Optimum rotatable designs for fitting second order response surface kronecker model

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Abstract

Response surface methodology is widely used for developing, improving, and optimizing processes in various fields. In this article, we present a method for constructing second order rotatable designs in order to explore and optimize response surfaces based on a set of fraction of factorial designs. The designs achieve both properties of rotatability and estimation efficiency.
We shall concentrate on the moment matrices and the related information surfaces based on the parameter subsystem of interest on the Kronecker model and their corresponding rotatable designs. The set of rotatable designs based on the central composite designs shall be presented. These designs shall be shown to be A-, D-, E- and T-optimal.

Keywords: *A- optimal, D- optimal, E- optimal, T- optimal, Response surface designs, Second-order designs, Information*

surface, Parameter system of interest, Kronecker model, Moment matrices, Rotatable designs, Central Composite Designs.

Introduction

Response surface designs is an experimental field in which treatments are various combinations of different levels of the factors that are quantitative. Here the main objective of the experimenter is usually to estimate the absolute response or the parameters of a model providing the relationship between the response and the factors. In many experimental situations this relationship is a

functional one. For example Y may be represented as a suitable function f of the levels $t_{1u}, t_{2u}, \ldots, t_{ku}$ of the k factors and, θ the set of parameters. A typical model may be of the form:

$$y_u = f(t_{1u}, t_{2u}, \ldots, t_{Vu}; \theta + e_u)' \qquad (1.1)$$

where $u = 1, 2, \ldots, N$ represents the N observations with t_{iu} representing the level of the ith factor ($i = 1, 2, \ldots, V$) in the uth observation. The residual e_u measures the experimental error of the uth observation. This particular function which describes the relationship in question is called the response surface. In practice this function is unknown as well as the set of the parameters and since the investigator attempts to approximate the response surface (the true functional relationship between response and factor levels), by using a derived polynomial equation, the object of the study now becomes the estimated response surface whose statistical properties are determined by the moment matrix

$$M(\xi) = \int f(t) f(t)^T d\xi \qquad (1.2)$$

for the Kronecker model which has all entries homogeneous.

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

$$i_m(t) = \frac{1}{f(t)^T M^{-1} f(t)} \quad for\ f(t) \in range\ M \quad and\ \ i_m(t) = 0\ otherwise. \qquad (1.3)$$

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

$$i_m(t) = C_{f(t)}(M(\xi)) \quad \text{(Pukelsheim, 2006)} \qquad (1.4)$$

In this study we concentrate on the matrices (1.2) and (1.4) based on the parameter subsystem of interest on the Kronecker model and their corresponding rotatable designs.

Response Surface Methodology

Response surface methodology (RSM) is a collection of mathematical and statistical techniques that are 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, 2001). RSM focuses on approximating the functional relationship between a given response and the factors involved as well as permitting a variety of experimental designs which allows one to achieve that estimate as efficiently and as economical as possible. (Clark and Williges, 1972).

Second-order designs are used in response surface methodology as acceptable approximation of true responses (Myers, 1971).Cornel (1990) lists numerous examples of applications of mixture experiments and provides a thorough discussion of both theory and practice. Early work done by Scheffe' (1958, 1963) suggested and analyzed canonical model forms when the regression function for the expected response is a polynomial of degree one, two or three.

In this study our focus is on the second degree Kronecker model suggested by Draper and Pukelsheim (1998) and as cited by Koech et.al. (2014):

Definition 1: In an $m - way$ second degree model $m \geq 2$, we take the regression function to be $f(t) = \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix} : \mathrm{T}_{\sqrt{m}} \rightarrow \mathbb{R}^k$

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.

Thus the second-degree Kronecker model is

$$E(Y_t) = f(t)'\theta = \theta_0 + \sum_{i=1}^{m} \theta_{ii}\, t_i^2 + \sum_{j=1}^{m} (\theta_{ij} + \theta_{ji})\, t_i t_j \qquad (1.6)$$

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

$\Theta = (\theta_0, \theta_1, \dots, \theta_{11}, \theta_{22}, \dots, \theta_{mm})^T \in \mathbb{R}^{m^2}$ is an unknown parameter. (1.7)

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

Rotatable Second-Degree Moment Matrices

In this study we make use of the following theorem as stated by Pukelsheim (2006) to check whether the constructed designs are second-order rotatable

Theorem1. Let M be a symmetric $(1+m+m^2)(1+m+m^2)$ matrix. Then M is a rotatable second-degree moment matrix on the experimental domain $T_{\sqrt{m}}$ if and only if for some

$$\mu_2 \in [0,1] \ \ and \ \ \mu_{22} \in \left[\frac{m}{m+2}\mu_2^2; \frac{m}{m+2}\mu_2\right],$$

We have

$$M = \begin{pmatrix} 1 & 0 & \mu_2 (vec\, I_m)^T \\ 0 & \mu_2 I_m & 0 \\ \mu_2 vec\, I_m & 0 & \mu_{22} F_m \end{pmatrix} \qquad (1.8)$$

Where $F_m = I_m \otimes I_m + I_{m,m} + \ (vec\, I_m)(vec\, I_m)^T$

The moment matrix in (1.7) is attained by a design $\tau \in T$ if and only if τ has all moments of

(i) $T\int_m ()etdforallim_i{}^{'2} \tau\mu = \leq_2$

(ii) $\int ()()ettedforallijm^{''22} \tau\mu = \neq \leq$

$T_{\sqrt{m}}\ ij\ 22$

(iii) ' 4 ()3etdforallimτμ=≤ , while all other
J i 22
T m √

moments up to order 4 vanish. (1.9)

The Design Problem

In this study, we present a method for constructing second order rotatable designs in order to explore and optimize response surfaces based on fractional factorial designs.

Optimality Criteria

The ultimate purpose of any optimality criterion is to measure the largeness of a non-negative definite $s \times s$ matrix C where C is the subset of M. In this study, for each of the constructed second order rotatble design, the matrix C will be the information matrix based on the parameter subsystem of interest on the Kronecker model. Hence the optimality criteria includes the popular D-, A-, E-, and T-criteria, corresponding to the parameter values 0, -1, -∞, and 1, respectively as defined below.

$\emptyset_0(C) = (\det C)^{-1}$, $\emptyset_{-1}(C) = \left(\frac{1}{s} trace\ C^{-1}\right)^{-1}$, $\emptyset_{-\infty}(C) = \lambda_{min}(C)$ and
$\emptyset_1(C) = \frac{1}{s} trace\ C$ (2.0)

for all C in PD $m+1$ / 2, the set of positive

definite $m+1$ × $m+1$ matrices.

2 2

Efficiency

The performance of designs comparing to the D-optimal design for model (1.6) are measured by the D-efficiency which is defined by:

$$D_{eff}(\xi^*) = \frac{v(\phi_0(\xi^*))}{v(\phi_0(\xi))} \qquad (2.1)$$

The Fractional factorial designs sets

The sets will be obtained from two-level fractional factorial designs.

Definition 3: The design that assigns uniform weight $\frac{1}{\ell}$ to each of the $\ell = 2^m$ vertices of $[-1;1]^m$ is called the complete factorial design and has a model matrix $X \in \mathbb{R}^{\ell\times(1+m)}$ satisfying $X^T X = \ell I_m$

Pukelheim (2006, pg 190) stated that there exists a $\phi - optimal\ design\ \xi$ for $K^T(\theta)$ in Ξ such that its support size is bounded according to $s \leq \#\ supp\ \xi \leq \frac{1}{2}s(s+1) + s(rank\ M - s)$.

For full parameter vector θ we have $m = k$. and the bound becomes $\frac{1}{2}k(k+1)$.

The support size 2^m of the complete factorial design quickly goes beyond the quadratic bound $\frac{1}{2}k(k+1) = \frac{1}{2}(m+1)(m+2)$ as $m\ becomes\ bigger$ (Pukelsheim 2006, pg 391).

$2^{m-p}\ fraction\ factorial\ design$ comprises of a 2^{-p} fraction of the complete factorial design 2^m in such a way that the associated model matrix X has orthogonal columns. This design has a support size that does not outgrow the quadratic bound thus giving rise to an optimal design for $K^T(\theta)$.

Construction of the designs

We now illustrate the construction of the designs by considering an experiment with $m = 3\ factors$, with a 2^{3-1} design generated using the highest confounding interaction. This yields the following fractions:

$$S_1 = \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \quad \text{and} \quad S_2 = \begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \end{pmatrix}. \qquad (2.2)$$

We now construct a set of rotatable designs based on (2.1) and the set of points S(,0,0) usual call star points in the central composite designs (CCD).

Central Composite Designs (CCD)

One of the most popular and commonly used classes of experimental designs for fitting the second order model are the central composite designs introduced by Box and Wilson (1951).

These designs are mixtures of three building blocks: cubes, stars and center points. (Pukelsheim 2006).

Assuming $m \geq 2$ design variables, the CCD consists of:

(i) The cube portion τ_c which is an $f = 2^{m-p}$ full ($p = 0$) or fractional ($p > 0$) factorial design of at least Resolution V with n_c replications. Each point is of the form $(t_1, t_2, \ldots, t_m) = S(\pm 1, \pm 1, \ldots, \pm 1)$.

(ii) The $2m$ axial points (star portion τ_s) with n_s replications that takes one observation at each of the vectors $\pm\alpha e_i$ for $i \le m$ for some star radius $\alpha > 0$.

(iii) The center portion τ_0 with n_0 replications which is the one point design in 0

The CCD has sample size $n = 2^{m-p}n_c + 2mn_s + n_0$. (2.3)

Each of the three types of design points in a CCD plays different roles:

a) The factorial points allow estimation of the first-order and interaction terms.
b) The axial points allow estimation of the squared terms.
c) The center points provide an internal estimate of pure error used to test for lack of fit and also contribute toward estimation of the squared terms.

In the second-degree moment matrices for the CCD, the only non-vanishing moments of the standardized design are:

$\mu_2(\tau) = \frac{n_c}{n}2^{m-p} + \frac{n_s}{n}2\alpha^2$, $\mu_{22}(\tau) = \frac{n_c}{n}2^{m-p}$ and
$\mu_4(\tau) = \frac{n_c}{n}2^{m-p} + \frac{n_s}{n}2\alpha^4$ (2.4)

To maintain rotatability, the value of α depends on the number of experimental runs in the factorial portion of the central composite design. Rotatability condition entails

$\mu_4(\tau) = 3\mu_{22}(\tau)$. (2.5)

Hence from (2.3)

$\alpha^4 = \frac{n_c}{n_s}2^{m-p}$ (2.6)

In this study we construct the set of rotatable central composite designs with the factorial portion comprising of design points generated from some supplementary difference sets of the form (2.1). The moment matrices and the related information surfaces based on the parameter subsystem of interest on the Kronecker model and their corresponding rotatable designs are obtained. The variations of the rotatable central composite designs are considered for three factors and D-, A-, E- and T- optimal values are obtained. The efficiency of the constructed designs is compared.

The following procedure is followed to obtain a rotatable central composite design for this study:

a) The cube portion (model matrix X of the difference set) is replicated 3 times i.e. $n_c = 3$.
b) The star portion is replicated once i.e. $n_s = 1$.
c) The replications of center point will be varied to obtain several variations of the central composite design with $n_0 = 0, 1, and\ 2$.
d) For rotatability, the value of α is obtained using the condition (2.4).

The set S_1 is used to illustrate the method of construction of optimal designs.

Design points for S_1

t_0	t_1	t_2	t_3
1	1	-1	-1
1	-1	1	-1
1	1	1	1
1	-1	-1	1

With reference to the $m-way$ second-degree Kronecker model (1.6), a three-factor second-degree Kronecker model is of the form:

$$\eta(\theta,t) = \theta_0 + \theta_1 t_1 + \theta_2 t_2 + \theta_3 t_3 + \theta_{11} t_1^2 + \theta_{12} t_1 t_2 + \theta_{13} t_1 t_3 + \theta_{21} t_2 t_1 + \theta_{22} t_2^2 + \theta_{23} t_2 t_3 + \theta_{31} t_3 t_1 + \theta_{32} t_3 t_2 + \theta_{33} t_3^2 \quad (2.7)$$

where $\eta(\theta,t)$ the response under experimental condition **t** is taken to be a real-valued random variable and θ=($\theta_0, \theta_1, \theta_2, \theta_3, \theta_{11}, \theta_{12}, \theta_{13}, \theta_{21}, \theta_{22}, \theta_{23}, \theta_{31}, \theta_{32}, \theta_{33})^T \varepsilon R^{m^2}$ an unknown parameter. All observations taken in an experiment are assumed to be uncorrelated and to have common unknown variance σ^2 $\varepsilon(0,\infty)$.

We use the central composite design to fit this model using conditions given in section 2.1 (i), (ii) and (iii) with $m = 3,\ p = 1, n_c = 3$, n_S =1 , $n_0 = 2;$ giving $n = 20$ experimental points and $\alpha = 1.861$.Thus for this set of conditions the design matrix X is given as t t t t t 1t t t1t3 2 1 t t 1 2

t 2 3 3 1 3 2 t t t t t t t

$$
\begin{bmatrix}
1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 \\
1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 \\
1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 \\
1 & -1.861 & 0 & 0 & 3.464 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1.861 & 0 & 0 & 3.464 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -1.861 & 0 & 0 & 0 & 0 & 0 & 3.464 & 0 & 0 & 0 & 0 \\
1 & 0 & 1.861 & 0 & 0 & 0 & 0 & 0 & 3.464 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & -1.861 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.464 \\
1 & 0 & 0 & 1.861 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.464 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

$(t_0 = 1)$ (2.8)

The corresponding moment matrix given in (1.8) is then obtained for m=3.

Parameter subsystem of interest for three factors

We consider the Euclidean unit vectors in $\mathbb{R}^m$ denoted by $e_1, e_2, \dots, e_m$ and the sets

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

Let K be a $k \times s$ coefficient matrix such that:

$K = (1, K_1, K_2,) \in \mathbb{R}^{m^2 \times s}$ for $m = 3$

(2.9)

where

$$K_1 = \sum_{I=1}^{3} e_{ii} e_i^T$$

and

$$K_2 = \frac{3}{\binom{4}{2}} \{(e_{ij} + e_{ji})e_i^T + (e_{ik} + e_{ki})e_j^T + (e_{jk} + e_{kj})e_k^T\}$$

The parameter subsystem considered in the following can be written as

$$K^T(\theta) = \left\{ \begin{array}{c} \theta_0 \\ \theta_{ii} \quad for\ 1 \le i \le 3 \\ \frac{3}{\binom{4}{2}} \begin{Bmatrix} (\theta_{ij} + \theta_{ji}) \\ (\theta_{ik} + \theta_{ki}) \\ \theta_{jk} + \theta_{kj} \end{Bmatrix} \quad for\ i < j < k \end{array} \right\} \varepsilon\ R^{\binom{m+1}{2}}\ for\ all\ \theta\ \varepsilon\ R^{m^2}$$

(m=3) $for\ i, j, k = \{1, 2, 3\}$

As is evident from equation (2.7), the Kronecker full parameter vector $\theta\ \varepsilon\ R^{m^2}$ is not estimable. The parameter system $K^T\theta$ is a maximal parameter system in model (2.7).

The amount of information which the design *T* contains on the parameter system is captured by the information matrix (1.4) is obtained as follows:

$$C_k(M(\xi)) = LM(\xi)L' \in NND(s)\ for\ K'\theta \qquad (2.10)$$

where *L* is the left inverse of coefficient matrix *K* and is defined by

$L^T = (K^T K)^{-1} K^T,$ and the information matrices for $K'\theta$ are linear transformation of moment matrices.

Now the problem considered in this study is a specific case as follows. For m=3 we have

$$L^T = (K^T K)^{-1} K^T = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}.$$

and from (1.4), (2.8), (2.9) and (2.10) the information matrix C is obtained . This is the moment matrix corresponding to the parameter system of interest. Hence the optimal values and their corresponding efficiencies are obtained by using (2.0) and (2.1) respectively. These are given in table 1 below.

Full factorial design ξ

We now construct a second order rotatable central composite design where the cube portion is a full factorial design 2^3 replicated $3\ times$.

we have $$S = \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

under the following conditions:

$n_c = 3$, $m = 3\ and\ p = 0$, and in which from (2.4) $\alpha = 2.213364 \approx 2.213$

Tbe CCD with these conditions is compared with the CCD $S_1$and the efficient values are given in Table 1.

Rotatability:

Using $S_j\ for\ j = 1,\ 2$ we obtain the rotatable designs $\xi_{n_{0i}}$ for 3 factors. For each $M(\xi_{n_{0i}}),\ (i = 0, 1, 2)$, rotatability conditions (1.8) are satisfied. Therefore the constructed designs are second order rotatable

Optimality and efficiency

We now present the set of rotatable designs based on the central composite designs and the corresponding D-, A-, T- and E- optimal values.

Table 1.

	Design	Number of center points	Determinant criterion $\varnothing_0(C_k$	Smallest Eigen value criterion $\varnothing_{-\infty}(C$ *(smallest positive Eigen value)*	Average-variance criterion $\varnothing_{-1}(C$	Trace criterion $\varnothing_1(C_k$	Determinant efficiency $D_{eff}(\xi_{n}$
S	ξ_{n0} ξ_{n0} ξ_{n0}	2 1 0	1.2986 1.2453 0.9152	0.0798 0.0439 0.0037	0.4459 0.2713 0.0255	1.9429 2.0376 2.1429	0.8224 0.8020 0.6139
S	ξ	2 1 0	1.5791 1.5527 1.4908	0.0866 0.0636 0.0394	0.4964 0.3848 0.2520	2.3924 2.4653 2.5424	

a) It can be observed that the optimal values $V(\varnothing_p(C_k(M)))\ for\ p = -\infty, -1, 0, 1$ for the designs $\xi_{n_{0i}}\ (i = 0, 1, 2)$ are less than the corresponding optimal values for the design ξ but irrespective of the design, the optimal values increase with increasing replicates of the center points except for the trace criterion whose value decreases as the replicates for center points increase.

b) For efficiency, this is obtained using the formula (2.1)

For example $D_{eff}(\xi_{n_{02}}) = \frac{v(\varnothing_0(\xi_{n_{02}}))}{v(\varnothing_0(\xi))}$

This means that the design ξ_{n02} is 17.76% more efficient. Comparing the three designs, design ξ_{n00} seems to be more efficient (38.61 %). This is a central composite design with no center points. We may therefore conclude that including or not including center points in a second-order rotatable central composite design does not affect the efficiency.

Conclusion

In this study, we have presented a method for constructing second order rotatable designs in order to explore and optimize response surfaces based on some class of supplementary difference sets. The constructed set of rotatable designs based on the central composite designs have achieved both properties of rotatability and estimation efficiency as shown by the results in relation to their moment matrices and the related information surfaces based on the parameter subsystem of interest on the Kronecker model. These designs have also proved to be A-, D-, E- and T-optimal.

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