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ON A – OPTIMILITY DESIGN FOR SOLVING SECOND - ORDER RESPONSE SURFACE DESIGN PROBLEMS

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ABSTRACT

Optimality criteria is a mechanism used for measuring the betterment of a design. Several traditional optimality criteria such as A, D, E, T, IV, etc, are the classes of optimal criterion for the test of optimum design. A – Optimality criterion as one of the traditional alphabetical criterion is used to examine the right selection of a design using second – order response surface models. In this paper, an algorithm and flowchart in line with a program to solve A – optimal design problem using second – order response surface model are developed. This paper also aimed to juxtaposing the accuracy between the manual and the programming technique in solving A – optimal problem. A six points of two designs with two explanatory variables were formulated to test the two methods. The result shows that the programming technique outperformed better than the manual method and it also minimizes error.

Keywords: Response surface, Optimal design, A – Optimum, Second-order model

INTRODUCTION

Response Surface Design (RSD) is an applied statistical and mathematical technique used for solving problems of responses influenced by various variables (Montgomery, 2013). In other words, response surface design is a design test technique established for the aim of detecting or obtaining the optimum response around the defined limit of the factors. RSD models are used to examine the influence of various expository factors on a dependent variable by estimating complex functional correlations using linear or quadratic multivariate polynomial regression models, which are usually designated as first or second - order response surface models (Jones and Nachtsheim, 2011). These designs are more effective to fit a second – order response surface model for the response and it is an integral part for constructing a model for modeling curve surface analysis (Myers et al., 2009). This method is necessary where different explanatory variables controls a response variable and it has become a standard statistical tool for analyzing experimental data. The independent variables are supposed to be continuous and influenced by the experimenter or designers (Victorbabu and Surekha, 2013). An appropriate model equation estimating the true functional correlation between the response variable and the set of independent variables to obtain rotatability in central composite design under response surface design was proposed by (Akpan and Akra, 2017)

Optimal designates a finding and controlling process that need to determine the optimum possible design selection. Optimal design is usually considered as the design process that seeks the "best" possible solution(s) for a mechanical structure, device, or system, satisfying the requirements and leading to the "best" performance, through optimization techniques. It also refers to the design points that best satisfy objective(s) which are in contrast to non-optimal design (Dieter and Schmidt, 2009). Optimal designs admit the evaluation of parameters without bias and with a least possible dispersion in the statistical model of an experiment. A design that is not optimal needs a larger number of experimental runs to estimate the parameters with the same precision as an optimal design. Practically, optimal design helps in reducing the costs of experimentation.

The optimality of a design is based on the statistical model and is estimated with respect to a statistical criterion, which is associated with the variance-matrix of the estimator. Optimal design for a bivariate efficacy-safety model when both responses are continuous is considered by (Magnusdottir, 2013; Schorning et al., 2017). A complete objective of optimality conditions is significant comprehend the performance of several numerical techniques (Jasbir, 2012). An algorithm and a program was developed to solve E – optimality criterion, where the result outperformed better than the manual traditional known method (Akra, et al., 2024). Optimal experimental design has as an aim to quest the optimal ways to perform an experiment considering the available resources and the statistical model (Magnusdottir and Nyquist, 2015; Magnusdottir, 2016). 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 (Renata, 2021). Relationship between E-, D- and A – optimality criteria and their relative efficiency to determine the best optimality criterion was established by (Akpan et al., 2017). 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 (Eric and Kwabena, 2022). E-optimal designs for the second-order response surface models on the k-dimensional cube and ball was studied by (Holger and Yuri, 2014).

In view of all the prominent contributions on A – optimality by different scholars, none has developed an easiest and simplified approach different from the manual traditional way of obtaining A – optimal design for second - order response surface model. Based on this fact, this paper seek to fill the shortfall by establishing a simplified algorithm and a program to compute A – optimal design. The significance of this algorithmic approach helps to reduce error in approximation than the existing manual method and also ease the computation of the above - mentioned optimality criterion.

Second - order response surface model

Response surfaces are mostly estimated by a second-order polynomial model as the higher-order effects are commonly insignificant. A second-order model for p - number of factors can be written as in Equation 1. The 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 $p*\frac{(p-1)}{2}$ interaction terms. To fit a second - order model, it require a design that several number of runs than the first - order design used to move close to the optimum. The second - order response surface model, in other words, known as a second-order response surface equation model denoted as;

$$y_r = \eta_o + \sum_{v=1}^{p}\eta_v t_v + \sum_{v=1}^{p}\eta_{vv}t_{vv}^2 + \sum_{v<j}^{p}\eta_{vj}\, t_v t_j + \varepsilon \quad (1)$$

Where b designated the $n\times 1$ vector of a non-quadratic parameter estimates, and t^{th} entry for all the parameters$\hat{\eta}_v$'s in the model. Let ηdesignate$n\times n$matrix with t^{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;

$$\hat{y}_v = \hat{\eta}_0 + t'r + t'\eta t \quad (2)$$

Equation (2) can be written as;

$$t = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ \vdots\ t_n \end{bmatrix}, r = \begin{bmatrix} \hat{\eta}_1 \\ \hat{\eta}_2 \\ \vdots \\ \vdots\ \hat{\eta}_n \end{bmatrix} \text{and}$$

$$\eta = \begin{bmatrix} \hat{\eta}_{11}\ \hat{\eta}_{12}/2 \cdots \hat{\eta}_{1n}/2 \\ \hat{\eta}_{12}/2\hat{\eta}_{22} \rightleftarrows\rightleftarrows\rightleftarrows\rightleftarrows\rightleftarrows\rightleftarrows\rightleftarrows\rightleftarrows \cdots\cdots \\ \vdots\vdots\vdots\vdots \\ \vdots\vdots\vdots\vdots \\ \hat{\eta}_{1n}/2 \cdots\cdots \hat{\eta}_{nn} \end{bmatrix}$$

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

$$t_s = -\frac{1}{2}\eta^{-1}r \quad (3)$$

Formation of Design Matrix for E - Optimal Criteria

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

$$f(t_1,t_2) = b_0 + b_1t_1 + b_2t_2 + b_3t_1^2 + b_4t_2^2 + b_5t_1t_2 + \ldots, a_{p-1}b_pt_it_j + e_{ij} \quad (4)$$

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

$$T = \begin{pmatrix} t_{11} & t_{12} & t_{13} & . & . & . & t_{1p} \\ t_{21} & t_{22} & t_{23} & . & . & . & t_{2p} \\ t_{31} & t_{32} & t_{33} & . & . & . & .t_{3p} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ t_{n1} & t_{n2} & t_{n3} & . & . & . & t_{np}. \end{pmatrix} \quad (5)$$

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

$$T = \begin{pmatrix} t_{11} & t_{21} \\ t_{21} & t_{22} \\ t_{31} & t_{32} \\ t_{41} & t_{42} \\ t_{51} & t_{52} \end{pmatrix} \quad (6)$$

For p = 2 the second - order response surface of equation (4) becomes;

$$f(t_1,t_2) = b_0 + b_1t_1 + b_2t_2 + b_3t_1^2 + b_4t_2^2 + b_5t_1t_2 + e \quad (7)$$

Design matrix of (7) is given by;

$$T = \begin{pmatrix} 1 & t_{11} & t_{12} & t_{11}^2 & t_{12}^2 & t_{11}t_{12} \\ 1 & t_{21} & t_{22} & t_{21}^2 & t_{22}^2 & t_{21}t_{22} \\ 1 & t_{31} & t_{32} & t_{31}^2 & t_{32}^2 & t_{31}t_{32} \\ 1 & t_{41} & t_{42} & t_{41}^2 & t_{42}^2 & t_{41}t_{42} \\ 1 & t_{51} & t_{52} & t_{51}^2 & t_{52}^2 & t_{51}t_{52} \\ 1 & t_{61} & t_{62} & t_{61}^2 & t_{62}^2 & t_{61}t_{62} \end{pmatrix} \quad (8)$$

Information matrix for the design

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

$$\tau(\varsigma) = \begin{cases} T^1T \\ \sum_{\underline{t}\in T} tt' \end{cases} \quad (9)$$

Normalized information matrix of (5) is designated as;

$$\tau(\varsigma) = \begin{cases} \frac{Np(T^1T)}{N^2}\frac{\sigma_t^2}{p} \\ p\sum_{t\in T} tt'h_v\frac{\sigma_t^2}{p} \end{cases} \quad (10)$$

Where $\frac{Np(T^1T)}{N^2}\frac{\sigma_t^2}{p}$ = if the weight are uniform or uniform probability measure.

$p\sum_{t\in T} tt'h_v\frac{\sigma_t^2}{p}$ = Non uniform probability measure and N = size of the matrix and p = number of factors

Conceptualization of Optimality Criteria in second - order response surface design

Design optimality is a variance-type criterion that involves optimizing various individual properties of the (T^1T)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 A – optimal design.

A-Optimality design for second – order response surface design

A nonlinear model of the form below is considered;

$$E(y/w) = f^T(w)\theta \quad (11)$$

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.

Hence, this criterion minimizes the trace of the dispersion matrix, $\tau(\varsigma)^{-1}$. Symbolically, a design $\varsigma$is said to be A-optimal if it gives $Min\{tr\tau(\varsigma)^{-1}\}$

A measure of the relative efficiency of design 1 to design 2 according to the A-rotatable criterion is given by;

$$A_e = \frac{tr[\tau_2(\varsigma)^{-1}]}{tr[\tau_1(\varsigma)^{-1}]}\times 100 \quad (12)$$

An algorithm for obtaining A – optimality Criterion

The following steps are adopted to obtain A – optimal design;

Step 1: Select the matrix called $(\varsigma_1)$for the first design.

Step 2: Take the transpose ofς_1 called ς_1'

Step 3: Take the product of the matrices $(\varsigma_1')$and (ς_1)called information matrix$\tau(\varsigma)$.

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

Step 5: Obtain the trace of the resulting matrix in (4).

Step 6: Repeat the same steps of (1) – (5) for the second design(ς_2).

Step 7: Hence, the minimum trace of the design i.e. $Mintrace(\tau(\varsigma))$ is A – optimal Criterion

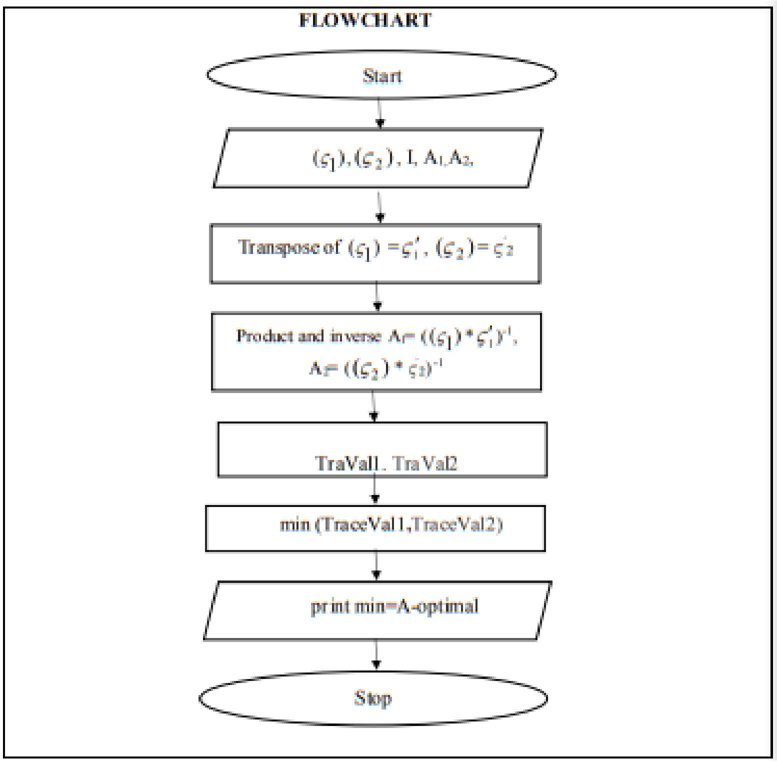


Figure 1: Flowchart of the algorithm for obtaining A- optimality criterion

Program Source for A – optimal design

```
MatrixManager.java
package dm;

importjama.Matrix;

public class MatrixManager
{
    public double matrixTrace(DataMatrix dm)
    {
        Matrix m = new Matrix(dm.elements);
        double d = m.trace();
        return d;
      }

    public double maxValue(double d[])
    {
        double v = d[0];
        for(inti = 0;i <d.length;i++){
          if(d[i] > v){
            v = d[i];
          }
        }
      return v;
    }
}

Program managé.
    private void solveACriterion()
    {
        String result = "";
        //Design Matrix 1
        DataMatrixmatTranspose =
        DataMatrix.transpose(curProblem.designMatrix1);
        //DataMatrix infoMat1 =
        curProblem.designMatrix1.multiplyBy(matTranspose);
        DataMatrix infoMat1 =
        matTranspose.multiplyBy(curProblem.designMatrix1);
        double trace1 = matMgr.matrixTrace(infoMat1);
        String v1 = "Trace of Design 1 = " + trace1;
        //DataMatrix.df.format(trace1);

        //Design Matrix 2
        matTranspose =
        DataMatrix.transpose(curProblem.designMatrix2);
        //DataMatrix infoMat2 =
        curProblem.designMatrix2.multiplyBy(matTranspose);
        DataMatrix infoMat2 =
        matTranspose.multiplyBy(curProblem.designMatrix2);
        double trace2 = matMgr.matrixTrace(infoMat2);
        String v2 = "Trace of Design 2 = " + trace2;
        //DataMatrix.df.format(trace2);

        //compare
        if(trace1 < trace2){
            result = "Design Matrix 1 is A-optimal";
        }else if(trace1 > trace2){
            result = "Design Matrix 2 is A-optimal";
        }else if(trace1 == trace2){
            result = "Both Design Matrices are A-optimal";
        }
        createReport("A-
        Criterion",infoMat1,infoMat2,v1,v2,result);
    }
```

RESULTS AND DISCUSSION

Consider a second - order response surface model for p = 2 and 6 – points of two designs given below;

$$f(t) = b_0 + b_1t_1 + b_2t_2 + b_3t_1^2 + b_4t_2^2 + b_5t_1t_2, t_1, t_2 = -1 \le t \le 2$$

$$X_1 = \begin{pmatrix} -1 & 1 \\ 0 & -1 \\ 2 & 0 \\ 0 & 2 \\ -1.4 & 0 \\ 0 & 1.4 \end{pmatrix}, \quad X_2 = \begin{pmatrix} -1 & 1 \\ 0 & -1 \\ 2 & 0 \\ -1.4 & 2 \\ 0 & 1.4 \\ 1 & 0 \end{pmatrix}$$

Let D_1 and D_2 represent the design matrices for X_1 and X_2 respectively. From (7), the design matrices are given as;

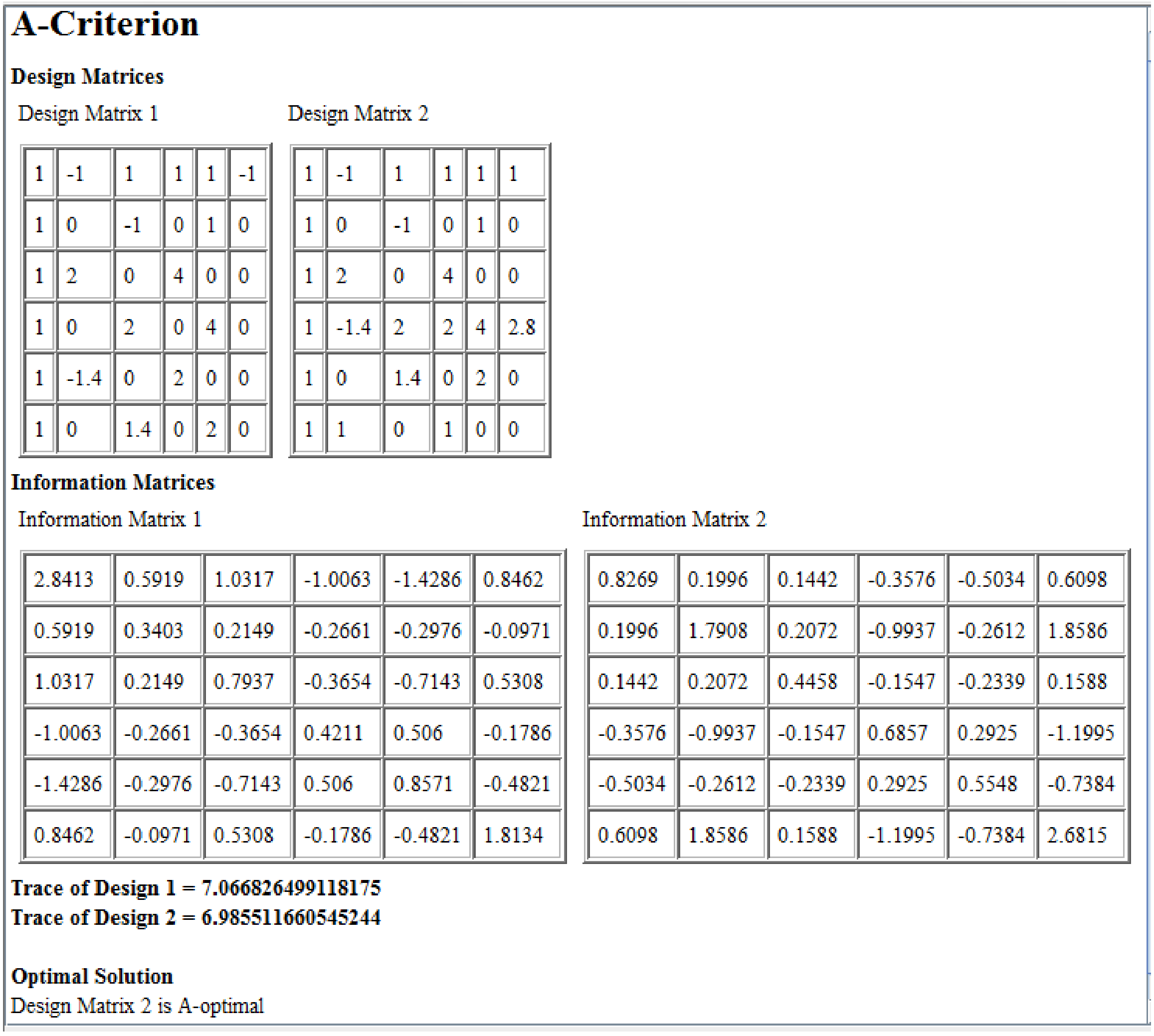
$$D_1 = \begin{pmatrix} 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 0 & -1 & 0 & 1 & 0 \\ 1 & 2 & 0 & 4 & 0 & 0 \\ 1 & 0 & 2 & 0 & 4 & 0 \\ 1 & -1.4 & 0 & 1.96 & 0 & 0 \\ 1 & 0 & 1.4 & 0 & 1.96 & 0 \end{pmatrix}, \qquad D_2 = \begin{pmatrix} 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 0 & 1 & 0 \\ 1 & 2 & 0 & 4 & 0 &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

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

$$D_1 = \begin{pmatrix} 2.8413 & 0.5919 & 1.0317 & -1.0063 & -1.4286 & 0.8462 \\ 0.5919 & 0.3403 & 0.2149 & -0.2661 & -0.2976 & -0.0971 \\ 1.0317 & 0.2149 & 0.7937 & -0.3654 & -0.7143 & 0.5308 \\ -1.0063 & -0.2661 & -0.3654 & 0.4211 & 0.506 & -0.1786 \\ -1.4286 & -0.2976 & -0.7143 & 0.506 & 0.8571 & 0.4821 \\ 0.8462 & -0.0971 & 0.5308 & -0.1786 & -0.4821 & 1.8134 \end{pmatrix},$$

$$D_2 = \begin{pmatrix} 0.8269 & 0.1996 & 0.1442 & -0.3576 & -0.5034 & 0.6098 \\ 0.1996 & 1.7908 & 0.2072 & -0.9937 & -0.2612 & 1.8586 \\ 0.1442 & 0.2072 & 0.4458 & -0.1547 & -0.2339 & 0.1588 \\ -0.3576 & -0.9937 & -0.1547 & 0.6857 & 0.2925 & -1.1995 \\ -0.5034 & -0.2612 & -0.2339 & 0.2925 & 0.5548 & -0.7384 \\ 0.6098 & 1.8586 & 0.1588 & -1.1995 & -0.7384 & 2.6815 \end{pmatrix}$$

Design 1: Trace(D_1) = 7.0669
Design 2: Trace(D_2) = 6.9855
Min trace {D} = 6.9855
Hence, design 2 is A – optimal.
From the above program, the result shows analysis of the two information matrices obtained from the six point designs using second – order response surface model. Hence, by definition of A – optimal design, the minimum trace of the information matrix gives the result of the design. Therefore, design 2 is A – optimal design as shown in Fig 2.



A-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

2.8413	0.5919	1.0317	-1.0063	-1.4286	0.8462
0.5919	0.3403	0.2149	-0.2661	-0.2976	-0.0971
1.0317	0.2149	0.7937	-0.3654	-0.7143	0.5308
-1.0063	-0.2661	-0.3654	0.4211	0.506	-0.1786
-1.4286	-0.2976	-0.7143	0.506	0.8571	-0.4821
0.8462	-0.0971	0.5308	-0.1786	-0.4821	1.8134

Information Matrix 2

0.8269	0.1996	0.1442	-0.3576	-0.5034	0.6098
0.1996	1.7908	0.2072	-0.9937	-0.2612	1.8586
0.1442	0.2072	0.4458	-0.1547	-0.2339	0.1588
-0.3576	-0.9937	-0.1547	0.6857	0.2925	-1.1995
-0.5034	-0.2612	-0.2339	0.2925	0.5548	-0.7384
0.6098	1.8586	0.1588	-1.1995	-0.7384	2.6815

Trace of Design 1 = 7.066826499118175
Trace of Design 2 = 6.985511660545244

Optimal Solution
Design Matrix 2 is A-optimal

Figure 2: The A - 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 (D_{EM})	New method(D_{NM})
1	7.0669	7.0668
2	6.9856	6.9855

Discussion
Second - order response surface model for p = 2 and 6 – points of two designs were considered for the analysis of both techniques (manual calculation and programming approach). Information matrices were formed in consonant with the A – optimality criterion and the results were obtained. The trace values of design 1 are 7.0669 and 7.0668 while the trace values of design 2 are 6.9856 and 6.9855. Therefore, the minimum trace occur in design 2.
In comparing the two methods, we observed a little variation in fractional part (i.e the new method differs from the existing method by 0.0001 and that the later approach has a minimum trace value which satisfied the condition of A – optimality criteria) which intuitively proven that the programming method of solving A – optimal design is better than the manual technique for solving second – order response surface design problem.

CONCLUSION
According to the above results, the minimum trace value of the dispersion matrix for design 2 is smaller than that of the design matrix 1 which fulfilled the postulate of A – optimum design criterion. Therefore the design (X_2) is A – optimal. It is very clear from the illustrations that the algorithmic approach for solving A – optimality problems surpass the existing manual method due to approximation and error minimization. In this paper, the newly algorithmic method is limited to second - order response surface model with two predictor variables. It is recommended that more explanatory variables higher than two variables be experimented using second – order response design to solve A – optimality problems for further study.

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