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On E–Optimality Design for Quadratic Response Surface Model

Ukeme Paulinus Akra*
Department of Statistics, Akwa Ibom State University, Ikot Akpaden, Mkpat Enin, Nigeria
Email: ukemeakra@gmail.com
ORCID iD: https://orcid.org/0000-0003-3097-2209
*Corresponding author

Edet Effiong Bassey
Department of Statistics, University of Calabar, Calabar, Nigeria
Email: basseyedet@gmail.com
ORCID iD: https://orcid.org/0009-0009-4852-3736

Ofong Edet Ntekim
Department of Mathematics, University of Calabar, Calabar, Nigeria
Email: offongntekim@gmail.com
ORCID iD: https://orcid.org/0009-0007-2801-6388

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Abstract: In response surface methodology, optimality criteria is a major tools used to measure the goodness of a design. Optimal experimental designs (or optimum designs) are a class of experimental designs that are optimal with respect to some statistical criterion. E – Optimality criterion is one of the traditional alphabetical criterion used to explore the right choice of a design in both linear and quadratic response surface models. In this paper, we investigated E – optimal experimental designs for a quadratic response surface model with two factor predictors. We developed an algorithm and a flowchart in line with a program to obtain E – optimal design and compare the result with an existing method. Two designs were formulated each with six points to illustrate the usefulness of the new method. The result revealed that the new technique outperformed better than the existing method. The significance of the later to the former technique is that, it minimizes error due to approximation and also make the computation of the aforementioned optimality easier. We, therefore recommended this method to be used at all length of points when E – optimality is to be evaluated.

Index Terms: Optimal design, Response surface, E – Optimality and Quadratic response surface

1. Introduction

Response Surface Methodology (RSM) is a design test method introduced for the purpose of determining the best response around the fixed limit of the factors. These designs are more efficient to fit a 2^{nd} – order predicted model for the response and more essential for designing a model for modeling curve surface analysis [1]. In other words, response Surface Methodology (RSM) is a statistical and mathematical method that are useful for analyzing problems in which a response of concern is influence by various variables [2]. The design is seek to relate a response variable to the levels of numbers of predictor. Response surface methodology has become a standard tool in the analysis of experimental data. These models are used to study the influence of several input factors on a response variable by approximating complex functional relationships by simple linear or quadratic multivariate polynomial regression models, which are usually denoted as first or second - order response surface models [3]. Response surface method is essential where various predicted variables control a response variable. The predicted variables are supposed to be non - discontinuous and influenced by the designers [4]. A suitable model approximation for the true functional relationship between the response and the set of predicted variables to obtain rotatability in Central Composite Design (CCD) was proposed by [5].

In the design of experiments for estimating statistical models, optimal designs allow parameters to be estimated without bias and with minimum variance. A non-optimal design requires a greater number of experimental runs to estimate the parameters with the same precision as an optimal design. In practical terms, optimal experiments can reduce the costs of experimentation. The optimality of a design depends on the statistical model and is assessed with respect to a statistical criterion, which is related to the variance-matrix of the estimator. Specifying an appropriate model and specifying a suitable criterion function both require understanding of statistical theory and practical knowledge with designing experiments. Optimal design for a bivariate efficacy-safety model when both responses are continuous is considered by [6, 7, 8]. A comprehensive idea of optimality conditions is fundamental for a clear understanding of the performance of many numerical techniques [15]. The optimality criteria are the conditions a function must satisfy at its minimum point. E-optimal designs for the second-order response surface models on the k-dimensional cube and ball was studied by [9]. Optimal designs for a multi-response Emax model: Optimal experimental design has as a goal to find the best ways to perform an experiment considering the available resources and the statistical model was presented by [10, 11]. Optimal designs are considered for the simultaneous response of efficacy and safety in a bivariate model, for the drug combination trials, and for general regression problems, including but not limited to dose-finding analysis [12]. Relationship between E-, D- and A – optimality criteria and their relative efficiency to determine the best optimality criterion was established by [13]. Optimal approximate designs that estimate main effects and interactions for the situation of both full and partial profiles when all attributes have common general number of levels, and also to generate exact designs with reduced pairs for the particular situation of two level attributes was constructed by [14]. Despite all the promising contributions on E – optimality by different authors, none have been able to establish the easiest way beyond the traditional method of computing E – optimal design for quadratic response surface model. Based on this situation, this article aim to fill the gap by providing a simple and precise algorithm to compute E – optimal design. The significance of this algorithm minimizes error due to approximation than the existing method and also make the computation of the aforementioned optimality easier.

2. Methodology

2.1. Quadratic response surface model

Response surfaces are usually approximated by a second-order regression model as the higher-order effects are usually unimportant. A second-order model (also known as the full quadratic) for k number of factors can be written as in Equation 1. This second order model includes linear terms, cross product terms and a second order term for each of the $x's$. The linear terms just have one subscript. The quadratic terms have two subscripts. There are $k*\frac{(k-1)}{2}$ interaction terms. To fit a quadratic model, the need of a response surface design that has more runs than the first order designs used to move close to the optimum. This quadratic model is the basis for response surface designs under the assumption that although the hill is not a perfect quadratic polynomial in k dimensions, it provides a good approximation to the surface near the maximum or a minimum. The quadratic response surface model is other words known as a second-order response surface polynomial model which is designated as;

$$y_r = \eta_o + \sum_{v=1}^{k} \eta_v w_v + \sum_{v=1}^{k} \eta_{vv} w_{vv}^2 + \sum_{v<j}^{k} \eta_{vj} w_v w_j + \varepsilon \tag{1}$$

Where t designated the $n \times 1$ vector of a non-quadratic parameter estimates, and v^{th} entry for all the parameters $\hat{\eta}_v$'s in the model. Let η designate $n \times n$ matrix with v^{th} diagonal element $\hat{\eta}_{vv}$ and with off-diagonal $(vj)^{th}$ entry $\hat{\eta}_{vj}/2$. To estimate the stationary point, equation (1) can be written as;

$$\hat{y}_V = \hat{\eta}_0 + w't + w'\eta w \tag{2}$$

Equation can be written as

$$w = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ \vdots w_n \end{bmatrix}, \ t = \begin{bmatrix} \hat{\eta}_1 \\ \hat{\eta}_2 \\ \vdots \\ \vdots \hat{\eta}_n \end{bmatrix} \text{ and } \eta = \begin{bmatrix} \hat{\eta}_{11} & \hat{\eta}_{12}/2 & \cdots & \hat{\eta}_{1n}/2 \\ \hat{\eta}_{12}/2 & \hat{\eta}_{22} & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \hat{\eta}_{1n}/2 & \cdots & \cdots & \hat{\eta}_{nn} \end{bmatrix}$$

Then the parameters for the stationary points can be calculated by the formula:

$$w_s = -\frac{1}{2}\eta^{-1}t \tag{3}$$

2.2. Formation of Design Matrix for E - Optimal Criteria

Given a k –parameter function, $f(w)$ on N-point design has a $N \times k$ design matrix such that each row of the matrix is a point in $\tilde{W}$. For example, consider n-points design for quadratic response model;

$$f(w_1, w_2) = a_0 + a_1 w_1 + a_2 w_2 + a_3 w_1^2 + a_4 w_2^2 + a_5 w_1 w_2 + \ldots, a_{k-1} a_k w_i w_j + e_{ij} \tag{4}$$

The n-points design matrix of equation (4) is given as;

$$W = \begin{pmatrix} w_{11} & w_{12} & w_{13} & \cdot & \cdot & \cdot & w_{1k} \\ w_{21} & w_{22} & w_{23} & \cdot & \cdot & \cdot & w_{2k} \\ w_{31} & w_{32} & w_{33} & \cdot & \cdot & \cdot & .w_{3k} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ w_{n1} & w_{n2} & w_{n3} & \cdot & \cdot & \cdot & w_{nk}. \end{pmatrix} \tag{5}$$

From equation (5), a 5-points design matrix is designated as;;

$$W = \begin{pmatrix} w_{11} & w_{21} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \\ w_{41} & w_{42} \\ w_{51} & w_{52} \end{pmatrix} \tag{6}$$

For k = 2 the for quadratic response surface of (4) becomes;

$$f(w_1, w_2) = a_0 + a_1 w_1 + a_2 w_2 + a_3 w_1^2 + a_4 w_2^2 + a_5 w_1 w_2 + e \tag{7}$$

Design matrix of (7) is given by;

$$W = \begin{pmatrix} 1 & w_{11} & w_{12} & w_{11}^2 & w_{12}^2 & w_{11}w_{12} \\ 1 & w_{21} & w_{22} & w_{21}^2 & w_{22}^2 & w_{21}w_{22} \\ 1 & w_{31} & w_{32} & w_{31}^2 & w_{32}^2 & w_{31}w_{32} \\ 1 & w_{41} & w_{42} & w_{41}^2 & w_{42}^2 & w_{41}w_{42} \\ 1 & w_{51} & w_{52} & w_{51}^2 & w_{52}^2 & w_{51}w_{52} \\ 1 & w_{61} & w_{62} & w_{61}^2 & w_{62}^2 & w_{61}w_{62} \end{pmatrix} \tag{8}$$

2.3. Information matrix for the design

The goodness of a design is measured by the magnitude of the information matrix. The information matrix $\tau(\varsigma)$ of the design is defined to be;

$$\tau(\varsigma) = \begin{cases} W^T W \\ \sum\limits_{\underline{w} \in \tilde{W}} \underset{\sim}{w} w' \end{cases} \tag{9}$$

Normalized information matrix of (5) is designated as;

$$\tau(\varsigma)=\begin{cases}\dfrac{N\,k\,(W^{T}W)}{N^{2}}\dfrac{\sigma_{w}^{2}}{k}\\ k\sum\limits_{w\in\tilde{W}}\underline{w}w'h_{v}\dfrac{\sigma_{w}^{2}}{k}\end{cases} \tag{10}$$

Where $\frac{N\,k\,(W^{T}W)}{N^{2}}\frac{\sigma_{w}^{2}}{k}$ = if the weight are uniform or uniform probability measure.

$k\sum\limits_{w\in\tilde{W}}\underline{w}w'h_{v}\frac{\sigma_{w}^{2}}{k}$ = Non uniform probability measure and N = size of the matrix and k = number of factors

2.4. Concept of Optimality Criteria in quadratic response surface model

Design optimality is a variance-type criterion that involves optimizing various individual properties of the $(W^{T}W)$ matrix. Optimal designs are experimental designs that are generated based on a particular optimality criterion and are generally optimal only for a specific statistical model. Optimal design methods use a single criterion in order to construct designs for Response Surface Design (RSD); this is especially relevant when fitting quadratic order models.

Therefore, an optimality criterion is a criterion which summarizes how good a design is, which could be either maximizing or minimizing a design. This design is often called the alphabetical optimality criteria because of the letters of the alphabet used. There are several optimality criteria in existence, but our interest is on E – optimal design

2.5. E-Optimal design for quadratic response surface model

A nonlinear model of the form below is considered;

$$E(y/w)=f^{T}(w)\theta \tag{11}$$

Where y is one – dimensional response, w is the predictor variable, f^{T} is a vector $f(w)=f_1(w),\ldots,f_n(w)$ which is the vector of the regression function and $\theta=(\theta_1,\ldots,\theta_n)$ is a vector of unknown model parameters.

This criterion arises as a special case of Kiefer's ϕ_p - optimality criterion, which is defined as;

$$\phi_k(M)=\left[M^{-1}tr\left(M^{k}(\rho)\right)\right]^{\frac{1}{k}}=\left(M^{-1}\sum_{i=1}^{n}\lambda_i^{k}(M(\rho))\right)^{\frac{1}{k}}\text{ for } k\in(-\infty,1) \tag{12}$$

When $\phi_{-\infty}(\rho)=\lim\limits_{k\to\infty}\phi_k(\varepsilon)$ of (12), the expression $\lambda_1(M(\rho)),\ldots,\lambda_n(M(\rho))$ designated the eigenvalues of the information matrix $M(\rho)$ and $\lambda_{\min}(M(\rho))$ corresponding to its minimum eigenvalue.

Hence, this criterion minimizes the maximum eigenvalue of the dispersion matrix $\tau(\varsigma)^{-1}$. Symbolically, a design ς is said to be E-rotatable if

$$\varsigma=Min\left\{Max\left(\lambda^{-1}\right)\right\} \tag{13}$$

Where λ the largest eigenvalue of the information matrix $\tau(\varsigma)$

2.6. An algorithm for obtaining E – optimality Criterion

The following steps are employed to obtain E – optimal design;

Step 1: Select the matrix called (ς_1) for the first design.

Step 2: Take the transpose of ς_1 called ς_1'

Step 3: Take the product of the matrices (ς_1') and (ς_1) called information matrix $\tau(\varsigma)$.

Step 4: Take inverse of the resulting matrix in (3).

Step 5: Obtain eigenvalue of the resulting matrix in (4). To obtain eigenvalue, put the matrix in the form $|A-\lambda I|=0$, where I = identity matrix, A = the design matrix of (4).

Step 6: Select the maximum eigenvalue of (5).

Step 7: Repeat the same steps from (1) – (6) above for the second design (ς_2).

Step 8: Compare the two maximum eigenvalue and select the minimum of the maximum eigenvalue

Step 9: Hence, $Min\{Max(\lambda^{-1})\}$ is E – optimal criterion.

Flowchart

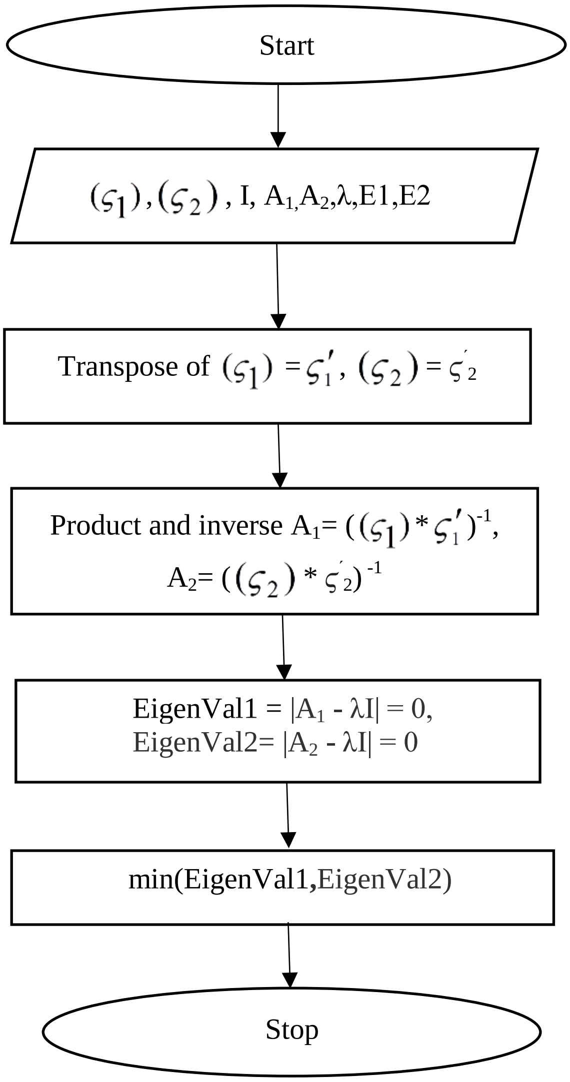


Fig. 1. Flowchart of the algorithm for obtaining E – optimality Criterion

2.7. Program Source for E – optimal design

DataMatrix.java

```
package dm;
import jama.*;
import java.text.DecimalFormat;
import org.apache.commons.math.fraction.*;

public class DataMatrix implements java.io.Serializable
{
	private static final long serialVersionUID = 1L;
	double elements[][];

	public DataMatrix(double d[][])
	{
		setAllElements(d);
```

```
}

public static DataMatrix transpose(DataMatrix m)
{
        double d[][] = new double[m.elements[0].length][m.elements.length];
        for(int i = 0;i < m.elements.length;i++){
                for(int j = 0;j < m.elements[i].length;j++){
                        d[j][i] = m.elements[i][j];
                }
        }
        return new DataMatrix(d);
}

public DataMatrix multiplyBy(DataMatrix m)
{
        Matrix m1 = new Matrix(elements);
        Matrix m2 = new Matrix(m.elements);
        Matrix rs = m1.times(m2);
        DataMatrix results = new DataMatrix(rs.getArray());
        return results;
}

public DataMatrix divideBy(double s)
{
        DataMatrix m = new DataMatrix(elements.length,elements[0].length);
        for(int i = 0;i < elements.length;i++){
                for(int j = 0;j < elements[i].length;j++){
                        m.elements[i][j] = elements[i][j]/s;
                }
        }
        return m;
}

public DataMatrix inverse()
{
        Matrix m2 = null;
        try{
                DataMatrix lm = copy();
           Matrix m = new Matrix(lm.elements);
           m2 = m.inverse();
        }catch(Exception ex){
                System.out.println("Inverse Error: " + ex.getMessage());
                return null;
        }
        return new DataMatrix(m2.getArray());
}

public double[] eigenValue()
{
        double d[];
        try{
                DataMatrix lm = copy();
           Matrix m = new Matrix(lm.elements);
           EigenvalueDecomposition e = m.eig();
           //Matrix D = e.getD();
           d = e.getRealEigenvalues();
        }catch(Exception ex){
                System.out.println("EigenValue: " + ex.getMessage());
                return null;
        }
        return d;
}
```

Program manager. Java

```
private void solveECriterion()
{
    String result = "";
    //Design Matrix 1
    DataMatrix matTranspose = DataMatrix.transpose(curProblem.designMatrix1);
    //DataMatrix infoMat1 = curProblem.designMatrix1.multiplyBy(matTranspose);
    DataMatrix infoMat1 = matTranspose.multiplyBy(curProblem.designMatrix1);
    DataMatrix div = infoMat1.divideBy(curProblem.matrixSize);
    DataMatrix matInv = div.inverse();
    double eigens[] = matInv.eigenValue();
    double maxEigen1 = matMgr.maxValue(eigens);
    String v1 = "Eigen of Design 1 = " + maxEigen1; //DataMatrix.df.format(maxEigen1);

    //Design Matrix 2
    matTranspose = DataMatrix.transpose(curProblem.designMatrix2);
    //DataMatrix infoMat2 = curProblem.designMatrix2.multiplyBy(matTranspose);
    DataMatrix infoMat2 = matTranspose.multiplyBy(curProblem.designMatrix2);
    div = infoMat2.divideBy(curProblem.matrixSize);
    matInv = div.inverse();
    eigens = matInv.eigenValue();
    double maxEigen2 = matMgr.maxValue(eigens);
    String v2 = "Eigen of Design 2 = " + maxEigen2; //DataMatrix.df.format(maxEigen2);

    //compare
    if(maxEigen1 < maxEigen2){
        result = "Design Matrix 1 is E-optimal";
    }else if(maxEigen1 > maxEigen2){
        result = "Design Matrix 2 is E-optimal";
    }else if(maxEigen1 == maxEigen2){
        result = "Both Design Matrices are E-optimal";
    }
    createReport("E-Criterion",infoMat1,infoMat2,v1,v2,result);
}
}
```

3. Result/Implementation

Consider a quadratic response surface model for k = 2 and the two designs with 6 – points given below;

$$f(w) = a_0 + a_1 w_1 + a_2 w_2 + a_3 w_1^2 + a_4 w_2^2 + a_5 w_1 w_2, \quad w_1, w_2 = -1 \le w \le 2$$

$$Y_1 = \begin{pmatrix} -1 & 1 \\ 0 & -1 \\ 2 & 0 \\ 0 & 2 \\ -1.4 & 0 \\ 0 & 1.4 \end{pmatrix}, \quad Y_2 = \begin{pmatrix} -1 & 1 \\ 0 & -1 \\ 2 & 0 \\ -1.4 & 2 \\ 0 & 1.4 \\ 1 & 0 \end{pmatrix}$$

Let D_1 and D_2 represent the design matrices for Y_1 and Y_2 respectively. From (7), the design matrices are given as;

$$D_1 = \begin{pmatrix} 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 0 & -1 & 0 & 1 & 0 \\ 1 & 2 & 0 & 4 & 0 & 0 \\ 1 & 0 & 2 & 0 & 4 & 0 \\ 1 & -1.4 & 0 & 1.96 & 0 & 0 \\ 1 & 0 & 1.4 & 0 & 1.96 & 0 \end{pmatrix}, \quad D_2 = \begin{pmatrix} 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 0 & 1 & 0 \\ 1 & 2 & 0 & 4 & 0 & 0 \\ 1 & -1.4 & 2 & 1.96 & 4 & -2.8 \\ 1 & 0 & 1.4 & 0 & 1.96 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Information matrix for design 1 and design 2 is given as;

$$D_1 = \begin{pmatrix} 6 & -0.4 & 3.4 & 7 & 8 & -1 \\ -0.4 & 6.96 & -1 & 4.2 & -1 & 1 \\ 3.4 & -1 & 7.96 & 1 & 10.8 & -1 \\ 7 & 4.2 & 1 & 21 & 1 & -1 \\ 8 & -1 & 10.8 & 1 & 22 & -1 \\ -1 & 1 & -1 & -1 & -1 & 1 \end{pmatrix}, D_2 = \begin{pmatrix} 6 & 0.6 & 3.4 & 8 & 8 & 3.8 \\ 0.6 & 7.96 & -3.8 & 5.2 & -6.6 & -4.92 \\ 3.4 & -3.8 & 7.96 & 5 & 10.8 & 6.6 \\ 8 & 5.2 & 5 & 22 & 9 & 6.6 \\ 8 & -6.6 & 10.8 & 9 & 22 & 12.2 \\ 3.8 & -4.92 & 6.6 & 6.6 & 12.2 & 8.84 \end{pmatrix}$$

Design 1: Eigenvalue (λ_1) = 3.8167 1.7443 0.3394 0.0860 0.0340 -0.0000

Max (λ_1^{-1}) = 29.4118

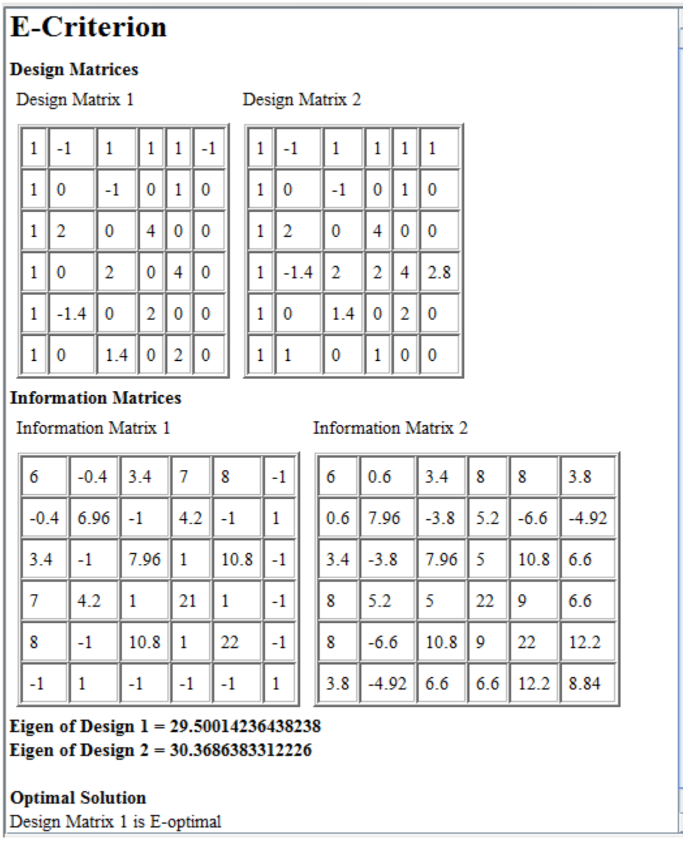
Design 2: Eigenvalue (λ_2) = 4.2628 1.5841 0.1237 0.0468 0.0330 0.0000

Max (λ_2^{-1}) = 30.3030

Min {max (λ^{-1}) } = 29.4118

Hence, design 1 is E – optimal.

From the above program, the result is obtained as;



E-Criterion

Design Matrices

Design Matrix 1

1	-1	1	1	1	-1
1	0	-1	0	1	0
1	2	0	4	0	0
1	0	2	0	4	0
1	-1.4	0	2	0	0
1	0	1.4	0	2	0

Design Matrix 2

1	-1	1	1	1	1
1	0	-1	0	1	0
1	2	0	4	0	0
1	-1.4	2	2	4	2.8
1	0	1.4	0	2	0
1	1	0	1	0	0

Information Matrices

Information Matrix 1

6	-0.4	3.4	7	8	-1
-0.4	6.96	-1	4.2	-1	1
3.4	-1	7.96	1	10.8	-1
7	4.2	1	21	1	-1
8	-1	10.8	1	22	-1
-1	1	-1	-1	-1	1

Information Matrix 2

6	0.6	3.4	8	8	3.8
0.6	7.96	-3.8	5.2	-6.6	-4.92
3.4	-3.8	7.96	5	10.8	6.6
8	5.2	5	22	9	6.6
8	-6.6	10.8	9	22	12.2
3.8	-4.92	6.6	6.6	12.2	8.84

Eigen of Design 1 = 29.50014236438238
Eigen of Design 2 = 30.3686383312226

Optimal Solution

Design Matrix 1 is E-optimal

Fig. 2. The E - optimality of two designs

From the analysis of the two methods, the result is summarized in Table 1

Table 1. The result for the new and existing method

Design	Existing method (λ_{EM})	New method (λ_{NM})
1	29.5001	29.4118
2	30.3686	30.3030

In comparing the two methods, we observed a little variation in fractional part which intuitively proven that the latter is better than the former.

4. Conclusion

Based on the above result, the minimum maximum eigenvalue of the dispersion matrix for design 1 is smaller than that of the design matrix 2 which satisfied the condition for E – optimality criterion. Therefore, the design (y_1) is E – optimal. It is obvious from the illustration that the algorithm technique for obtaining E – optimality is better than the existing method by way of minimizing errors. The newly algorithm technique is limitation to quadratic response model with two predictor variables. It is suggested that more than two predictors of quadratic response surface design and higher design with E – optimal can be experimented for further study.

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Authors' Profiles

Ukeme Paulinus Akra is a Lecturer at the Department of Statistics, Akwa Ibom State University, Ikot Akpaden, Mkpat Enin. He had his Ph.D in Statistics (Experimental Design), M.Sc (Statistics), B.Sc (Maths/Stats) at the University Calabar, Calabar, Ngieria, and ND (Maths/Stats) at Akwa Ibom State Polytechnic, Ikot Osurua, Ikot Ekpene. He research interest is Design of Experiment, Block Design, Response surface, Optimal design and Multivariate analysis. However, he research interest is not limited to the above - mentioned areas. He mentored many undergraduate and postgraduate students and other researchers in the field. He has published many papers in peer – reviewed Journals and conferences. He is a reviewer in many reputable Journals.

Edet Effiong Bassey is a Lecturer and a researcher at the Department of Statistics, University of Calabar, Calabar, Nigeria. He obtained his B.Sc. (Maths/Stats) from Cross River University of Technology (CRUTECH), Calabar and M.Sc (Statistics) at University of Calabar, Calabar, Nigeria. He is currently on his Doctorate degree in Statistics at Ignatius Ajuru University of Education, Port Harcourt, Nigeria. His research interest is Multivariate analysis, Experimental design and Operation research.

Offong Edet Ntekim is a Lecturer and a researcher at the Department of Mathematics, University of Calabar, Calabar, Nigeria. He obtained his B.Sc (Maths/Stats) and M.Sc (Maths) from University of Calabar, Calabar, Nigeria. He is currently doing his Doctorate degree in Applied Mathematics from the same University. He research interests is Differential Equation, Partial Differential Equation, Integral Equation and Combinatoric. He served as a coordinator; Mathematics for Social Sciences, Advance Mathematics and presently serving as undergraduate Project Coordinator. He was served as a resource person at FGN – UBE 2012 Teachers Professional Development Program. He has many publications in both foreign and local journals and is a member of Mathematical Association of Nigeria.

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