International Journal of Mathematics and Statistics Studies
Vol.1, Issue 4, pp.48-58, December 2013
Published by European Centre for Research Training and Development UK (www.ea-journals.org)

ON THE COMPARISON OF BOUNDARY AND INTERIOR SUPPORT POINTS OF A RESPONSE SURFACE UNDER OPTIMALITY CRITERIA

Thomas Adidaumbe Ugbe[1] and Stephen Sebastian Akpan[2]
[1,2]Department Of Mathematics/Statistics And Computer Science, University Of Calabar, Calabar, Cross River State, Nigeria

ABSTRACT: *The performance of the design matrices obtained from boundary and interior support points of a response surface is compared within a specified experimental area based on first order response surface model. This is achieved by determining the values of the desired optimal design criteria with respect to their corresponding information matrices. These optimality criteria are: D- optimality, G- optimality, A –optimality and E- optimality. Four designs arbitrarily chosen from both boundary and interior support points were used for the study. The designs obtained from boundary support points were found to be better than the designs obtained from interior support points with respect to the aforementioned design optimality criteria considered in this work.*

KEYWORDS: Boundary Support Points, Optimality Criteria, Information Matrix, response surface, Interior Support Points

INTRODUCTION

One of the first to state criteria and obtain optimum experimental designs for regression problems was Smith (1918). Many years thereafter, Kiefer (1959) developed meaningful computational procedures for finding optimum designs in regression problems of statistical inference. An optimality criterion showed how good a design is and it is maximized or minimized by an optimal design. Numerous papers by { Kiefer (1959), Kiefer (1961), Kiefer (1962) and Kiefer (1972) } and { Kiefer and Wolfowitz (1959), Kiefer and Wolfowitz (1960) and Kiefer and Wolfowitz (1964) } and most recently Vrdoljak (2010), Emmett et al (2011) and Gilmour and Trinca (2012) play a central role- in the development of optimality criteria. In Kiefer and Wolfowitz (1959), their theoretical approach to design optimality and their introduction of the D- and E- optimality criteria for the linear regression model laid the ground work for other design criteria; A-, F-, G- and D- optimality criteria. See for example, Yang (2008). Many of these design criteria were originally developed for the homogeneous variance linear models, but most have been adopted for use in a non-linear and non-homogeneous variance situation as well. See for example, Ugbe and Chigbu (2012).

There are many optimality criteria, these criteria are: D-, A- , E-, G-, V-, I-, T-, optimality criteria etc. They are sometimes called alphabetical optimality criteria. A comprehensive and accessible description of optimality criteria and their applications is found in Atkinson et al (2007).The aim of this work is to compare designs from boundary and interior support points of the response surface using the D-, G-, A-, and E-, optimality criteria for first order response surface model.

NOTATIONS AND DEFINITIONS

NOTATIONS

To define each optimality criteria used in this study some notations are needed. Thus, we consider a design, ζ, to be represented by a matrix M, and for the same design, ζ, the information matrix is defined to be $\varphi(Mo) = M(\zeta) = X'X$; Mo = M= information matrix, φ is some optimality characteristic measure function. The determinant of the information matrix, $X'X$ is $\det(X'X)$; the variance of the estimated variance surface at X, is $d(X,\zeta)$ $= f'(x)M^{-1}(\zeta)f(x)$

DEFINITIONS

D-optimality criterion: A design that maximizes the determinant of the information matrix, $X'X$ is called a D-optimal design. Symbolically, a design is D-optimal if it gives $\varphi(Mo)=$ max $\det(X'X)$. By a D-optimal design, the generalized variance of the best, linear, unbiased estimates of the parameters is minimized, regardless of the actual parameterization of the regression function.

G-optimality criterion: A design that minimizes the maximum variance of the estimated response function over the design region is called a *G- optimality criterion*. Symbolically, i.e min{ max d (X, ζ)}. The experimeter optimizing a design according to the G- optimality criterion intends to get a good estimate of all the observed responses.

A-optimality criterion: A design that minimizes the trace of the dispersion matrix,$(X'X)^{-1}$ is called an *A- optimality criterion*. Symbolically, a design is A- optimal if it gives min tr$(X'X)^{-1}$
E-optimality criterion: A design that minimizes the maximum eigenvalues of the dispersion matrix, $(X'X)^{-1}$ is called an E-optimal design. Symbolically, a design is E-optimal if it gives min λ^{-1}, where X is the largest eigenvalue of information matrix.

GENERAL APPROACH OF THE INVESTIGATION

Introduction

We shall make comparison under (D-,G-, A-, and E-) optimality criteria between the boundary and interior support points of the response surface for first order response surface model in the closed interval [0,1].

The design matrix obtained from the boundary and interior support points are defined as follows:
X_b- design matrix of boundary support points
X_t – design matrix of interior support points
All the designs are obtained from **figure 1**

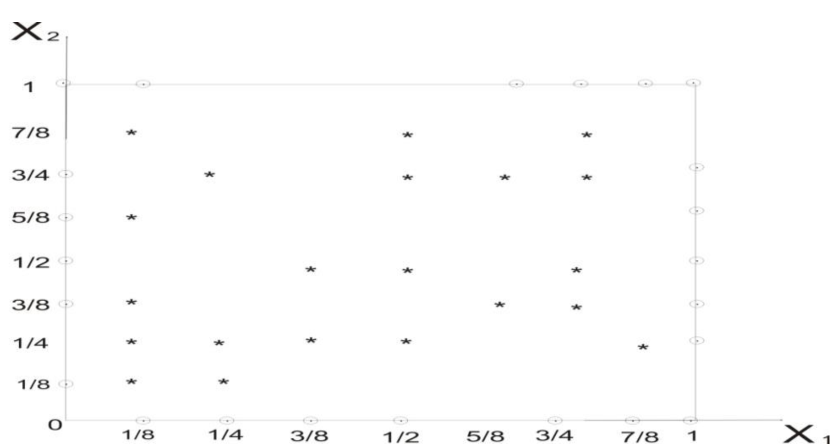

Figure 1 Experimental region (Response Surface)

First order response surface model is given by $f(x_1,x_2) = a_o + a_1x_1 + a_2x_2 + e$.

In **figure 1** points 'circled' are the boundary support points while points with 'asterisks' are interior support points.

Design matrices for boundary support points are:

(Note; four design matrices are arbitrary chosen for the study)

$$X_{b_1} = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \\ 1 & \frac{1}{2} & 0 \\ 1 & 1 & \frac{1}{2} \\ 1 & \frac{3}{8} & 0 \\ 1 & 1 & 0 \end{pmatrix}, \qquad X_{b_2} = \begin{pmatrix} 1 & \frac{5}{8} & 1 \\ 1 & 0 & \frac{1}{8} \\ 1 & 0 & \frac{3}{8} \\ 1 & 1 & \frac{3}{8} \\ 1 & \frac{3}{4} & 1 \\ 1 & 1 & \frac{5}{8} \end{pmatrix}, \qquad X_{b_3} = \begin{pmatrix} 1 & \frac{3}{4} & 0 \\ 1 & \frac{1}{8} & 0 \\ 1 & 0 & \frac{1}{2} \\ 1 & \frac{1}{8} & 1 \\ 1 & \frac{7}{8} & 1 \\ 1 & 1 & \frac{5}{8} \end{pmatrix},$$

$$X_{b_4} = \begin{pmatrix} 1 & 0 & \frac{5}{8} \\ 1 & 0 & \frac{3}{4} \\ 1 & 1 & \frac{3}{4} \\ 1 & 1 & \frac{1}{4} \\ 1 & \frac{7}{8} & 0 \\ 1 & \frac{1}{4} & 0 \end{pmatrix}.$$

Design matrix for interior support points are: (Note; four design matrices are arbitrarily chosen for the study).

$$X_{t_1} = \begin{pmatrix} 1 & \frac{1}{8} & \frac{1}{4} \\ 1 & \frac{1}{4} & \frac{1}{4} \\ 1 & \frac{1}{8} & \frac{1}{8} \\ 1 & \frac{1}{8} & \frac{3}{8} \\ 1 & \frac{1}{2} & \frac{1}{4} \\ 1 & \frac{1}{4} & \frac{3}{4} \end{pmatrix}, \qquad X_{t_2} = \begin{pmatrix} 1 & \frac{1}{8} & \frac{5}{8} \\ 1 & \frac{1}{8} & \frac{7}{8} \\ 1 & \frac{1}{4} & \frac{1}{8} \\ 1 & \frac{1}{2} & \frac{1}{2} \\ 1 & \frac{1}{2} & \frac{3}{4} \\ 1 & \frac{1}{2} & \frac{7}{8} \end{pmatrix}, \qquad X_{t_3} = \begin{pmatrix} 1 & \frac{3}{8} & \frac{1}{4} \\ 1 & \frac{3}{8} & \frac{1}{2} \\ 1 & \frac{7}{8} & \frac{1}{4} \\ 1 & \frac{3}{4} & \frac{1}{2} \\ 1 & \frac{3}{4} & \frac{3}{4} \\ 1 & \frac{5}{8} & \frac{3}{8} \end{pmatrix},$$

$$X_{t_4} = \begin{pmatrix} 1 & \frac{1}{8} & \frac{5}{8} \\ 1 & \frac{1}{8} & \frac{7}{8} \\ 1 & \frac{1}{4} & \frac{1}{8} \\ 1 & \frac{5}{8} & \frac{3}{4} \\ 1 & \frac{3}{4} & \frac{3}{8} \\ 1 & \frac{3}{4} & \frac{7}{8} \end{pmatrix}$$

3.2 Comparing design from boundary and interior support points under D- optimality

Recall now from the definition of D- optimality criterion, $\varphi(Mo)$= max $\det(X'X)$. In this context, the set of information matrices, $X_b{}'X_b$ and $X_t{}'X_t$, between these matrices, the one that gives a maximum determinant is optimal. In other words, we need to establish numerically that one of the following inequalities, det ($X_b{}'X_b$)< det ($X_t{}'X_t$) and det ($X_t{}'X_t$) < det ($X_b{}'X_b$) holds.

Thus four different designs for both boundary and interior support points were used for the illustrations as given earlier. The designs are X_{b_1}, X_{b_2}, X_{b_3}, X_{b_4} and X_{t_1}, X_{t_2} X_{t_3} and X_{t_4}

The design and information matrices from boundary support points, X_{b_1} for first order response surface model are:

$$X_{b_1} = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \\ 1 & \frac{1}{2} & 0 \\ 1 & 1 & \frac{1}{2} \\ 1 & \frac{3}{8} & 0 \\ 1 & 1 & 0 \end{pmatrix} , \qquad \frac{X_{b_1}' X_{b_1}}{N} = \begin{pmatrix} 1 & .6458 & .4167 \\ .6458 & .5651 & .2500 \\ .4167 & .2500 & .3750 \end{pmatrix}$$ (where N is the no. of design points) .

$\det\left\{\frac{1}{N}\left(X_{b_1}' X_{b_1}\right)\right\}$ = .0294. The corresponding design and information matrices from interior support points, i.e

$$X_{t_1} = \begin{pmatrix} 1 & \frac{1}{8} & \frac{1}{4} \\ 1 & \frac{1}{4} & \frac{1}{4} \\ 1 & \frac{1}{8} & \frac{1}{8} \\ 1 & \frac{1}{8} & \frac{3}{8} \\ 1 & \frac{1}{2} & \frac{1}{4} \\ 1 & \frac{1}{4} & \frac{3}{4} \end{pmatrix} , \qquad \frac{X_{t_1}' X_{t_1}}{N} = \begin{pmatrix} 1 & .2083 & .6042 \\ .2083 & .0469 & .1250 \\ .6042 & .1250 & .3932 \end{pmatrix}$$

$\det\left\{\frac{1}{N}\left(X_{t_1}' X_{t_1}\right)\right\} = .00009720.$

Obviously, the inequality $\det\left(X_{t_1}'X_{t_1}\right) < \det\left(X_{b_1}'X_{b_1}\right)$ holds.

By the same token, det $\left(X_b'X_b\right)$ and det $\left(X_t'X_t\right)$ for the designs, 2, 3 and 4 given earlier are obtained. For each of the designs under consideration the maximum values of $\det\left(X_b'X_b\right)$ and $\det\left(X_t'X_t\right)$ are given in table 1. Just as we have seen in the case of the designs 1, that the inequality det $\left(X_t'X_t\right) < \det\left(X_b'X_b\right)$ holds, the inequality det $\left(X_t'X_t\right) < \det\left(X_b'X_b\right)$ also holds for the designs 2,3 and 4.

Thus, with respect to the D-optimality criterion, designs obtained from the boundary support points are better in fitting a first order response surface model than those of interior support points.

Comparing designs from boundary and interior support points under G-optimality criterion

Given a design, X, let d(X_b,X) denote the variance of the estimated regression function of boundary support points designs. And let d(X_t, X) denote the variance of the estimated regression function of interior support points designs. In comparing the functions under G-optimality criterion, we need to established that one of the following inequalities,

Max d(X_b, X)<Max d(X_t, X) and Max d(X_t, X)<Max d(X_b, X) holds. For design, 1 the variance of the estimated regression function of boundary support points designs, d(X_b, X),

is d(X_b, X)= $f'(X_b)(X_b'X_b)^{-1}f(X_b)$

For design 1, $\left(\frac{1}{N}X_{b_1}'X_{b_1}\right)^{-1}$=$\begin{pmatrix} 5.0743 & -4.6867 & -2.5141 \\ -4.6867 & 6.8386 & 0.6488 \\ -2.5141 & 0.6488 & 5.0278 \end{pmatrix}$

The maximum of d(X_b, X)= $f'(X_b)(X_b'X_b)^{-1}f(X_b), for\ design\ 1$ is Max d(X_{b_1}, X)= Max$\left\{f'\left(X_{b_1}\right)\left(X_{b_1}'X_{b_1}\right)^{-1}f\left(X_{b_1}\right)\right\}$=5.0739

The corresponding variance of the estimated regression function of interior support points design, d(X_t,X)= $f'(X_t)(X_t'X_t)^{-1}f(X_t)$, the maximum for design, 1, ie Max d(X_{t_1}, X) = Max $\left\{f'\left(X_{t_1}\right)\left(X_t'X_{t_1}\right)^{-1}f\left(X_{t_1}\right)\right\}$ = 5.3482. Obviously, the inequality Max d(X_b, X)<Max d(X_t, X) holds. By the same token d(X_b, X) and d(X_t, X) for the designs, 2,3 and 4 are obtained. For each of the designs under consideration the maximum values of d(X_b, X) and d(X_t, X) are given in

table 2. Similarly, the inequality holds for the designs 2, 3 and 4. Thus, with respect to G-optimality criterion, designs obtained from boundary support points are better in fitting first order response surface model than those from interior support points.

Comparing designs from boundary and interior support points under A-optimality criterion.

The comparison between boundary and interior support points designs based on the A-optimality criterion considers the trace values of the dispersion matrices, $(X_b{'}X_b)^{-1}$ and $(X_t{'}X_t)^{-1}$. Here, we are to established that one of the following inequalities tr$(X_b{'}X_b)^{-1}$ < tr$(X_t{'}X_t)^{-1}$ and tr $(X_t{'}X_t)^{-1}$< tr$(X_b{'}X_b)^{-1}$ holds. For the designs 1, 2, 3 and 4, the values of tr$(X_b{'}X_b)^{-1}$ and tr$(X_t{'}X_t)^{-1}$ have been obtained in table 3.

We shall continue our illustration here as in the preceding section.

Thus, $\left(\frac{1}{N}X_{b_1}{'}X_{b_1}\right)^{-1}=\begin{pmatrix} 5.0743 & -4.6867 & -2.5141 \\ -4.6867 & 6.8386 & 0.6488 \\ -2.5141 & 0.6488 & 5.0278 \end{pmatrix}$

Thus, tr$\left(\frac{1}{N}X_{b_1}{'}X_{b_1}\right)^{-1}$ = 16.9407

For the corresponding interior support points design, the dispersion matrix is

$$\left(\frac{1}{N}X_t{'}X_t\right)^{-1}=\begin{pmatrix} 6.3834 & -12.1150 & -7.8211 \\ -12.1150 & 56.4345 & -2.4537 \\ -7.8211 & -2.4537 & 25.1502 \end{pmatrix}$$

Thus, tr$\left(\frac{1}{N}X_{t_1}{'}X_{t_1}\right)^{-1}$ = 87.9681. obviously, the inequality tr$(X_b{'}X_b)^{-1}$ < tr$(X_t{'}X_t)^{-1}$ holds. For the rest of the designs adopted for illustration in the work, inspection of table 3 reveals that the values of $\varphi(Mo)$ correspond to the values of tr$(X_b{'}X_b)^{-1}$ which shows that the inequality tr$(X_b{'}X_b)^{-1}$ < tr$(X_t{'}X_t)^{-1}$ holds. Thus, with respect to A-optimality criterion, designs obtained from boundary support points are better in fitting first order respond surface model.

Comparing designs from boundary and interior support points under E-optimally criterion.

We shall use the result in table 4 to consider the E-optimality criterion. This table shows maximum eigenvalues taken of the matrix $(X_b{'}X_b)^{-1}$ and the maximum $(X_t{'}X_t)^{-1}$ for the designs;1, 2, 3 and 4.

Given a design, let ${\lambda_b}^{-1}$ denote the maximum eigenvalues of the dispersion matrix, $(X_b'X_b)^{-1}$ and let ${\lambda_t}^{-1}$ denote the maximum eigenvalues of dispersion matrix, $(X_t'X_t)^{-1}$. In comparing boundary and interior support points designs under E-optimality criterion, we need to establish that one of the following inequalities, ${\lambda_b}^{-1} < {\lambda_t}^{-1}$and ${\lambda_t}^{-1} < {\lambda_b}^{-1}$ holds. For design, 1, the maximum eigenvalue of ${\lambda_b}^{-1}$ of the corresponding dispersion matrix, $(X_b'X_b)^{-1}$ is 11.4411. The maximum eigenvalue ${\lambda_t}^{-1}$ of the corresponding dispersion matrix, $(X_t'X_t)^{-1}$ is 59.2254. Clearly, the inequality${\lambda_b}^{-1} < {\lambda_t}^{-1}$ holds. In the same manner, the values of ${\lambda_b}^{-1}$ and ${\lambda_t}^{-1}$ for the designs 2, 3, and 4 are obtained. From table 4, we observed that for these designs the inequality ${\lambda_b}^{-1} < {\lambda_t}^{-1}$ holds. Thus, with respect to E-optimality criterion designs obtained from boundary support points are better in fitting first order response surface model than those from interior support points.

Table 1 **D-optimality values for the given design used in comparison**

Designs	**number of points**	**Max det$(X_b'X_b)$**	**Max det$(X_t'X_t)$**	**$\varphi(Mo)$**
1	6	0.02940	0.0007076	0.02940
2	6	0.0143	0.00020	0.0143
3	6	0.0272	0.0011	0.0272
4	6	0.0197	0.0057	0.0197

Table 2 **G-optimality values of the given design used in comparison**

Designs	**Number of points**	**Max d$(X_b'X)$**	**Max d$(X_t'X)$**	**$\varphi(Mo)$**
1	6	5.0739	5.3482	5.0739
2	6	3.8302	4.7615	3.8302
3	6	3.4275	4.4204	3.4274
4	6	4.1911	4.3371	4.1911

Table 3 A-optimality values for the given designs used in comparison

Designs	**Number of points**	**Tr$(X_b'X_b)^{-1}$**	**Tr$(X_t'X_t)^{-1}$**	$\varphi(Mo)$
1	6	16.9407	87.9681	16.9407
2	6	24.2175	58.8853	24.2175
3	6	15.9039	78.2356	25.9039
4	6	20.4203	34.3360	20.4203

Table 4 E-optimality values for the given design used in comparison

Designs	**Number of points**	**Max $\lambda_b{}^{-1}$**	**Max $\lambda_t{}^{-1}$**	$\varphi(Mo)$
1	6	11.4411	59.2254	11.4411
2	6	16.0634	37.7583	16.0634
3	6	8.3623	41.2908	8.3623
4	6	14.6537	19.4825	14.6537

CONCLUSION

It can be concluded that for each of the optimality criteria considered, designs obtained from boundary support points are better in fitting and estimating first order response surface model than designs obtained from interior support points. Furthermore, a design that is D-optimal minimizes the generalized variance of the estimate of the treatment parameters and the one that is G-optimal minimizes the maximum variance of the estimate of the surface or response. It can be deduced that design obtained from boundary support points are minimum variance design. Therefore, they are efficient in estimating first order response surface model.

REFERENCES

Atkinson, A. C., Donev, A. N. and Tobias.(2007). Optimum Experimental Designs, with SAS, Oxford: Oxford University Press.

Emmett, M., Goos, P. and Stillman, E .C.(2011). A Weighted Prediction-Based Selection Criterion for Response Surface Designs. Quality Reliab. Eng. Int.27, 719-729.

Gilmour, S.G. and Trinca, L. A. (2012). Optimum Designs of Experiments for Statistical Inference. Journ. Roy. Statistics. Soc. C. 61,345-401.

Kiefer, J. (1959) .Optimum Experimental Design. Journ. Roy. Statist Soc. B, 21, 272-319.

Kiefer, J. (1961). Optimum Designs in Regression Problems. Annal of Maths Statist. 32,298-325.

Kiefer, J. (1962).Two More Criteria Equivalent to D-optimality Designs. Annal of Maths Statist.33,792-796

Kiefer, J. (1974).General Equivalence Theory for Optimal Designs (Approximate Theory). Annals of Maths Statist:12, 849-879.

Kiefer, J. and Wolfowitz, J. (1959). Optimum Designs in Regression Problems. Annals of Maths. Statist 30, 271-294.

Kiefer, J.and Wolfowitz, J. (1960).The Equivalence of Two Extremum Problems. Canad J. Math. 12, 363-366.

Kiefer, J. and Wolfowitz, J. (1964). Optimum Extrapolation and Interpolation Designs, I. Annals Inst. Statist. Math. 16, 79-108.

Smith, K. (1918). On the Standard Deviation of Adjusted and Interpolated Values of an Observed Polynomial Function and its Constant and the Guidance they give towards a Proper Choice of the Distribution of Observations. Biometrika. 12, 1-85.

Ugbe, T.A. and Chigbu, P. E. (2012). On D-optimality Criterion of Non-overlapping and Overlapping Segmentation of the Response Surface. Research Journ. of Maths and Statist. 4, 1-5.

Vrdoljak, M. (2010). Optimality Criteria Method for Optimal Designs in Hyperbolic Problems. Mathematical Communications. 15,555-572.

Yang, M. (2008). A-optimal Designs for Generalized Linear Models with Two Parameters. Journ. of Statist. Plann. And In*f*.138,624-641.