

# Comparative Analysis of the Existing and Modified Techniques for Solving Second Order Response Surface Design Problems

<sup>1</sup>Stephen Sebastian Akpan, <sup>2</sup>John Usen and <sup>3</sup>Thomas Adidaumbe Ugbe

<sup>1,2,3</sup>Department of Maths/Statistics and Computer Science, University of Calabar, Cross-River State, Nigeria

<sup>1</sup>[steveakpan@yahoo.com](mailto:steveakpan@yahoo.com), <sup>2</sup>[usen@yahoo.com](mailto:usen@yahoo.com) and [ugbe\\_thomas@yahoo.com](mailto:ugbe_thomas@yahoo.com)

## Abstract

Comparative analysis of the existing and the modified techniques for solving second-order response surface design problems is considered in this paper. The new technique proffers a better solution procedure with regards to the exploration of near-optimal factors settings as well as the location of the optimum as compared to the “gambling nature” of the already existing method which explores the optimal region with little or no guarantee of precision. Numerical illustration using a second order response surface design problem confirms this assertion.

**Key words:** Response Surface Design, Central Composite Design, Mean-Centre Algorithm, Newton-Raphson Algorithm, Steepest Ascent method, First order model.

## 1. Introduction

Response Surface Methodology is a collection of mathematical and statistical techniques for analysing problems where several factors assumed continuous and controllable by the process engineer with negligible error influence a response variable and the goal is to optimize the response, Montgomery [1995]. The method was invented by G.E.P Box and K.B. Wilson in 1951 primarily for optimizing processes. It usually starts with fitting First Order Models to Response Surface design problems in small regions remote from the optimum and progressively moves to the optimal region using the Method of Steepest Ascent or Descent as the case may be. The prompting to continue or discontinue the fitting of First-order models to the design problem is usually indicated by a Lack-of-Fit Test. If this test indicates inadequacy of First-order models, then Second-order models are fit to cater for

curvature, Cochran [2] and Montgomery [1]. This inadequacy also implies that we are near the optimum. In this event, the design problem becomes a Second-order Response Surface Design Problem but no more a First-order Response Surface Design Problem, Montgomery [1].

Designs used for fitting first and second order models in response surface methodology are called Response Surface Designs, Cochran [3] and Montgomery [1]. The ones used for fitting first order models are called First Order Designs while those used for fitting second order models are called Second Order Designs, Cochran [3]. The most commonly used first order design is the  $2^k$  - factorial design since it possesses the feature of rotation. While the most commonly used efficient second order design is the Central Composite Design, Montgomery [1] and Buyske and Trout [4]. This particular design is a  $2^k$  - factorial design augmented with centre and axial points Cochran [3], Draper et al. [5] and Wu and Yuan [6].

To explore for near-optimal factors settings in the optimal region especially in events where the process experiences spontaneous momentary shifts from the optimum the existing RSM procedure implements a canonical analysis. This procedure is unsure and involves gambling with near-optimal factors settings on the part of the process engineer. Akpan & Usen (2013) has proposed an improvement of the Response Surface Methodology procedure for combating this problem with improved precision. The proposed improvement utilized the fusion of two iterative algorithms – Newton-Raphson and Mean-Centre algorithms. In this paper, we have implemented both procedures on a selected case study based on which we have compared both procedures. The proposed procedure corrects the observed deficiency.

## **2. Numerical Illustration Using the Existing Procedure**

To illustrate the use of the existing and proposed procedures we shall consider the case study below from Montgomery [1].

Case Study:

A chemical engineer was interested in determining the operating conditions that maximize the yield of his process. Two controllable variables influenced process yield – Reaction time and Reaction Temperature. He was operating the process with reaction time of 35 minutes and reaction temperature of 155 degrees Fahrenheit which resulted in yields around 40 percent. Since it was unlikely that this region contained the optimum, a First Order Model was fit and the Method of Steepest Ascent applied. The engineer decided that the region of exploration for fitting the FOM should be (30, 40) minutes of reaction time and (150, 160) degrees Fahrenheit of reaction temperature.

To simplify the calculations, we coded the independent variables to a  $-1$  to  $1$  interval. Thus if  $\xi_1$  denotes the natural variable time and  $\xi_2$  denotes the natural variable temperature, then the coded variables are

$$x_1 = \frac{\xi_1 - 35}{5}, \quad x_2 = \frac{\xi_2 - 155}{5}$$

Table I shows the data display.

TABLE I – Process Data for Fitting of the first FOM

Natural Variables		Coded Variables		Responses
$\xi_1$	$\xi_2$	$x_1$	$x_2$	$y$
30	150	-1	-1	39.3
30	160	-1	1	40.0
40	150	1	-1	40.9
40	160	1	1	41.5
35	155	0	0	40.3
35	155	0	0	40.5
35	155	0	0	40.7
35	155	0	0	40.2
35	155	0	0	40.6

The design used to collect the data is a  $2^2$  factorial augmented by 5 centre points. Repeat observations at the centre were used to estimate the experimental error. The design is centred about the current operating conditions for the process. Using MINITAB we obtained the following:

The first regression equation is

$$y = 40.4 + 0.775 x_1 + 0.325 x_2$$

Predictor	Coef	SE Coef	T	P
Constant	40.4444	0.0573	705.99	0.000
x1	0.77500	0.08593	9.02	0.000
x2	0.32500	0.08593	3.78	0.009

S = 0.171863 R-Sq = 94.1% R-Sq(adj) = 92.1%

#### Analysis of Variance

Source	DF	SS	MS	F	P
Regression	2	2.8250	1.4125	47.82	0.000
Residual Error	6	0.1772	0.0295		
Lack of Fit	2	0.0052	0.0026	0.06	0.942
Pure Error	4	0.1720	0.0430		
Total	8	3.0022			

Source	DF	Seq SS
x1	1	2.4025
x2	1	0.4225

No evidence of lack of fit ( $P \geq 0.1$ ).

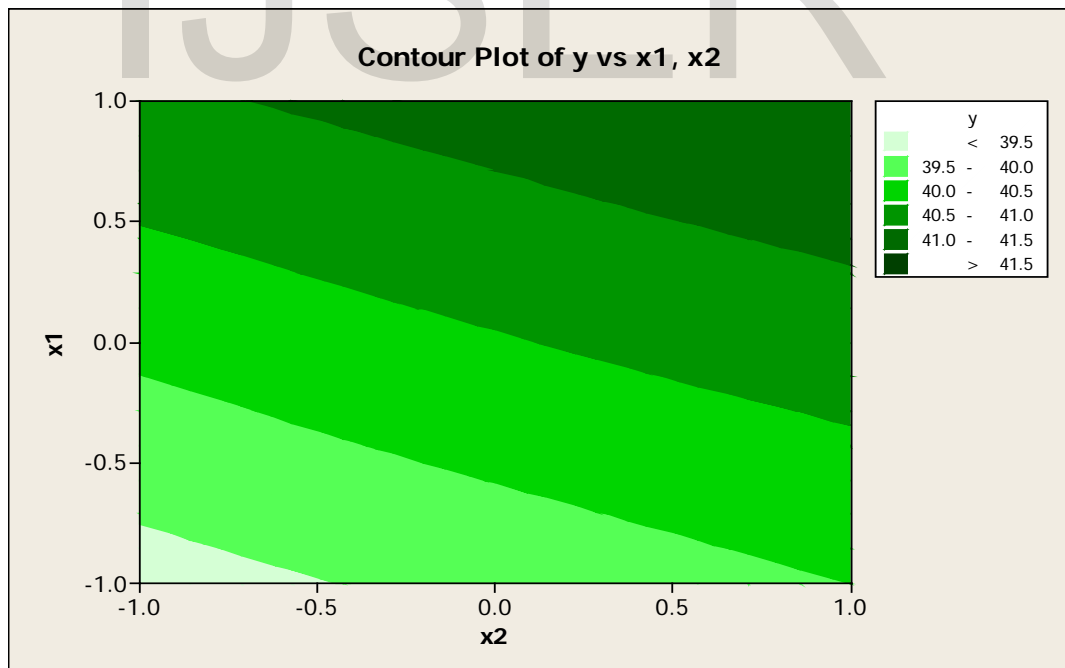


FIG. I - Contour graph for the First First-order Model

To move away from the design centre [the point  $(x_1 = 0, x_2 = 0)$ ] along the path of steepest ascent, we moved 0.775 units in the  $x_1$  - direction for every 0.325 units in the  $x_2$  - direction. Thus, the path of steepest ascent passed through the points  $(x_1 = 0, x_2 = 0)$  and had slope  $-\frac{x_2}{x_1} = \frac{0.325}{0.775}$ .

We decided to use five minutes of reaction time as the basic step size. Using the relationship between  $\xi_1$  and  $x_1$  we observed that five minutes of reaction time is equivalent to a step in the coded variable  $x_1$  of  $-\Delta x_1 = 1$ . Therefore, the steps along the path of steepest ascent are  $\Delta x_1 = 1.0000$  and  $-\Delta x_2 = \left(\frac{0.325}{0.775}\right)\Delta x_1 = 0.4194$ .

We computed points along this path and observed yields at these points until a decrease in response was noted. The results are shown in Table II. The steps are shown in both coded and natural variables. While the coded variables are easier to manipulate mathematically, the natural variables must be used in running the process. Increase in response was observed through the tenth step. However, the eleventh step produced a decrease in yield. Therefore, another first-order model had to be fit in the general vicinity of the point  $-(\xi_1 = 85, \xi_2 = 175.970)$ .

TABLE II – Steepest Ascent Experiment for the First First-order Model

	Coded variables		Natural variables		Response
	$x_1$	$x_2$	$\xi_1$	$\xi_2$	$y$
<i>Origin</i>	0	0	35	155	
$\Delta$	1.0000	0.4194			
<i>Origin + <math>\Delta</math></i>	1.0000	0.4194	40	157.097	41.0
<i>Origin + 2<math>\Delta</math></i>	2.0000	0.8388	45	159.194	41.9
<i>Origin + 3<math>\Delta</math></i>	3.0000	1.2582	50	161.291	43.1
<i>Origin + 4<math>\Delta</math></i>	4.0000	1.6776	55	163.388	43.7
<i>Origin + 5<math>\Delta</math></i>	5.0000	2.0970	60	165.485	44.1
<i>Origin + 6<math>\Delta</math></i>	6.0000	2.5164	65	167.582	44.3
<i>Origin + 7<math>\Delta</math></i>	7.0000	2.9358	70	169.679	52.1
<i>Origin + 8<math>\Delta</math></i>	8.0000	3.3552	75	171.776	63.8
<i>Origin + 9<math>\Delta</math></i>	9.0000	3.7746	80	173.873	78.3
<i>Origin + 10<math>\Delta</math></i>	10.0000	4.1940	85	175.970	80.3
<i>Origin + 11<math>\Delta</math></i>	11.0000	4.6134	90	178.067	79.2

A second FOM was fit about the point - ( $\xi_1 = 85, \xi_2 = 175$ ). The region of exploration for  $\xi_1$  was (80, 90) and for  $\xi_2$  it was - (170, 180). Thus the coded variables were

$$x_1 = \frac{\xi_1 - 85}{5}, \quad x_2 = \frac{\xi_2 - 175}{5}$$

The data is shown in Table III below.

TABLE III – Data for Fitting the Second First-order Model

Natural variables		Coded variables		Responses
$\xi_1$	$\xi_2$	$x_1$	$x_2$	$y$
80	170	-1	-1	76.5
80	180	-1	1	77.0
90	170	1	-1	78.0
90	180	1	1	79.5
85	175	0	0	79.9
85	175	0	0	80.3
85	175	0	0	80.0
85	175	0	0	79.7
85	175	0	0	79.8

Again, the design used to collect the data is a  $2^2$  factorial augmented by 5 centre points. Repeat observations at the centre were used to estimate the experimental error. The design was centred about the current operating conditions for the process. Using MINITAB we obtained the following:

The regression equation is

$$y = 79.0 + 1.00 x_1 + 0.500 x_2$$

Predictor	Coef	SE Coef	T	P
Constant	78.9667	0.4538	174.02	0.000
x1	1.0000	0.6807	1.47	0.192
x2	0.5000	0.6807	0.73	0.490

S = 1.36137 R-Sq = 31.0% R-Sq(adj) = 8.0%

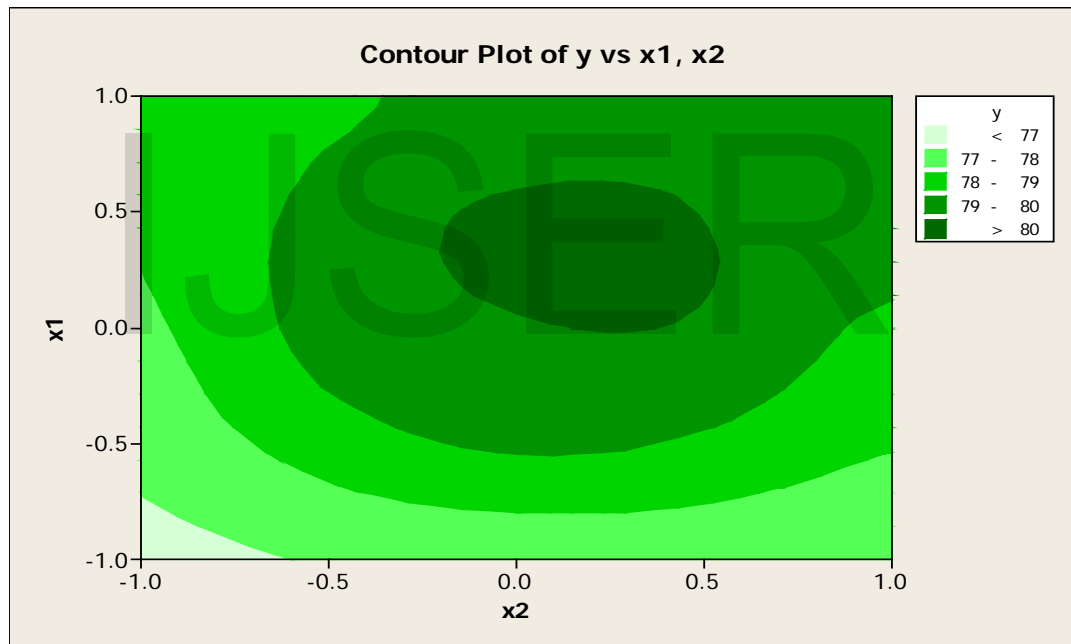
**Analysis of Variance**

Source	DF	SS	MS	F	P
Regression	2	5.000	2.500	1.35	0.328
Residual Error	6	11.120	1.853		
Lack of Fit	2	10.908	5.454	102.91	0.000
Pure Error	4	0.212	0.053		
Total	8	16.120			

Source	DF	Seq SS
x1	1	4.000
x2	1	1.000

**Lack of fit test**

Possible curvature in variable x1 (P-Value = 0.012)  
 Possible curvature in variable x2 (P-Value = 0.012)  
 Possible lack of fit at outer x-values (P-Value = 0.011)  
 Overall lack of fit test is significant at P = 0.011



**FIG. II - Contour graph for the Second First-order Model**

This curvature in the true surface may indicate that we are near the optimum. At this point, additional analysis had to be done to locate the optimum more precisely.

A second-order model in the variables -  $x_1, x_2$  cannot be fitted using the data in Table III. We decided to augment these data with enough points to fit a second-

order model. To do this, we obtained four observations at  $(x_1 = 0, x_2 = \pm 1.414)$  and  $(x_1 = \pm 1.414, x_2 = 0)$ . The complete data set is shown in Table IV.

TABLE IV – Central Composite Design for the Case Study

Natural Variables		Coded Variables		Responses
$\xi_1$	$\xi_2$	$x_1$	$x_2$	$y$
80	170	-1	-1	76.5
80	180	-1	1	77.0
90	170	1	-1	78.0
90	180	1	1	79.5
85	175	0	0	79.9
85	175	0	0	80.3
85	175	0	0	80.0
85	175	0	0	79.7
85	175	0	0	78.4
92.07	175	1.414	0	78.4
77.93	175	-1.414	0	75.6
85	182.07	0	1.414	78.5
85	167.93	0	-1.414	77.0

Using MINITAB we obtained the following:

The regression equation is

$$y = 79.9 + 0.995 x_1 + 0.515 x_2 - 1.38 x_1^2 - 1.00 x_2^2 + 0.250 x_1 x_2$$

Predictor	Coef	SE Coef	T	P
Constant	79.9400	0.1191	671.26	0.000
x1	0.99505	0.09415	10.57	0.000
x2	0.51520	0.09415	5.47	0.001
x1 <sup>2</sup>	-1.3764	0.1010	-13.63	0.000
x2 <sup>2</sup>	-1.0013	0.1010	-9.92	0.000
x1x2	0.2500	0.1331	1.88	0.103

S = 0.266290 R-Sq = 98.3% R-Sq(adj) = 97.0%

Analysis of Variance

Source	DF	SS	MS	F	P
Regression	5	28.2467	5.6493	79.67	0.000
Residual Error	7	0.4964	0.0709		
Lack of Fit	3	0.2844	0.0948	1.79	0.289
Pure Error	4	0.2120	0.0530		
Total	12	28.7431			



Source	DF	Seq SS
x1	1	7.9198
x2	1	2.1232
x1^2	1	10.9816
x2^2	1	6.9721
x1x2	1	0.2500

No evidence of lack of fit ( $P \geq 0.1$ ).

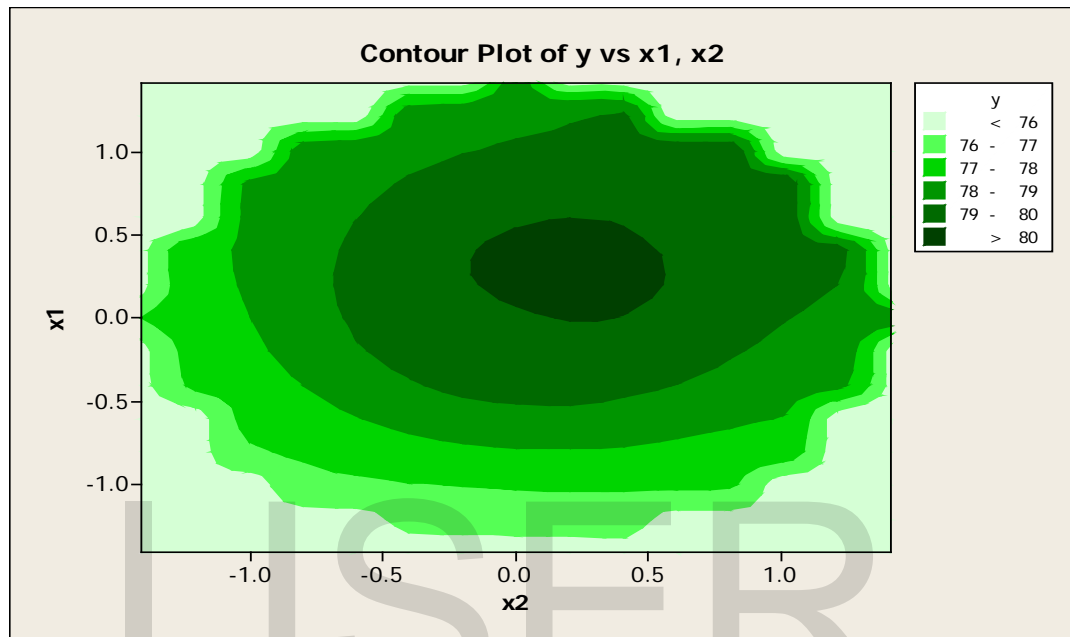


FIG. III - Contour graph for the Second-order Model

To obtain the optimum operating condition using the existing procedure, we recall that the second-order model is

$$\hat{y} = 79.9 + 0.995x_1 + 0.5151x_2 - 1.38x_1^2 - 1.00x_2^2 + 0.250x_1x_2$$

We now perform the canonical analysis. Note that

$$\mathbf{b} = \begin{pmatrix} 0.995 \\ 0.5151 \end{pmatrix} \quad \mathbf{B} = \begin{pmatrix} -1.38 & 0.125 \\ 0.125 & -1.00 \end{pmatrix}$$

The stationary point is

$$\mathbf{x}_0 = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b}$$

But

$$\mathbf{B}^{-1} = \begin{pmatrix} -0.732936326 & -0.09161704 \\ -0.09161704 & -1.01145213 \end{pmatrix}$$

$$\Rightarrow \mathbf{x}_0 = -\frac{1}{2} \begin{pmatrix} -0.732936326 & -0.09161704 \\ -0.09161704 & -1.01145213 \end{pmatrix} \begin{pmatrix} 0.995 \\ 0.5151 \end{pmatrix}$$

$$= -\frac{1}{2} \begin{pmatrix} -0.776463581 \\ -0.612157947 \end{pmatrix}$$

$$= \begin{pmatrix} 0.38823179 \\ 0.306078973 \end{pmatrix}$$

That is,  $\mathbf{x}_{1,0} = 0.38823179$  and  $\mathbf{x}_{2,0} = 0.306078973$ . In terms of the natural variables, the stationary point is

$$0.38823179 = \frac{\xi_1 - 35}{5} \quad 0.306078973 = \frac{\xi_2 - 175}{5}$$

which yields  $\xi_1 = 86.94115895$  and  $\xi_2 = 176.5303949$ . The predicted response at the stationary point is  $\hat{y}_0 = 80.17197596$  and is gotten as follows.

$$\hat{y}_0 = 79.9 + \frac{1}{2} (0.38823179 \quad 0.306078973) \begin{pmatrix} 0.995 \\ 0.5151 \end{pmatrix}$$

$$= 80.17197596$$

To further characterize the stationary point we obtain the canonical form of the fitted model. The eigen values  $\lambda_1$  and  $\lambda_2$  are the roots of the determinant equation

$$|\mathbf{B} - \lambda \mathbf{I}| = 0$$

$$\begin{vmatrix} -1.38 - \lambda & 0.125 \\ 0.125 & -1.00 - \lambda \end{vmatrix} = 0$$

which reduces to

$$\begin{aligned} \Rightarrow \lambda^2 + 2.38\lambda + 1.364375 &= 0 \\ \Rightarrow \lambda &= \frac{-2.38 \pm \sqrt{(2.38)^2 - 4(1)(1.364375)}}{2(1)} \\ &= -0.962568692 \quad \text{or} \quad -1.417431308 \end{aligned}$$

The roots of this quadratic equation are  $\lambda_1 = -0.962568692$  and  $\lambda_2 = -1.417431308$ . Thus the canonical form of the fitted model is

$$\hat{y} = 80.17197596 - 0.962568692w_1^2 - 1.417431308w_2^2$$

Since both  $\lambda_1$  and  $\lambda_2$  are negative and the stationary point is within the region of exploration, we conclude that the stationary point is a maximum.

Now, as an illustration, suppose that a process engineer could not operate the process at  $\xi_1 = 86.94115875$  and  $\xi_2 = 176.5303949$  owing to machine deterioration overtime. We now wish to “back away” from the stationary point to a point of lower cost, but without large losses in yield. The canonical form of the model indicates that the surface is less sensitive to yield loss in the  $w_1$  direction. Exploration of the canonical form requires converting points in the  $(w_1, w_2)$  space to points in the  $(x_1, x_2)$  space.

We illustrate the procedure using the fitted second-order model. For  $\lambda_1 = -0.962568692$ , we have

$$\begin{bmatrix} (-1.38 + 0.96256869) & 0.125 \\ 0.125 & (-1.00 + 0.96256869) \end{bmatrix} \begin{bmatrix} m_{11} \\ m_{21} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{aligned} -0.41743131m_{11} + 0.125m_{21} &= 0 \\ 0.125m_{11} - 0.03743131m_{21} &= 0 \end{aligned}$$

We wish to obtain the normalized solution to these equations, that is, the one for which  $m_{11}^2 + m_{21}^2 = 1$ . There is no unique solution to these equations, and it is most convenient to assign an arbitrary value of one of the unknowns, solve the system, and then normalize the solution. Letting  $m_{21}^* = 1$  we find

$m_{11}^* = 0.299450465$ . To normalize this solution divide  $m_{11}^*$  and  $m_{21}^*$  by -  
 $\sqrt{(m_{11}^*)^2 + (m_{21}^*)^2}$ .

$$\begin{aligned} \sqrt{(m_{11}^*)^2 + (m_{21}^*)^2} &= \sqrt{(0.299450465)^2 + 1^2} \\ &= 1.043872876 \end{aligned}$$

This yields the normalized solutions

$$m_{11} = \frac{m_{11}^*}{1.043872876} = \frac{0.299450465}{1.043872876} = 0.286864877$$

$$m_{21} = \frac{m_{21}^*}{1.043872876} = \frac{1}{1.043872876} = 0.957971054$$

which is the first column of the **M** matrix.

We now use -  $\lambda_2 = -1.417431308$ . Thus we have

$$\begin{aligned} \begin{bmatrix} (-1.38 + 1.417431308) & 0.125 \\ 0.125 & (-1.00 + 1.417431308) \end{bmatrix} \begin{bmatrix} m_{12} \\ m_{22} \end{bmatrix} &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ -0.037431308m_{12} + 0.125m_{22} &= 0 \\ 0.125m_{12} - 0.417431308m_{22} &= 0 \end{aligned}$$

Letting  $m_{22}^* = 1$  we find -  $m_{12}^* = -3.339450494$ . To normalize this solution, divide  
 $m_{12}^*$  and  $m_{22}^*$  by  $\sqrt{(m_{12}^*)^2 + (m_{22}^*)^2}$

$$\begin{aligned} \sqrt{(m_{12}^*)^2 + (m_{22}^*)^2} &= \sqrt{(-3.339450494)^2 + 1^2} \\ &= 3.485961789 \end{aligned}$$

This yields the normalized solutions

$$m_{12} = \frac{m_{12}^*}{3.48596179} = \frac{-3.339450494}{3.48596179} = -0.957971055$$

$$m_{22} = \frac{m_{22}^*}{3.48596179} = \frac{1}{3.48596179} = 0.286864877$$

which is the second column of the **M** matrix. Thus, we have

$$\mathbf{M} = \begin{bmatrix} 0.286864877 & -0.957971055 \\ 0.957971054 & 0.286864877 \end{bmatrix}$$

The relationship between the -  $\mathbf{w}$  and  $\mathbf{x}$  variables is

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0.286864877 & 0.957971054 \\ -0.957971055 & 0.286864877 \end{bmatrix} \begin{bmatrix} x_1 - 0.38823179 \\ x_2 - 0.306078973 \end{bmatrix}$$

If the process engineer wished to explore the response surface in the vicinity of the stationary point, he would determine appropriate points (by experience or gambling) to take observations in the  $(w_1, w_2)$  space and then use the above relationship to convert these points into the  $(x_1, x_2)$  space so that the runs may be made.

### 3. Numerical Illustration Using the Proposed Procedure

Define  $f(\mathbf{x}_t)$  the second-order model.

$$f(\mathbf{x}_t) = 79.9 + 0.995x_1 + 0.5151x_2 - 1.38x_1^2 - 1.00x_2^2 + 0.250x_1x_2$$

Define  $\mathbf{x}_0 = (x_{01}, x_{02}, x_{03}, \dots, x_{0n})$  the design centre.

$$\mathbf{x}_0 = (0, 0)$$

Define Optimum (Opt), the optimum yield gotten by classical technique.

$$Opt = 80.17192693$$

Step1: Input  $\mathbf{x}_0 = (x_{t1}, x_{t2}, x_{t3}, \dots, x_{tm})$  in  $f(\mathbf{x}_t)$

$$\mathbf{x}_0 = (0, 0)$$

Step 2: Evaluate  $\mathbf{E}_0 = f(\mathbf{x}_0)$  at  $\mathbf{x}_0$

$$\mathbf{E}_0 = f(\mathbf{x}_0) = 79.9$$

Step 3: Evaluate Allowed Error

$$\begin{aligned} AErr &= Opt - f(\mathbf{x}_0) \\ &= 80.17192693 - 79.9 \\ &= 0.27192693 \end{aligned}$$

Step 4: Evaluate the Jacobian gradient  $\mathbf{g}_0$  at the root  $\mathbf{x}_0$

$$\begin{aligned} \mathbf{g}_t = \nabla f(\mathbf{x}_t) &= \begin{pmatrix} \frac{\partial f(\mathbf{x}_t)}{\partial x_1} \\ \frac{\partial f(\mathbf{x}_t)}{\partial x_2} \end{pmatrix} \\ &= \begin{pmatrix} 0.995 - 2.76x_1 + 0.250x_2 \\ 0.5151 - 2.00x_2 + 0.250x_1 \end{pmatrix} \end{aligned}$$

At the point  $\mathbf{x}_0$

$$\mathbf{g}_0 = \nabla f(\mathbf{x}_0) = \begin{pmatrix} 0.995 \\ 0.5151 \end{pmatrix}$$

Step 5: Evaluate the Hessian  $\mathbf{H}_t$  and its inverse  $\mathbf{H}_t^{-1}$  at  $\mathbf{x}_t$

$$\mathbf{H}_t = \begin{pmatrix} \frac{\partial^2 f(\mathbf{x}_t)}{\partial x_1^2} & \frac{\partial^2 f(\mathbf{x}_t)}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f(\mathbf{x}_t)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(\mathbf{x}_t)}{\partial x_2^2} \end{pmatrix}$$

$$\Rightarrow \mathbf{H}_0 = \begin{pmatrix} -2.76 & 0.250 \\ 0.250 & -2.00 \end{pmatrix}$$

$$\mathbf{H}_t^{-1} = \begin{pmatrix} -0.366468163 & -0.04580852 \\ -0.04580852 & -0.505726065 \end{pmatrix}$$

Step 6: Evaluate the direction of improvement

$$\mathbf{U}_t = \Delta \mathbf{x}_t = \frac{\mathbf{H}_t^{-1} \mathbf{g}_t}{|\mathbf{H}_t^{-1} \mathbf{g}_t|}$$

Where

$$\|\mathbf{H}_t^{-1} \mathbf{g}_t\| = \sqrt{(x_1^*)^2 + (x_2^*)^2 + (x_3^*)^2 \cdots + (x_n^*)^2}$$

$$\begin{aligned} \mathbf{H}_0^{-1} \mathbf{g}_0 &= \begin{pmatrix} -0.366468163 & -0.04580852 \\ -0.04580852 & -0.505726065 \end{pmatrix} \begin{pmatrix} 0.995 \\ 0.5151 \end{pmatrix} \\ &= \begin{pmatrix} -0.38823179 \\ -0.306078973 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \|\mathbf{H}_0^{-1} \mathbf{g}_0\| &= \sqrt{(-0.38823179)^2 + (-0.306078973)^2} \\ &= 0.494376638 \end{aligned}$$

$$\mathbf{U}_0 = \frac{\begin{pmatrix} -0.38823179 \\ -0.306078973 \end{pmatrix}}{0.494376638}$$

$$= \begin{pmatrix} -0.785295582 \\ -0.619121029 \end{pmatrix}$$

Step 7: Evaluate the optimum step length  $\lambda_t$  in the direction  $\mathbf{U}_t$

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \lambda_t \mathbf{U}_t$$

$$\Rightarrow \mathbf{x}_t = \mathbf{x}_0 + \lambda_0 \mathbf{U}_0$$

$$= \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \lambda_0 \begin{pmatrix} -0.785295582 \\ -0.619121029 \end{pmatrix}$$

$$= (-0.785295582\lambda_0 \quad -0.619121029\lambda_0)$$

$$\Rightarrow f(\mathbf{x}_t) = f(-0.785295582\lambda_0 \quad -0.619121029\lambda_0)$$

$$\Rightarrow f(\mathbf{x}_t) = 79.9 - 1.100278346\lambda_0 - 1.112793769\lambda_0^2$$

$$\frac{\partial f(\mathbf{x}_t)}{\partial \lambda_0} = 0$$

$$\frac{\partial f(\mathbf{x}_t)}{\partial \lambda_0} = -1.100278346 - 2.225587538\lambda_0$$

$$\Rightarrow \lambda_0 = -\frac{1.100278346}{2.225587538}$$

$$= -0.494376575$$

$$\mathbf{x}_t = \begin{pmatrix} 0 \\ 0 \end{pmatrix} + (-0.494376575) \begin{pmatrix} -0.785295582 \\ -0.619121029 \end{pmatrix}$$

$$= \begin{pmatrix} 0.38823174 \\ 0.306078933 \end{pmatrix}$$

$$f(\mathbf{x}_t) = 80.17197596$$

This procedure gives us our optimum in one iterates. We now use the Mean-Centre algorithm with the design centre  $\mathbf{x}_0 = (0, 0)$  and the optimal setting  $\mathbf{x}^* = (0.38823174, 0.306078933)$  as initial approximations to explore for near-optimal settings in the optimal region. We have done this for two iterates.

Step 8: Explore for near-optimal settings in the optimal region

$$f(\mathbf{x}^*) = 80.1719759$$

Input  $\mathbf{x}_0 = (x_{01}, x_{02}, x_{03}, \dots, x_{0n})$  and  $\mathbf{x}^* = (x_1^*, x_2^*, x_3^*, \dots, x_n^*)$

$$\mathbf{x}_0 = (0, 0) \text{ and } \mathbf{x}^* = (0.38823174, 0.306078933)$$

Step 9: Evaluate  $\mathbf{x}_{t+1} = \frac{\mathbf{x}_t + \mathbf{x}^*}{2}$  at  $t = 0$

$$\mathbf{x}_1 = \frac{\mathbf{x}_0 + \mathbf{x}^*}{2} = \frac{\begin{pmatrix} 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0.38823174 \\ 0.306078933 \end{pmatrix}}{2} = \begin{pmatrix} 0.19411587 \\ 0.153039466 \end{pmatrix}$$



Step 10: Evaluate  $f(\mathbf{x}_{t+1})$  at  $t = 0$

$$f(\mathbf{x}_1) = 80.10398195$$

Step 11: If  $f(\mathbf{x}_{t+1}) < f(\mathbf{x}^*)$  increase  $t$  by one and go to step nine. Else, stop and set  $\mathbf{x}_{t+1} = \mathbf{x}^*$  if  $f(\mathbf{x}_{t+1}) = f(\mathbf{x}^*)$

Since  $f(\mathbf{x}_1) < f(\mathbf{x}^*)$  we go to step nine

$$\mathbf{x}_2 = \frac{\mathbf{x}_1 + \mathbf{x}^*}{2} = \frac{\begin{pmatrix} 0.19411587 \\ 0.153039466 \end{pmatrix} + \begin{pmatrix} 0.38823174 \\ 0.306078933 \end{pmatrix}}{2} = \begin{pmatrix} 0.291173805 \\ 0.229559199 \end{pmatrix}$$

Evaluating -  $f(\mathbf{x}_{t+1})$  at  $t = 1$  we have

$$f(\mathbf{x}_2) = 80.14569389$$

Since  $f(\mathbf{x}_2) < f(\mathbf{x}^*)$  the procedure continues until the termination criterion is satisfied. As we progress, in this routine, we obtain several near-optimal operating conditions before reaching the optimum itself.

#### 4. Comparison of the Existing and Proposed Procedures

Using the existing response surface technique the optimal operating condition is located with the Classical Derivative Technique whereas using the proposed improvement the optimal operating condition is located with the Newton-Raphson Technique. In this case, the design centre is used as a good initial approximation which guarantees that the optimum operating condition is obtained in one iterate or one more.

Exploration of optimal region for near-optimal settings is achieved with Canonical Transformation Procedure using the existing response surface technique. The existing procedure for achieving this is more or less a gambling process. Hence guarantees no precision. However, it is flexible. But exploration of optimal region for near-optimal settings is achieved with the Mean Centre Algorithm using the proposed improvement. It requires no transformation or gambling. Hence, it guarantees precision and gives near-optimal yields. However, it is not flexible.

## 5. Conclusion

An improvement of the existing response surface technique has been proposed for solving second-order response surface design problems. It comprises the fusion of two iterative algorithms - Newton-Raphson and Mean-Centre. The improvement unravels the design centre in the optimal region as a good initial approximation for starting the Newton-Raphson iteration; it also affords process engineers the ease and liberty of exploring near-optimal operating conditions in the optimal region.

## References

- [1] D. C. Montgomery, "Regression Analysis and Response Surface Methodology. Design and Analysis of Experiments," pp. 305-368, *New York: John Wiley & Sons*. Website: <http://www.stat.purdue.edu/~bacraig/note1/topic26.pdf>, 1995
- [2] W. G. Cochran and G. M. Cox "Response Surface Methodology, Experimental Design," *New York: John Wiley & Sons, Inc*, pp. 335-375, 1992.
- [3] S. Buyske and R. Trout, "Response Surface Methodology II," Website: <http://www.stat.rutgers.edu/home/buyske/591/Lect06.pdf>
- [4] N. R. Draper, D. K. J. Lin, S. Ghosh and Rao, C. R. Rao, "Response Surface Designs." *Handbook of Statistics - Elsevier Science B*, Vol. 13, pp. 343-374 Website: <http://www.personal.psu.edu/users/j/x/jxz203/im/linpub/HandbkStat/13Ch11.pdf>, 1996.
- [5] C. F. J. Wu and D. Yuan, "Construction of Response Surface Designs for Qualitative and Quantitative Factors." *IIQP Response Report RR-91-03* Website: <http://www.sciencedirect.com/science/article/pii/S0378375898000032>, 1998.