The difference of the variance functions between two estimated responses for a fourth order rotatable design in two dimensions

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Abstract. In this paper the difference of the variance functions between two estimated responses for a fourth order design at any two points in the factor space is developed. In particular, the variance function is considered in two dimensions when the design used is rotatable. The variance function in this situation is a function of the distances of the points from the origin of the design and the angle subtending the points at the origin. The variance function of this approach is discussed in detail when the two points are equidistant from the origin of the design. The criterion for the choice of an optimal design is given.

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1 Introduction

It is often seen that the difference between estimated responses at two points for a phenomena is a greater interest as compared to the actual response. The variance function and the difference of variances of two estimated responses assist in providing further insight about the criterion under investigation. Herzberg (1967) described the variance function depending on the length of the straight line joining the selected points to the origin and the angle between these two lines. The assumption of rotatability in design helps in determining the appropriate form for the product of the design matrix and its transpose (Box and Draper, 1980).

Huda and Mukerjee (1984) derived optimal design under the criterion for second order polynomial models when the design space is spherical in nature.

Gilmour (2006) provided the summary of use of response surface methodology (RSM) in various biological inductions and discussed in details the applications of RSM to experiments on biotechnological processes. The utility of subset designs is highlighted. In this paper the difference of variance functions between two estimated responses for a fourth order rotatable design has been studied. The extent to which the angle between the lines can be varied is determined.

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2 Fourth order rotatable model

Consider the problem in response surface designs for investigating the relationship between a responce y and two explanatory factors, say x_1 and x_2. Assuming all factors to be continuous in nature and the form of the functional relationship between them as unknown but within the range of interest, such that the function may be represented by a polynomial of moderately low order. In particular, we chose the combinations of levels of independent factors which will:

(i) enable an experimenter to approximate a functional relationship by fitting a polynomial through the terms of order four, and

(ii) have the property of rotatability.

Such a choice of combination of the various levels of the independent factors will provide a fourth order rotatable design.
Let us consider a general model

$$y_i = f'(x_i)\beta + \epsilon_i \tag{2.1}$$

whose matrix equivalent is,

$$Y = X'\beta + \varepsilon \tag{2.2}$$

where, Y is an $(n \times 1)$ vector of observations,
X is an $(n \times k)$ design matrix,
β is a $(k \times 1)$ vector of unknown parameters, and
ε is a $(n \times 1)$ vector of independently identically distributed random variables with mean zero and variance σ^2.
Specifically, for N observations let y_u be the response at the u^{th} run, for a polynomial equation of order four this maybe written as

$$\begin{aligned} y_u &= \beta_0 x_{0u} + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \beta_{ii} x_{iu}^2 + \sum_{i=1}^{k}\sum_{j=1}^{k} \beta_{ij} x_{iu} x_{ju} \\ &+ \sum_{i=1}^{k}\sum_{j=1}^{k}\sum_{l=1}^{k} \beta_{ijl} x_{iu} x_{ju} x_{lu} + \sum_{i=1}^{k}\sum_{j=1}^{k}\sum_{l=1}^{k}\sum_{r=1}^{k} \beta_{ijlr} x_{iu} x_{ju} x_{lu} x_{ru} + \varepsilon_u \end{aligned}$$

where, $\varepsilon_u \sim N(0, \sigma^2)$, $Cov(\varepsilon_u \varepsilon'_u) = 0,\ u \neq u' = 1, 2, \cdots, N$. The expectation of the response at the u^{th} run is given by $E[y_u] = x'_u\beta$. The estimated response is given by $\hat{y} = X'\hat{\beta}$, with matrix $X = (x_1, x_2, \cdots, x_N)'$ of order $N \times L^*$ (see appendix) and $\hat{\beta}$ is the least square estimate of β.

The algebra of estimating β is involving and tedious, therefore we make use of *Schlafflian Vectors* and *Matrices* to estimate β (([1]). For $k = 2$, $x' = (x_1, x_2)$, and defining the vector $x^{[4]}$, we use the expanded results with,

$$\begin{aligned} \mathbf{x}^{[4]'} x^{[4]} &= x_0^8 + x_1^8 + x_2^8 + 4[x_0^6 x_1^2 + x_0^6 x_2^2 + x_1^6 x_2^2 + x_0^2 x_1^6 + x_0^2 x_2^6 + x_1^2 x_2^6] \\ &+ 6[x_0^4 x_1^4 + x_0^4 x_2^4 + x_1^4 x_2^4] + 12[x_0^4 x_1^2 x_2^2 + x_0^2 x_1^4 x_2^2 + x_0^2 x_1^2 x_2^4], \end{aligned}$$

(2.3)

which implies that

$$\mathbf{x}^{[4]'} = [x_0^8, x_1^8, x_2^8, 2(x_0^3x_1, x_0^3x_2, x_1^3x_2, x_0x_1^3, x_0x_2^3, x_1x_2^3), \sqrt{6}(x_0^2x_1^2, x_0^2x_2^2, x_1^2x_2^2), 2\sqrt{3}(x_0^2x_1x_2, x_0x_1^2x_2, x_0x_1x_2^2)],$$

(2.4)

and the parameter β is expressed as

$$\beta' = [\beta_0, \beta_1, \beta_2, \beta_{11}, \beta_{22}, \beta_{12}, \beta_{111}, \beta_{222}, \beta_{112}, \beta_{122}, \beta_{1111}, \beta_{2222}, \beta_{1122}, \beta_{1112}, \beta_{1222}]. \tag{2.5}$$

Applying the model given in (2.1), and Schlafflian vectors approach, the least square estimate is given by

$$\hat{\beta} = (\sum_{u=1}^{N} x^{[4]'}x^{[4]})^{-1}x^{[4]'}y. \tag{2.6}$$

The estimated response $\hat{y}_u$ at any point is given by $\hat{y}_u = x_u^{[4]'}\hat{\beta}$, and the variance of the estimated response will be given by

$$Var(\hat{y}_u) = x_u^{[4]'}\ Var(\hat{\beta})\ x_u^{[4]} = x_u^{[4]'}\ (X'X)^{-1}\ x_u^{[4]}\sigma^2\ . \tag{2.7}$$

We generate vectors D_1, D_2 and D_3, to workout the moment matrix with two predictor variables ([1]). For the design with two predictor variables we write,

$$N^{-1}(X'X) = N^{-1}\sum_{u=1}^{N} x^{[4]}x^{[4]'} = N^{-1}\sum_{=1}^{N}\begin{pmatrix} D_1 \\ D_2 \\ D_3 \end{pmatrix}[D'_1, D'_2, D'_3]$$

(2.8)

Therefore the moment matrix is given by

$$N^{-1}(X'X) = \sum_{u=1}^{N}\begin{pmatrix} D_1D_1' & D_1D_2' & D_1D_3' \\ D_2D_1' & D_2D_2' & D_2D_3' \\ D_3D_1' & D_3D_2' & D_3D_3' \end{pmatrix}$$

(2.9)

Our focus lies on the main diagonal of (2.9) since the off diagonals elements will be 0 with regard to conditions of rotability. That is to say

$$N^{-1}(X'X) = diag\sum_{u=1}^{N}[D_1D_1'\ \ D_2D_2'\ \ D_3D_3'] \tag{2.10}$$

The final form of the moment matrix obtained will be ([1]),

$$N^{-1}(X'X) = diag[\ B\ M\ L\ ]. \tag{2.11}$$

3 Parameter estimates

In order to obtain the paramenter estimate ($\hat{\beta}$) we consider the expression for the inverse of the matrix $X'X$, by rewriting (2.11) as

$$(X'X) = N\ diag[\ B \quad M \quad L\ ] \tag{3.1}$$

whose inverse will be of the form

$$(X'X)^{-1} = N^{-1} diag\ [B^{-1} \quad M^{-1} \quad L^{-1}], \tag{3.2}$$

obtained by working out the inverses of B, M and L ([1]). Using (2.11) in (2.6) we have

$$\hat{\beta} = N^{-1} \quad diag\ [B^{-1} \quad M^{-1} \quad L^{-1}]\ X'y \tag{3.3}$$

using $x^{[4]'}$ of (4) in (14) we get

$$\hat{\beta} = N^{-1} \quad diag\ [B^{-1} \quad M^{-1} \quad L^{-1}] \begin{pmatrix} D_1 \\ D_2 \\ D_3 \end{pmatrix} y = \begin{pmatrix} \hat{\beta}_{*1} \\ \hat{\beta}_{*2} \\ \hat{\beta}_{*3} \end{pmatrix}$$

(3.4)

where

$$\hat{\beta}_{*1} = [\hat{\beta}_0, \frac{1}{\sqrt{6}}\hat{\beta}_{11}, \frac{1}{\sqrt{6}}\hat{\beta}_{22}, \hat{\beta}_{1111}, \hat{\beta}_{2222}, \frac{1}{\sqrt{6}}\hat{\beta}_{1122}]' \tag{3.5}$$

$$\hat{\beta}_{*2} = [\frac{1}{2}\hat{\beta}_1, \frac{1}{2}\hat{\beta}_2, \frac{1}{\sqrt{12}}\hat{\beta}_{122}, \frac{1}{\sqrt{12}}\hat{\beta}_{112}, \frac{1}{2}\hat{\beta}_{111}, \frac{1}{2}\hat{\beta}_{222}]' \tag{3.6}$$

$$\hat{\beta}_{*3} = [\frac{1}{2}\hat{\beta}_{1112}, \frac{1}{2}\hat{\beta}_{1222}, \frac{1}{\sqrt{12}}\hat{\beta}_{12}]' \quad . \tag{3.7}$$

The main interest is that of finding the estimates of the coefficients of the general mean and the linear factors β_0, β_1 and β_2 ([1]).

4 The estimated response

The estimated response $\hat{y}_u$ at a point $(x_{0u},\ x_{1u},\ x_{2u})$ from a general situation will be

$$\hat{y}_u = x_u^{[4]'}\hat{\mu}, \tag{4.1}$$

our focus being that of the coefficients of the main effects only where $x_u^{[4]'}$ is as provided in (2.4) and μ giving our parameter system of interest given as $\mu = J'\beta$ [for μ and J see paper1].

Using equation (4.1) we get

(4.2) $$\hat{y}_u = x_u^{[4]'} J' \hat{\beta} = [D_1' \ D_2' \ D_3'] diag[\ R\ S\ T\ ]\hat{\beta} = [D_1'R \quad D_2'S \quad D_3'T]\hat{\beta}$$

we get the expression for the estimated response of a fourth order rotatable design in two dimensions as,

(4.3) $$\hat{y}_u = \hat{\beta}_0 \sum_{u=1}^{N} x_{0u}^4 + \hat{\beta}_1 \sum_{u=1}^{N} x_{1u}^4 + \hat{\beta}_2 \sum_{u=1}^{N} x_{2u}^4,$$

with the variance of estimated response being constant ([1]).

5 Difference of the variance functions of two estimated responses

Suppose that x_a' and x_b' are two distinct points identified on the two response surface of different radii. The two points are given as

(5.1) $$\hat{y}(x_a') = x_a'\hat{\beta} \ , \qquad \hat{y}(x_b') = x_b'\hat{\beta}$$

where $\hat{\beta}$ is the Least Square Estimate of β. The standardized variance of these two estimated responses will be

(5.2) $$V_a = x_a'(X'X)^{-1}x_a \ , \qquad V_b = x_b'(X'X)^{-1}x_b$$

With reference to a rotatable design, $X'X$ has a special form, Box and Hunter (1957). Taking into consideration equation (2.4) where now $x_a' = (\rho_1, 0, 0, ..., 0)$ is taken as a vector of order (15×1) of a row of the design matrix X arising from a point in the predictor variable space. If we express the vector as;

(5.3) $$x_a' = [d_1' \ \ d_2' \ \ d_3']$$

where
$d_1' = (\rho_1,\ 0,\ 0,\ 0,\ 0,\ 0)$, $d_2' = (0,\ 0,\ 0,\ 0,\ 0,\ 0)$ and $d_3' = (0,\ 0,\ 0)$
then the standardized variance function of the estimated response at x_a' will be given as

$$\begin{aligned} V_a &= x_a'\ J'(X'X)^{-1}J\ x_a \\ &= d_1'\ R'\ B^{-1}R\ d_1 \ + \ d_2'\ S'\ M^{-1}\ S\ d_2 \ + \ d_3\ T'\ L^{-1}T\ d_3 \\ &= \rho_1^2\triangle^{-1}\ S_0 = \frac{24\rho_1^2\beta_1^*}{\mu^*} \end{aligned}$$

(5.4)

which on substituting the values of β_1^*, μ^* and k gives

$$V_a = \frac{24\rho_1^2[8\lambda_4\lambda_8 - 6\lambda_6^2]}{24[8\lambda_4\lambda_8 - 6\lambda_6^2] - 12\lambda_2[8\lambda_2\lambda_8 - 4\lambda_4\lambda_6] + 8\lambda_4[6\lambda_2\lambda_6 - 4\lambda_4^2]} \tag{5.5}$$

Let

$$x_b' = [d_1^{*'}\ d_2^{*'}\ d_3^{*'}] \tag{5.6}$$

be a vector of order (15×1) of a row of the design matrix X arising from a point in the predictor variable space. We observe that this is a particular point on the response surface which must not be along the axes of the predictor variable space. However the vector makes an angle θ with the axis x_1 where
$d_1^{*'} = (\rho_2 \cos\theta,\ 0,\ 0,\ 0,\ 0,\ 0)$, $d_2^{*'} = (\rho_2 \sin\theta,\ 0,\ 0,\ 0,\ 0,\ 0)$, and $d_3^{*'} = (0,\ 0,\ 0)$
then the standardized variance of the estimated response at x_b will be expressed as

$$\begin{aligned} V_b &= x_b'\ J'(X'X)^{-1}J\ x_b \\ &= d_1^{*'}\ R'\ B^{-1}R\ d_1^* \quad + \quad d_2^{*'}\ S'\ M^{-1}\ S\ d_2^* \\ &= \frac{\rho_2^2 \cos^2\theta\beta_1^*}{\mu^*} + \rho_2^2 \sin^2\theta {\beta_3^*}^{-1}\alpha \end{aligned}$$

(5.7)

which on substituting the values of β_1^*, β_3^*, μ^*, α and k we have

(5.8)

$$V_b = \frac{24\rho_2^2\cos^2\theta[8\lambda_4\lambda_8 - 6\lambda_6^2]}{24[8\lambda_4\lambda_8 - 6\lambda_6^2] - 12\lambda_2[8\lambda_2\lambda_8 - 4\lambda_4\lambda_6] + 8\lambda_4[6\lambda_2\lambda_6 - 4\lambda_4^2]} + \frac{\frac{3}{2}\lambda_6\rho_2^2\sin^2\theta}{6\lambda_2\lambda_6 - 4\lambda_4^2}$$

With reference to conditions of rotatability we have

$\omega_1 = 24[8\lambda_4\lambda_8 - 6\lambda_6^2]$
$\omega_2 = 12\lambda_2[8\lambda_2\lambda_8 - 4\lambda_4\lambda_6]$
$\omega_3 = 8\lambda_4[6\lambda_2\lambda_6 - 4\lambda_4^2]$

then

$$V_a = \frac{\omega_1\rho_1^2}{\omega_1 - \omega_2 + \omega_3} \tag{5.9}$$

and

$$V_b = \frac{\omega_1\rho_1^2\cos^2\theta}{\omega_1 - \omega_2 + \omega_3} + \frac{\frac{3}{2}\lambda_6\rho_2^2\sin^2\theta}{[6\lambda_2\lambda_6 - 4\lambda_4^2]} \tag{5.10}$$

The difference of the variance functions of the two estimated responses will be

$$V_c = V_a - V_b = \frac{\omega_1(\rho_1^2 - \rho_1^2\cos^2\theta)}{\omega_1 - \omega_2 + \omega_3} - \frac{\frac{3}{2}\rho_2^2\sin^2\theta}{[6\lambda_2\lambda_6 - 4\lambda_4^2]}\ , \tag{5.11}$$

which is a function of θ.

6 Discussion

The results in (5.11) can optimized by finding the first order condition and solving for θ. After which we explore the second order condition to evaluate the nature of the function.

Suppose we let

$$\frac{\omega_1}{\omega_1 - \omega_2 + \omega_3} = h_1$$

and

$$\frac{\frac{3}{2}\lambda_6}{[6\lambda_2\lambda_6 - 4\lambda_4^2]} = \frac{12\lambda_4\lambda_6}{\omega_3} = h_2,$$

which we use to re-expressed (5.11) as,

$$V_c = h_1(\rho_1^2 - \rho_1^2 \cos^2\theta) - h_2\rho_2^2 \sin^2\theta. \tag{6.1}$$

The first order of condition of (6.1) will be

$$f_1'(\theta) = \frac{\partial V_c}{\partial \theta} = 2h_1\rho_2^2 \cos\theta \sin\theta - 2h_2\rho_2^2 \cos\theta \sin\theta = 0,$$

on solving we get

$$\theta = \{0, 90\}. \tag{6.2}$$

With regard to rotatability we only need to evaluate θ for values of $0^o \leq \theta \leq 90^o$ since by rotating the points around the sphere the angle remains invariant as well as first quadrant can be used to give values in other quadrants. The second derivative of (6.1) will be

$$f_c''(\theta) = \frac{\partial^2 V_c}{\partial \theta^2} = 2[h_1 - h_2]\rho_2^2[1 - 2\sin^2\theta] \tag{6.3}$$

On substitution for values of θ from the set in (6.2) we have two conditions;

(i) for $\theta = 0^o$

$$f_c''(\theta) = 2[h_1 - h_2]\rho_2^2[1 - 0] = 2[h_1 - h_2]\rho_2^2$$

By letting $\lambda_2 < \frac{1}{k}$ and $\lambda_4 \leq \frac{\lambda_2}{k+2}$ from the results of Huda and Mukerjee (1984), while evaluating the values of λ_6 and λ_8 with regard to conditions and same procedures we have, $\lambda_2 < \frac{1}{2}$, $\lambda_4 = \frac{\lambda_2}{4}$;on considering the equality, $\lambda_2\lambda_6 = \frac{\lambda_4}{k+4}$; therefore $\lambda_6 = \frac{\lambda_4}{6\lambda_2}$ and $\lambda_4\lambda_8 = \frac{\lambda_6}{k+6}$ thus $\lambda_8 = \frac{\lambda_6}{8\lambda_4}$ We therefore need only evaluate the values of λ_2 say λ_2^* in order to compute h_1 and h_2. For $\lambda_2^* = 0.4396$ from the results of Huda and Mukerjee we find that

$$h_1 = 34.76694889, \quad h_2 = 1.014808732 \tag{6.4}$$

hence if the vectors are equidistant and the distance is unitary then,

$$f_c''(\theta) = 2[h_1 - h_2]\rho_2^2 = 67.5042805 > 0^o \tag{6.5}$$

which implies that the difference of the variance functions for two estimated responses is minimized when $\theta = 0^o$.

(ii) for $\theta = 90^o$ we have

$$f_c''(\theta) = 2[h_1 - h_2]\rho_2^2[1 - 2\sin 90^o] = -67.50572314 < 0^o \tag{6.6}$$

which implies that the difference of the variance functions for two estimated responses is maximized when $\theta = 90^o$.
We now evaluate the extent to which the angle θ can be varied while still minimizing the functions in V_c of (6.1). We tabulate the results as follows;

Table of Values

θ	$f_c''(\theta)$	θ	$f_c''(\theta)$
0	67.5042805	44	2.355865415
5	66.4787388	45	0
10	63.43327426	46	-2.355865415
15	58.46042178	47	-4.70886057
20	51.71127896	48	-7.056118705
25	43.39091511	49	-9.394780045
30	33.75214025	50	-11.72199529
35	23.08782369	55	-23.08782369
40	11.72199529	60	-33.75214025
41	9.394780045	70	-51.71127896
42	7.056118705	80	-63.43327426
43	4.70886057	90	-67.5042805

Where, $f_c''(\theta)$ is the second derivative of the function V_c, that is the difference of the variance functions of two estimated responses.

7 Conclusions

The aim of every experimenter is to minimize the variance function, therefore we conclude that for the difference of the variance functions for two estimated responses we may achieve a global minimum while others exogenous factors assumed constant by letting the angle between the two vectors θ to be as close as possible to 45^o.

If differences of points close together in the factor space are involved, based on our results, an optimal design for a fourth order rotatable design in two dimensions from the this approaches will be chosen on the basis of minimum variance function criterion as emphasized by Herzberg (1967), Box and Draper (1980), Huda (1985) and Huda and Mukerjee (1984).

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