x_k dx, \quad g = \sqrt{3} \int x_i x_j dx$$

$$n = \sqrt{3} \int x_i^3 x_j dx \quad \text{in each case } i \neq j \neq k \quad (13)$$

From [4],

$$\left(C_K(M(\xi)) \right)^{-1} = \begin{bmatrix} 25 & -10 & -10 & -10 & 0 & 0 & 0 \\ -10 & 5 & \frac{15}{4} & \frac{15}{4} & 0 & 0 & 0 \\ -10 & \frac{15}{4} & 5 & \frac{15}{4} & 0 & 0 & 0 \\ -10 & \frac{15}{4} & \frac{15}{4} & 5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{5}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{5}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{8} \end{bmatrix} \quad (14)$$

$$(C_K(M(\xi)))^{-1} L_3 = \begin{bmatrix} r & b & b & b & c & c & c \\ b & d & e & e & f & f & t \\ b & e & d & e & f & t & f \\ b & e & e & d & t & f & f \\ \frac{5g}{8} & \frac{5n}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5h}{8} & \frac{5a}{8} & \frac{5a}{8} \\ \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} \\ \frac{5g}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5h}{8} & \frac{5a}{8} \\ \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} \\ \frac{5g}{8} & \frac{5a}{8} & \frac{5n}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5a}{8} & \frac{5h}{8} \\ \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} & \frac{8}{8} \end{bmatrix} \quad (15)$$

Where

$$r = 25 - 30v, \quad b = -10w + 25v - 20h,$$

$$c = -20n + 25g - 10a$$

$$d = \frac{10w-20v+15h}{2}, \quad e = \frac{15w-40v+35h}{4}, \quad t =$$

$$\frac{15n-20g+10a}{2}, \quad f = \frac{35a-40g+15a}{4}$$

From (15) *I* – optimal value is equal to:

$$\begin{aligned} \text{tr}[(C_K(M(\xi)))^{-1} L_3] &= r + 3d + 3 \times \frac{5h}{8} \\ &= \frac{200-480v+120w+195h}{8} \end{aligned} \quad (16)$$

where *v*, *w* and *h* are as defined in (13).

Then using (13) and (16)

$$\begin{aligned} \text{tr}[(C_K(M(\xi)))^{-1} L_3] &= \frac{200}{8} - \frac{480}{8} \int x_1^2 dx + \frac{120}{8} \int x_1^4 dx + \frac{195}{8} \int x_1^2 x_2^2 dx \\ & \quad (17) \end{aligned}$$

Using (11)

$$\begin{aligned} \int x_1^2 dx &= \int_0^1 \frac{\prod_{i=1}^3 p_i!}{(3-1+\sum_{i=1}^3 p_i)!} \\ &= 2! \times \frac{2!}{(3-1+2)!} = \frac{1}{6} \end{aligned}$$

Similarly

$$\int x_1 x_2 dx = \frac{1}{12}$$

$$\int t_1^4 dx = \frac{1}{15}$$

$$\int x_1^2 x_2^2 dx = \frac{1}{90}$$

$$\int x_1^3 x_2 dx = \frac{1}{60}$$

$$\int x_1^2 x_2 x_3 dx = \frac{1}{180}$$

Thus

$$L_3 = \begin{bmatrix} 1 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{6} & \frac{1}{15} & \frac{1}{90} & \frac{1}{90} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} \\ \frac{1}{6} & \frac{1}{15} & \frac{1}{90} & \frac{1}{90} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} \\ \frac{1}{6} & \frac{1}{15} & \frac{1}{90} & \frac{1}{90} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{18} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{18} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{18} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{18} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{18} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{18} & \frac{1}{18} \end{bmatrix} \quad (18)$$

and

$$I - \text{optimal value} = 16.2708 \quad (19)$$

4.2. Four Factors I-Optimal Rotatable CCD

For *m* = 4

$$\begin{aligned} f(x) &= [1 \quad x_1^2 \quad x_2^2 \quad x_3^2 \quad x_4^2 \quad x_1 x_2 + x_3 x_4 \quad x_1 x_3 + x_2 x_4 \quad x_1 x_4 + x_2 x_3]' \\ & \quad (20) \end{aligned}$$

Let *x*₁ = *a*, *x*₂ = *b*, *x*₃ = *c*, *x*₄ = *d*

Then *C_K*(*M*(*ξ*)) is obtained. (see appendix 4).

From (7)

$$L_4 = \sqrt{4} \times B$$

where

$$\begin{aligned} B &= \int x_1^{p_1} x_2^{p_2} x_3^{p_3} x_4^{p_4} dx dx dx dx \\ &= \frac{1}{\prod_{i=1}^4 (p_i + 1)} = \frac{1}{\prod_{i=1}^4 p_i!} \\ &= \frac{1}{(4 + \sum_{i=1}^4 p_i)!} = \frac{1}{(4 - 1 + \sum_{i=1}^4 p_i)!} \end{aligned} \quad (21)$$

where *p* is the power of the factors and

$$\int dx = \frac{1}{\sqrt{4}}$$

Thus

$$L_4 = \begin{bmatrix} 1 & p & p & p & p & q & q & q \\ p & r & g & g & g & t & t & t \\ p & g & r & g & g & t & t & t \\ p & g & g & r & g & t & t & t \\ p & g & g & g & r & t & t & t \\ q & t & t & t & t & u & t & t \\ q & t & t & t & t & t & u & t \\ q & t & t & t & t & t & t & u \end{bmatrix} \quad (22)$$

where

$$\begin{aligned}
 p &= \sqrt[4]{4} \int x_i^2 dx, \quad i = 1, 2, 3, 4, \quad g = \sqrt[4]{4} \int x_1^2 x_2^2 dx, \quad i \neq j \\
 u &= \sqrt[4]{4} \int (x_i x_j + x_k x_l)^2 dx, \quad r = \sqrt[4]{4} \int x_i^4 dx \\
 q &= \sqrt[4]{4} \int (x_i x_j + x_k x_l) dx \quad (\text{Sum of two-factor interactions}) \\
 t &= \sqrt[4]{4} \int x_i^2 (x_i x_j + x_k x_l) dx, \\
 &u = \sqrt[4]{4} \int (x_i x_j + x_k x_l)^2 dx \quad (23)
 \end{aligned}$$

And in each case $i \neq j \neq k \neq l$

And from [4],

$$\left(C_K(M(\xi)) \right)^{-1} = \begin{bmatrix} \frac{300}{11} & -\frac{85}{11} & -\frac{85}{11} & -\frac{85}{11} & -\frac{85}{11} & 0 & 0 & 0 \\ -\frac{85}{11} & \frac{133}{44} & \frac{89}{44} & \frac{89}{44} & \frac{89}{44} & 0 & 0 & 0 \\ -\frac{85}{11} & \frac{89}{44} & \frac{133}{44} & \frac{89}{44} & \frac{89}{44} & 0 & 0 & 0 \\ -\frac{85}{11} & \frac{89}{44} & \frac{89}{44} & \frac{133}{44} & \frac{89}{44} & 0 & 0 & 0 \\ -\frac{85}{11} & \frac{89}{44} & \frac{89}{44} & \frac{89}{44} & \frac{133}{44} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} \end{bmatrix} \quad (24)$$

Therefore

$$\left(C_K(M(\xi)) \right)^{-1} L_4 = \begin{bmatrix} a & b & b & b & b & b & b & b \\ c & d & e & e & e & f & f & f \\ c & e & d & e & e & f & f & f \\ c & e & e & d & g & f & f & f \\ c & e & e & e & d & t & t & t \\ \frac{q}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{u}{8} & \frac{t}{8} & \frac{t}{8} \\ \frac{q}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{u}{8} & \frac{t}{8} & \frac{t}{8} \\ \frac{q}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{u}{8} & \frac{t}{8} & \frac{t}{8} \\ \frac{q}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{u}{8} & \frac{t}{8} & \frac{t}{8} \end{bmatrix} \quad (25)$$

where

$$\begin{aligned}
 a &= -\frac{340p-300}{11}, \quad b = \frac{-85r-300p+255g}{11}, \\
 c &= \frac{100p-85}{11} \\
 d &= \frac{133r-340p+267g}{44}, \quad e = \frac{89r-340p+311g}{44}, \\
 f &= \frac{100t-85q}{11}
 \end{aligned}$$

From (8) I – optimal value is equal to:

$$\begin{aligned}
 \text{tr} \left[\left(C_K(M(\xi)) \right)^{-1} L_4 \right] &= -\frac{340p-300}{11} + 4 \times \\
 &\frac{133r-340p+267g}{44} + 3 \times \frac{u}{8} \\
 &= \frac{300-680p+133r+267g}{11} + \frac{3u}{8} \quad (26)
 \end{aligned}$$

where p, r, g and u are as defined in (23).

Thus using (23) and (26)

$$\begin{aligned}
 \text{tr} \left[\left(C_K(M(\xi)) \right)^{-1} L_4 \right] &= \frac{300}{11} - \frac{680}{11} \sqrt[4]{4} \int x_1^2 dx + \frac{133}{11} \sqrt[4]{4} \int x_1^4 dx + \frac{267}{11} \sqrt[4]{4} \\
 &\int x_1^2 x_2^2 dx + \frac{3}{8} \sqrt[4]{4} \int (x_i x_j + x_k x_l)^2 dx \quad (27) \\
 &\text{for } i \neq j \neq k \neq l
 \end{aligned}$$

Using (11)

$$\begin{aligned}
 \sqrt{m} \int x_1^2 dx &= \sqrt[4]{4} \frac{\prod_{i=1}^4 p_i!}{(4-1 + \sum_{i=1}^4 p_i)!} 3! \\
 &\times \frac{1}{(4-1+2)!} = \frac{1}{10}
 \end{aligned}$$

Similarly

$$\sqrt{m} \int x_1 x_2 dx = \frac{1}{20}$$

$$\sqrt{m} \int x_1^4 dx = \frac{1}{35}$$

$$\sqrt{m} \int x_1^2 x_2^2 dx = \frac{1}{210}$$

$$\sqrt{m} \int x_1^3 x_2 dx = \frac{1}{140}$$

$$\sqrt{m} \int x_1^2 x_2 x_3 dx = \frac{1}{420}$$

$$\sqrt{m} \int x_1 x_2 x_3 x_4 dx = \frac{1}{840} \quad (28)$$

Thus

$$L_4 = \begin{bmatrix} 1 & \frac{1}{10} & \frac{1}{210} & \frac{1}{35} & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} \\ \frac{1}{10} & \frac{1}{35} & \frac{1}{210} & \frac{1}{210} & \frac{1}{210} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{210} & \frac{1}{35} & \frac{1}{210} & \frac{1}{210} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{210} & \frac{1}{210} & \frac{1}{35} & \frac{1}{210} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{210} & \frac{1}{210} & \frac{1}{210} & \frac{1}{35} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{84}{105} & \frac{105}{105} & \frac{105}{105} \\ \frac{1}{10} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{84}{105} & \frac{105}{105} \\ \frac{1}{10} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{84}{105} \end{bmatrix} \quad (29)$$

And

$$I - \text{optimality} = \frac{300}{11} - \frac{680}{11} \times \frac{1}{10} + \frac{133}{11} \times \frac{1}{35} + \frac{267}{11} \times \frac{1}{210} + \frac{3}{8} \times \frac{1}{84} = 21.556 \quad (30)$$

5.0. I- optimal Rotatable Weighted Central Composite Designs (IWCCDs)

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

$$\xi_{IWCCD}(w) = \sum_{i=1}^2 w_i \xi_i \text{ with } w = (w_1, w_2)' \in T_2 \quad (31)$$

is called a weighted central composite design with weight vector $\sum_{i=1}^2 w_i = 1$.

Then using linearity mapping property of the information matrix $C_k(M(\xi)) = LM(\xi)L'$, for every $w \in T_2$

$$C_K(M(\xi(w))) = \sum_{i=1}^2 w_i C_K(M(\xi_i)) \quad i = 1, 2 \quad (32)$$

In this paper the rotatable WCCD ($\alpha^4 = 2^{m-p}$) is expressed as:

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

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 or IV) and ξ_s is the design with $2m$ distinct support points (the star portion) and thus the total support points is $n = n_F + 2m$.

[3] used the General Equivalence Theorem for I-optimality to investigate V-optimal mixture designs for the q th degree model using the simplex centroid design. In this section, this theorem is adapted to investigate the Central Composite Design where the cube portion is constructed through resolution R.

Assuming that all runs of the experiment based on the simplex-centroid design with weights w_1, w_2, \dots, w_q are independent and that the responses have equal variance (which is assumed to be one, without loss of generality), the best linear unbiased estimator of β is the ordinary least squares estimator. The corresponding information matrix is:

$$C = X^T \Lambda X \quad (33)$$

with $X = [f(x_1), f(x_2), \dots, f(x_q)]'$ the $q \times s$ model matrix (in this case comprising of regression vectors in the parameter subsystem of interest)

corresponding to the s points of the second kronecker model central composite design and Λ is a diagonal matrix such that

$$\Lambda = \begin{bmatrix} \frac{w_1}{F} I_F & 0 \\ 0 & \frac{w_2}{2m} I_{2m} \end{bmatrix} \quad (34)$$

where I_F is an $F \times F$ identity matrix, F is the number of experimental runs in the fractional factorial portion, I_{2m} is a $2m \times 2m$ identity matrix, $2m$ is the number of runs in the star portion and m is the number of factors and $w_i, i = 1, 2$ are the weights assigned to each design portion.

[1] explains that a continuous design with information matrix M is I- optimal if and only if $f'(x)C^{-1}LC^{-1}f(x) \leq tr(C^{-1}L)$ (35)

for each point x in the experimental region χ . The general equivalence theorem states that for a design to be I- optimal, the inequality (35) when evaluated at each of the design points becomes

$$f'(x)C^{-1}LC^{-1}f(x) = tr(C^{-1}L) \quad (36)$$

The relation (36) is used to determine the values of the weights for optimal rotatable design ξ_{WCCD} .

5.1. Three Factors I - Optimal Rotatable WCCD

I- optimal WCCD for three factors based on the parameter subsystem of interest is derived in this section. The corresponding optimal value is also computed for the purpose of comparison.

From [4], the parameter subsystem of interest dealt with in this paper for $m = 3$ is the vector $K'(\theta) =$

$$\begin{bmatrix} \theta_0 \\ \theta_{11} \\ \theta_{22} \\ \theta_{33} \\ \frac{\theta_{12} + \theta_{21}}{2} \\ \frac{\theta_{13} + \theta_{31}}{2} \\ \frac{\theta_{23} + \theta_{32}}{2} \end{bmatrix}$$

The corresponding regression vector of factors in the parameter subsystem of interest is

$$f(x) = [1 \quad x_1^2 \quad x_2^2 \quad x_3^2 \quad x_1x_2 \quad x_1x_3 \quad x_2x_3]' \quad (37)$$

This gives rise to the matrix X with the following entries;

$$X = [1 \quad f(x_1) \quad f(x_2) \quad f(x_3) \quad f(x_4) \quad f(x_5) \quad f(x_6)]' \quad (38)$$

Thus

$$X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 0 & 0 & 0 \end{bmatrix} \quad (39)$$

The design ξ_{IWCCD} (31) is such that

$$\xi_{IWCCD} = w_1 \xi_F + w_2 \xi_S, \quad w_1 + w_2 = 1 \quad \text{and} \quad w_1, w_2 \geq 0 \quad (40)$$

Then each of the design points in the cube portion is assigned a mass of $\frac{1}{4}w_1$ while each of the design points in the star portion is assigned a mass of $\frac{1}{6}w_2$.

Then (34) becomes

$$\Lambda = \begin{bmatrix} \frac{w_1}{4} I_4 & \mathbf{0} \\ \mathbf{0} & \frac{w_2}{6} I_6 \end{bmatrix} \quad (41)$$

Letting $w_2 = 1 - w_1$ then

$$C = X^T \Lambda X = \begin{bmatrix} 1 & \frac{w_1+2}{3} & \frac{w_1+2}{3} & \frac{w_1+2}{3} & 0 & 0 & 0 \\ \frac{w_1+2}{3} & -\frac{w_1-4}{3} & w_1 & w_1 & 0 & 0 & 0 \\ \frac{w_1+2}{3} & w_1 & -\frac{w_1-4}{3} & w_1 & 0 & 0 & 0 \\ \frac{w_1+2}{3} & w_1 & w_1 & -\frac{w_1-4}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & w_1 \end{bmatrix} \quad (42)$$

And

$$C^{-1} = \begin{bmatrix} \frac{5w_1+4}{w_1^2-w_1} & \frac{w_1+2}{w_1-w_1} & \frac{w_1+2}{w_1-w_1} & \frac{w_1+2}{w_1-w_1} & 0 & 0 & 0 \\ \frac{w_1+2}{w_1^2-w_1} & -\frac{w_1+2}{2w_1^2-2w_1} & \frac{w_1+2}{4w_1^2-4w_1} & \frac{w_1+2}{4w_1^2-4w_1} & 0 & 0 & 0 \\ \frac{w_1+2}{w_1^2-w_1} & \frac{w_1-4}{4w_1^2-4w_1} & -\frac{w_1+2}{2w_1^2-2w_1} & \frac{w_1-4}{4w_1^2-4w_1} & 0 & 0 & 0 \\ \frac{w_1+2}{w_1^2-w_1} & \frac{w_1-4}{4w_1^2-4w_1} & \frac{w_1-4}{4w_1^2-4w_1} & -\frac{w_1+2}{2w_1^2-2w_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{w_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{w_1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{w_1} \end{bmatrix} \quad (43)$$

From (39), point x_1 in the cube portion is used such that

$$f(x_1) = [1 \ 1 \ 1 \ 1 \ 1 \ -1 \ -1]'$$

Then the relation (36) results in

$$\frac{211}{90w_1^2} = -\frac{81w_1 + 46}{20w_1^2 - 20w_1}$$

Giving $w_1 = 0.379318$ or -1.526094

But $w_1 > 0$, therefore:

$$w_1 = 0.38 \quad \text{and hence} \quad w_2 = 1 - 0.38 = 0.62 \quad (44)$$

Similarly, from (39), if point x_9 in the star portion design is used such that

$$f(x_9) = [1 \ 0 \ 0 \ 2 \ 0 \ 0 \ 0]'$$

the same results are obtained.

Therefore substituting the values of w_1 and w_2 in

$$\xi_{WCCD} = w_1 \xi_F + w_2 \xi_S,$$

the I -optimal Rotatable Weighted Central

Composite Design (ξ_{IWCCD}) for three factors can be expressed as:

$$\xi_{IWCCD} = 0.38\xi_F + 0.62\xi_S \quad (45)$$

Now on substituting the values of the weights (44),

the information matrix (42) for a design that is I -optimal becomes:

$$C = \begin{bmatrix} 1 & 0.79 & 0.79 & 0.79 & 0 & 0 & 0 \\ 0.79 & 1.21 & 0.38 & 0.38 & 0 & 0 & 0 \\ 0.79 & 0.38 & 1.21 & 0.38 & 0 & 0 & 0 \\ 0.79 & 0.38 & 0.38 & 1.21 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.38 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.38 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.38 \end{bmatrix} \quad (46)$$

Then from (6) the corresponding I -optimal value is

$$tr(C^{-1}L) = 16.2942 \quad (47)$$

5.2. Four Factors I - Optimal WCCD

I -optimal WCCD for three factors based on the parameter subsystem of interest is derived in this section. The corresponding optimal value is also computed for the purpose of comparison. From [4], the parameter subsystem of interest dealt with in this study for $m = 4$ is the vector

$$K'(\theta) = \begin{bmatrix} \theta_0 \\ \theta_{11} \\ \theta_{22} \\ \theta_{33} \\ \theta_{44} \\ \frac{\theta_{12} + \theta_{21} + \theta_{34} + \theta_{43}}{4} \\ \frac{\theta_{13} + \theta_{31} + \theta_{24} + \theta_{42}}{4} \\ \frac{\theta_{14} + \theta_{41} + \theta_{23} + \theta_{32}}{4} \end{bmatrix}$$

The corresponding regression vector of factors in the parameter subsystem of interest is:

$$f(x) = [1 \ x_1^2 \ x_2^2 \ x_3^2 \ x_4^2 \ x_1x_2 + x_3x_4 \ x_1x_3 + x_2x_4 \ x_1x_4 + x_2x_3]'$$

(48)

This gives rise to the matrix X with the following entries;

$$X = [1 \ f(x_1) \ f(x_2) \ f(x_3) \ f(x_4) \ f(x_5) \ f(x_6) \ f(x_7)]'$$

(49)

Thus

$$X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 & 1 & -2 & -2 & 2 \\ 1 & 1 & 1 & 1 & 1 & -2 & 2 & -2 \\ 1 & 1 & 1 & 1 & 1 & 2 & -2 & -2 \\ 1 & 1 & 1 & 1 & 1 & 2 & -2 & -2 \\ 1 & 1 & 1 & 1 & 1 & -2 & 2 & -2 \\ 1 & 1 & 1 & 1 & 1 & -2 & -2 & 2 \\ 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 2.83 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2.83 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2.83 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2.83 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2.83 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2.83 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2.83 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2.83 & 0 & 0 & 0 \end{bmatrix}$$

(50)

Let the design ξ_{IWCCD} (31) be such that $\xi_{IWCCD} = w_1\xi_F + w_2\xi_S$, $w_1 + w_2 = 1$ and $w_1, w_2 \geq 0$

(51)

Then each of the design points in the cube portion is assigned a mass of $\frac{1}{8}w_1$ while each of the design points in the star portion is assigned a mass of $\frac{1}{8}w_2$.

Then from (34)

$$\Lambda = \begin{bmatrix} \frac{w_1}{8}I_8 & \mathbf{0} \\ \mathbf{0} & \frac{w_2}{8}I_8 \end{bmatrix}$$

(52)

Letting $w_2 = 1 - w_1$ then

$$C = X^T\Lambda X =$$

$$\begin{bmatrix} 1 & \frac{117w_1+283}{400} & \frac{117w_1+283}{400} & \frac{117w_1+283}{400} & \frac{117w_1+283}{400} & 0 & 0 & 0 \\ \frac{117w_1+283}{400} & \frac{8089-4054w_1}{4045} & W_1 & W_1 & W_1 & 0 & 0 & 0 \\ \frac{117w_1+283}{400} & W_1 & \frac{8089-4054w_1}{4045} & W_1 & W_1 & 0 & 0 & 0 \\ \frac{117w_1+283}{400} & W_1 & W_1 & \frac{8089-4054w_1}{4045} & W_1 & 0 & 0 & 0 \\ \frac{117w_1+283}{400} & W_1 & W_1 & W_1 & \frac{8089-4054w_1}{4045} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4w_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4w_1 \end{bmatrix}$$

(53)

From (50), point x_1 in the cube portion is used such that

$$f(x_1) = [1 \ 1 \ 1 \ 1 \ 1 \ 2 \ 2 \ 2]'$$

(54)

Thus the relation (36) results in

$$\frac{255297073200251213w^2 + 3606468774w + 13}{68679720204928560w^4 - 12403329120w^3 + 560w^2 + 52041413029541w^2 + 43505732610558w - 8099} = -\frac{10045456254288w^3 - 10045457161376w^2 + 907088w}{10045456254288w^3 - 10045457161376w^2 + 907088w}$$

And this gives

$$w_1 = -1.926 \text{ or } 0.3725$$

(55)

But $w_1 > 0$, therefore:

$$w_1 = 0.3725 \implies w_2 = 1 - 0.3725 = 0.6275$$

(56)

On evaluating at other points in the factorial portion of the design, the following weights are obtained:

$$f(x_1) \text{ and } f(x_7) \implies w_1 = 0.3725$$

$$f(x_2), f(x_3), f(x_4), f(x_5) \text{ and } f(x_6) \implies w_1 = 0.4122$$

Similarly on working out the relation (36) using a point in the star portion design say

$$f(x_{13}) = [1 \ 0 \ 2.83 \ 0 \ 0 \ 0 \ 0 \ 0]'$$

$$w_2 = 0.5976 \implies w_1 = 1 - 0.5976 = 0.4024$$

(57)

But a uniform weight is assigned to each design point in the factorial portion for optimality. We therefore take an average of the different weights and this gives:

$$w_1 = 0.4024$$

Therefore substituting the values of w_1 and w_2 in $\xi_{IWCCD} = w_1\xi_F + w_2\xi_S$, the I -optimal Rotatable Weighted Central Composite Design (ξ_{IWCCD}) for four factors can be expressed as:

$$\xi_{IWCCD} = 0.4024 \xi_F + 0.5976 \xi_S$$

(58)

Now on substituting the values of the weights in (57), the information matrix for a design that is I -optimal becomes:

$$C = X^T\Lambda X = \begin{bmatrix} 1 & 0.825 & 0.825 & 0.825 & 0.825 & 0 & 0 & 0 \\ 0.825 & 1.596 & 0.402 & 0.402 & 0.402 & 0 & 0 & 0 \\ 0.825 & 0.402 & 1.596 & 0.402 & 0.402 & 0 & 0 & 0 \\ 0.825 & 0.402 & 0.402 & 1.596 & 0.402 & 0 & 0 & 0 \\ 0.825 & 0.402 & 0.402 & w_1 & 1.596 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.609 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.609 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.609 \end{bmatrix}$$

(59)

Consequently, the optimal value for the $I - optimal$ weighted rotatable central composite design is:

$$tr(C^{-1}L_4) = 26.78 \quad (60)$$

6.0. Results and conclusion

Optimal rotatable WCCD for three and four factors were derived and optimality was accomplished through application of I-optimality criteria which follows from the General Equivalence Theorem [2]. I-optimal rotatable WCCD were found to exist for both resolution III and IV designs. Optimal values were computed and a general form of I- optimal value was derived. Efficiency of the constructed designs was computed relative to the corresponding Uniformly Weighted Central Composite Designs as shown in Table 1.

Table 1: I-optimal Rotatable Designs

m-Factors	Resolution	Uniformly weighted CCD	WC CD	Efficiency	Weights	
					w_1	w_2
3	III	16.27	16.29	1.001	$w_1 = 0.38$	$w_2 = 0.62$
4	IV	21.56	26.78	1.24	$w_1 = 0.37$	$w_2 = 0.63$

I-optimal WCCD for both resolution III and IV designs exists and the relative efficiency is near one. These results show that none of the designs namely: Resolution III Uniformly Weighted CCD and WCCD and Resolution IV Uniformly Weighted CCD and WCCD, could be said to be uniformly superior to the other with respect to the I-optimality criterion efficiency. Further a greater weight is assigned to the star portion than the cube portion in both designs indicating that the star portion plays a greater role under the I-optimality criterion.

Recommendations

It is recommended that further research can be done on the practicability of the optimal rotatable Weighted Central Composite Designs investigated in this study. Further, this paper was restricted to CCD with no center points. It would be interesting to observe what happens if a similar study is carried out with center points added to both the cube and the star portions.

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Appendices

1.

Table 2: 2_{III}^{3-1} Design

Run	Factors		
	x_1	x_2	$x_3 = x_1x_2$
1	-1	-1	+1
2	+1	-1	-1
3	-1	+1	-1
4	+1	+1	+1

2.

Table 3: 2_{IV}^{4-1} Design

Run	Factors			
	x_1	x_2	x_3	$x_4 = x_1x_2x_3$
1	-1	-1	-1	-1
2	+1	-1	-1	+1
3	-1	+1	-1	+1
4	+1	+1	-1	-1
5	-1	-1	+1	+1
6	+1	-1	+1	-1
7	-1	+1	+1	-1
8	+1	+1	+1	+1

3.

Three Factors Central Composite Design $X =$

1	-1	-1	1	1	1	-1	1	1	-1	-1	-1	1
1	1	-1	-1	1	-1	-1	-1	1	1	-1	1	1
1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1
1	1	1	1	1	1	1	1	1	1	1	1	1
1	-1.4142	0	0	2	0	0	0	0	0	0	0	0
1	1.4142	0	0	2	0	0	0	0	0	0	0	0
1	0	-1.4142	0	0	0	0	0	2	0	0	0	0
1	0	1.4142	0	0	0	0	0	2	0	0	0	0
1	0	0	-1.4142	0	0	0	0	0	0	0	0	2
1	0	0	1.4142	0	0	0	0	0	0	0	0	2

4.

$C_K(M(\xi))$

$$= \begin{bmatrix} 1 & a^2 & b^2 & c^2 & d^2 & cd + ab & bd + ac & ad + bc \\ a^2 & a^4 & a^2b^2 & a^2c^2 & a^2d^2 & a^2(cd + ab) & a^2(bd + ac) & a^2(ad + bc) \\ b^2 & a^2b^2 & b^4 & b^2c^2 & b^2d^2 & b^2(cd + ab) & b^2(bd + ac) & b^2(ad + bc) \\ c^2 & a^2c^2 & b^2c^2 & c^4 & c^2d^2 & c^2(cd + ab) & c^2(bd + ac) & c^2(ad + bc) \\ d^2 & a^2d^2 & b^2d^2 & c^2d^2 & d^4 & d^2(cd + ab) & d^2(bd + ac) & d^2(ad + bc) \\ cd + ab & a^2(cd + ab) & b^2(cd + ab) & c^2(cd + ab) & d^2(cd + ab) & (cd + ab)^2 & y & y \\ bd + ac & a^2(bd + ac) & b^2(bd + ac) & c^2(bd + ac) & d^2(bd + ac) & y & (bd + ac)^2 & 0 \\ ad + bc & a^2(ad + bc) & b^2(ad + bc) & c^2(ad + bc) & d^2(ad + bc) & y & y & (ad + bc)^2 \end{bmatrix}$$

where $y = (bd + ac)(cd + ab)$