

Solution of optimization of a 3^K experimental settings using the technique of Newton Raphson

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ABSTRACT

Computer spreadsheet is used in solving optimization problem of several variables involving four factors that are varied at three levels each. The fitted equation obtained from the regression analysis has an $R-Sq = 98.5$ and $R-Sq (adj) = 96.9$. Multivariate optimization technique of Newton Raphson is used to locate the maximum of the function which contains several variables, starting at an initial points $(0,0,0,0)$, the final optimal and physically realistic economically acceptable combinations are found at $y = f(0.2, 0.1, 0.1, 0.1) 0.9684$. Which clearly demonstrated that the principle of normal curve is depicted. Recommendations are made which include the advantage of this method in determining or locating the optimum in case of minimum or saddle points in the response.

Key words: spreadsheets, Optimization, varied, response.RSM.

INTRODUCTION

As an important subject in the statistical design of experiments, the *Response Surface Methodology (RSM)* is a collection of mathematical and statistical techniques useful for the modeling and analysis of problems in which a response of interest is influenced by several variables and the objective is to optimize this response [1]. For example, the growth of a plant is affected by a certain amount of combination of a fertilizer like Nitrogen (N), Phosphorus (P), Sulphur (S) and Potassium (K). The plant can grow under any combination of a treatment. When treatments are from a continuous range of values, then a Response Surface Methodology is useful for developing, improving, and optimizing the response variable. In this case, if the plant growth y is the response variable as a function of x_1, x_2, x_3 and x_4 . It can be expressed as:

$$y = f(x_1, x_2, x_3, x_4) + e \quad \dots (1.0)$$

The variables N, P, S and K are independent variables where the response y depends on the various combination of them. The dependent variable y is a function of x_1, x_2, x_3 and x_4 , where $x_1 = N, x_2 = P, x_3 = S$ and $x_4 = K$, and the experimental error term is denoted as 'e'.

In most *RSM* problems, the true response function f is unknown. In order to develop a proper approximation for f , usually starts with a low-order polynomial in some small region.

If the response can be defined by a linear function of independent variables, then the approximating function is a first-order model. A first-order model with 2 independent variables can be expressed as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + e \quad \dots (2.0)$$

If there is a curvature in the response surface, which is clearly our own case, then a higher degree polynomial should be used. The approximating function with 2 variables is called a second-order model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + e \quad \dots (3.0)$$

In general all *RSM* problems use either one of these models. In each model, the levels of each factor are independent of the levels of other factors. [2]. The response surface analysis is performed by using the fitted surface. The response surface designs are types of designs for fitting response surface. Therefore, the objective of studying *RSM* can be accomplished by:

- (1) Understanding the topography of the response surface (local maximum, local minimum, ridge lines), and
- (2) Finding the region where the optimal response occurs.

The goal is to move rapidly and efficiently along a path to get to a maximum or a minimum response so that the response is optimized.

Computer spreadsheet is used throughout this work, using Newton's Raphson multivariate optimization procedure.[2]

METHODS

Steepest Ascent method and Steepest Descent Method:

The steepest ascent method and steepest descent method can be used to locate the maximum and the minimum respectively, of a function of several variables,[3] and [4].

The steepest ascent method is the most straightforward of the gradient search techniques. In this method we start with an initial point (x_0, x_0, x_0, x_0) , at this point; we determine the direction of the steepest ascent, that is, the gradient. We then search along the direction of the gradient, h_0 , until we find a maximum. The process is then repeated. The same approach can be used for minimization, in which case the terminology steepest descent is used. Starting at (x_0, x_0, x_0, x_0) the coordinates of any point in the gradient direction can be expressed as follows:

$$\begin{aligned} x_1 &= x_{10} + \frac{\partial f}{\partial x_1} h \\ x_2 &= x_{20} + \frac{\partial f}{\partial x_2} k \\ x_3 &= x_{30} + \frac{\partial f}{\partial x_3} l \\ x_4 &= x_{40} + \frac{\partial f}{\partial x_4} m \end{aligned} \quad \dots (5.0)$$

where h, k, l and m are distance along the I, j, k and l axis, and f is a function of x_1, x_2, x_3 and x_4 , and y , and the gradient is

$$\nabla f = \frac{\partial f}{\partial x_1} \hat{i} + \frac{\partial f}{\partial x_2} \hat{j} + \frac{\partial f}{\partial x_3} \hat{k} + \frac{\partial f}{\partial x_4} \hat{l} \quad \dots (6.0)$$

To find the maximum, we would search along the gradient direction, that is, along direction of this vector. The function can be expressed along the axis as;

$$f(x_1, x_2, x_3, x_4) = g(h, k, l, m) \quad \dots (7.0)$$

Now we have developed a function along the path of steepest ascent. How far along this path do we move?.

One approach might be to move along this path until we find the maximum of this function. This is the value of the step that maximizes $g(h, l, k, m)$ and hence, $f(x_1, x_2, x_3, x_4)$ in the gradient direction.

This method is called steepest ascent when an arbitrary step size h, l, k, m are used. If a value of a single step h^* is found that brings us directly to the maximum along the gradient direction, the method is called the optimal steepest ascent. [5], [6] and [7].

Whether a maximum or a minimum occurs involves not only the first partial derivatives of $f(x, x_2, x_3, x_4)$ with respect to x, x_2, x_3 and x_4 but also the second partial derivatives. Assuming that these derivatives are continuous at and near the point being evaluated, the determinant can be computed:

$$|H| = \frac{\partial^2 f}{\partial x_i^2} - \left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right)^2 \quad i \neq j. \text{H is Hessian Matrix} \quad \dots (8.0)$$

Three cases can occur:

1. If $|H| > 0$ and $\frac{\partial^2 f}{\partial x_i^2} > 0$, then $f(x, x_2, x_3, x_4)$ has a local minimum.
2. If $|H| > 0$ and $\frac{\partial^2 f}{\partial x_i^2} < 0$, then $f(x, x_2, x_3, x_4)$ has a local maximum. ... (9.0)
3. If $|H| < 0$, then $f(x, x_2, x_3, x_4)$ has a saddle point. (a saddle point is a point where all the first partial derivatives of a function vanish but which is not a local maximum or minimum.)

The quantity $|H|$ is equal to the determinant of a matrix made up of the second derivatives:

$$H = \begin{bmatrix} y_{11} & y_{21} & y_{31} & y_{41} \\ y_{12} & y_{22} & y_{32} & y_{42} \\ y_{13} & y_{23} & y_{33} & y_{43} \\ y_{14} & y_{24} & y_{34} & y_{44} \end{bmatrix}, \text{ is also known as the Hessian matrix of } f(x, x_2, x_3, x_4) \quad \dots (10.0a)$$

$$\text{Where } y_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j} \quad \dots (10.0b)$$

RESULTS

Application of Newton's procedure for multivariate optimization

The above named method is now applied to our valid and statistically fitted model as follows;

Recall from our seminar II that our selected model is the following:

$$Y = 0.975 + 0.129 X_1 + 0.0859 X_2 - 0.166 X_3 - 0.116 X_4 + 0.0367 X_1^2 - 0.0694 X_3^2 - 0.0170 X_4^2 - 0.150 X_1 X_2 - 0.0416 X_1 X_3 - 0.0842 X_1 X_4 - 0.0876 X_2 X_3 + 0.0569 X_2 X_4 - 0.0134 X_3 X_4. \quad \dots (11.0)$$

Now

$$\frac{\partial f}{\partial x_1} = y_1 = 0.129 + 0.0734 X_1 - 0.150 X_2 - 0.416 X_3 - 0.0842 X_4$$

$$\frac{\partial f}{\partial x_2} = y_2 = 0.0859 - 0.150 X_1 - 0.0876 X_3 + 0.0569 X_4$$

$$\frac{\partial f}{\partial x_3} = y_3 = -0.166 - 0.1388 X_3 - 0.416 X_1 - 0.0876 X_2 - 0.0134 X_4 \quad \dots (12.0)$$

$$\frac{\partial f}{\partial x_4} = y_4 = -0.116 - 0.0340X_4 - 0.0842X_1 + 0.0569X_2 - 0.0134X_3.$$

Now solving these equation using matlab 7.0, we obtain

$$\Rightarrow X_1 = -0.5539$$

$$X_2 = 0.1222$$

$$X_3 = 0.5866$$

$$X_4 = 02.0668$$

Since $Hx = y \Rightarrow x = yH^{-1}$

Therefore, we have our matrix as follows:

$$\begin{bmatrix} 0.0734 & -0.15 & -0.416 & -0.0842 \\ -0.15 & 0 & -0.0876 & 0.0569 \\ -0.416 & -0.0876 & -0.1388 & -0.0134 \\ -0.0842 & 0.0569 & -0.0134 & -0.034 \end{bmatrix} \quad \dots (13.0)$$

Now $\text{Det}(H) = 0.0012$

This implies that our determinant is positive. i.e. $\text{Det}(H) > 0$. It clearly implies that this is a case of local minimum since condition 1 is satisfied hence the need to apply Steepest ascent.

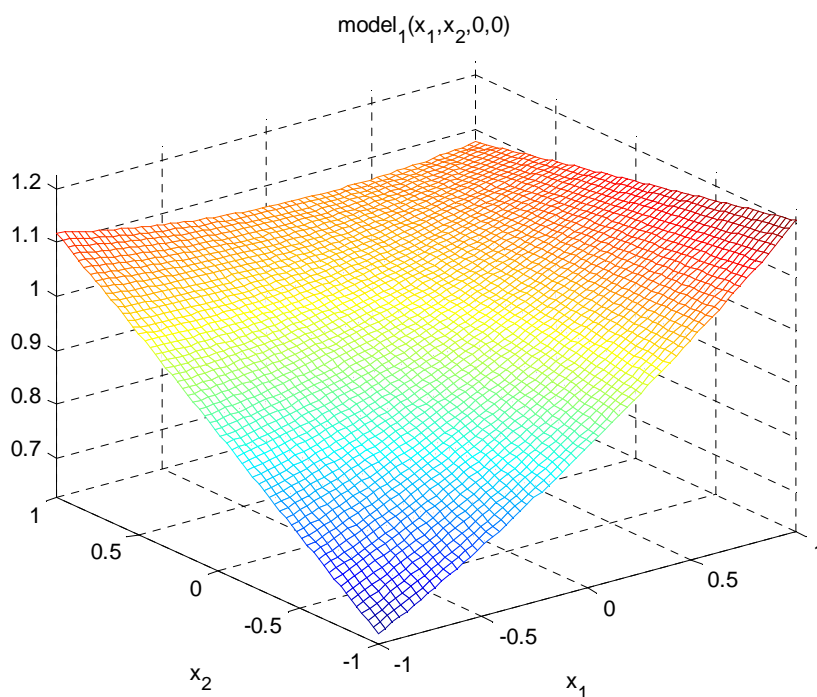


Figure 1: Plot of N and P interactions with Yield

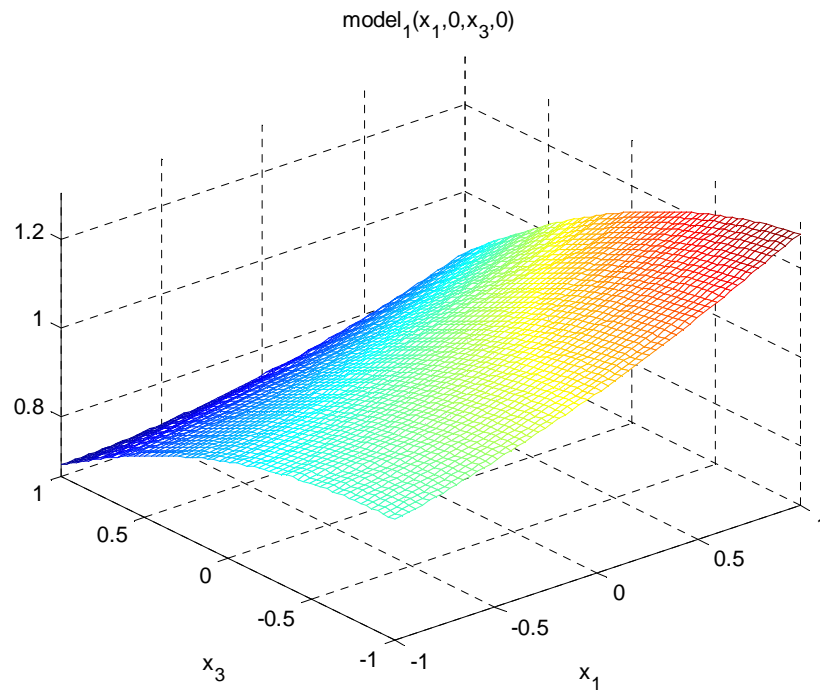


Figure 2 plot of N and S interaction against yield.

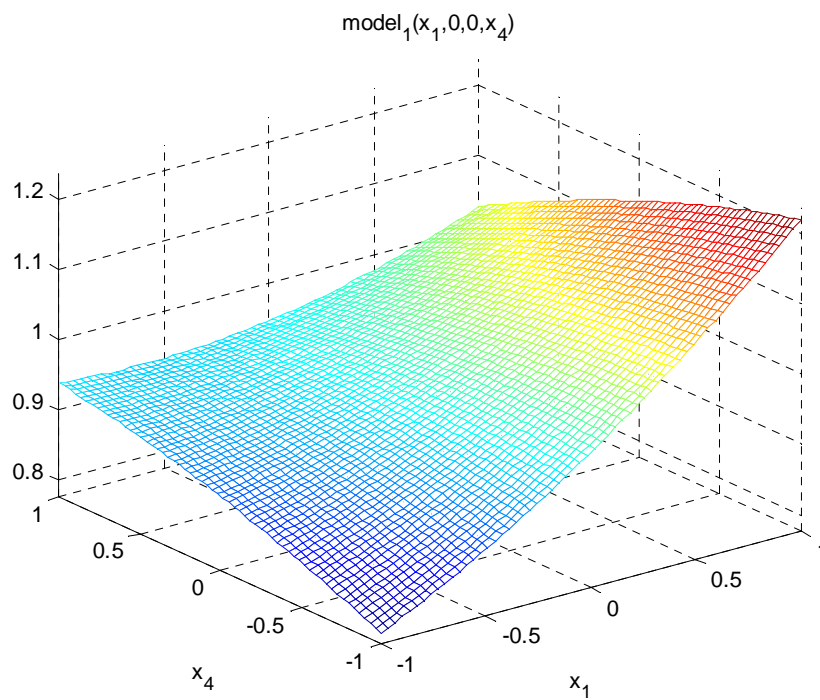


Figure 3: Plot of N and K against response Y

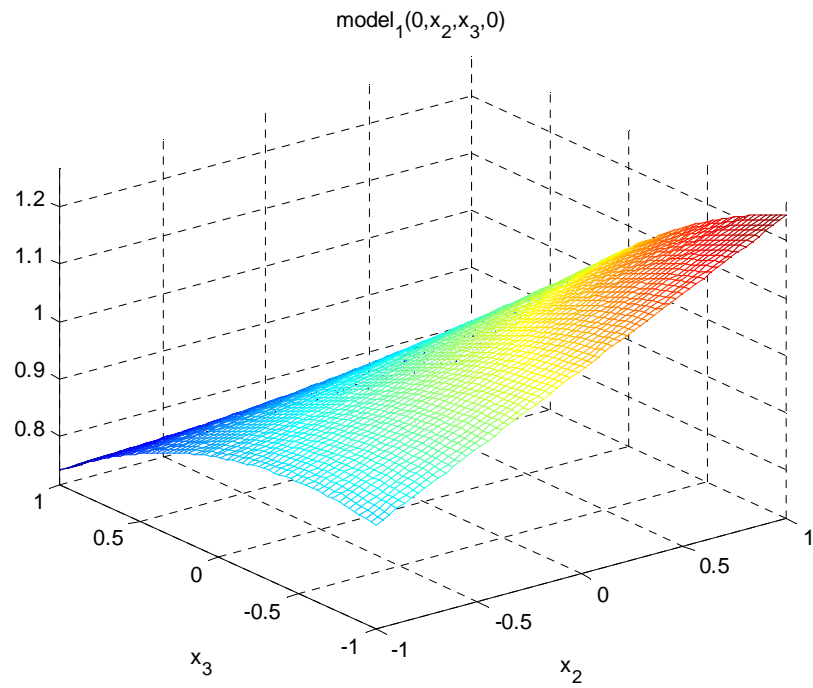


Figure 4: plot of P and S against response Y
 $\text{model}_1(0, 0, x_3, x_4)$

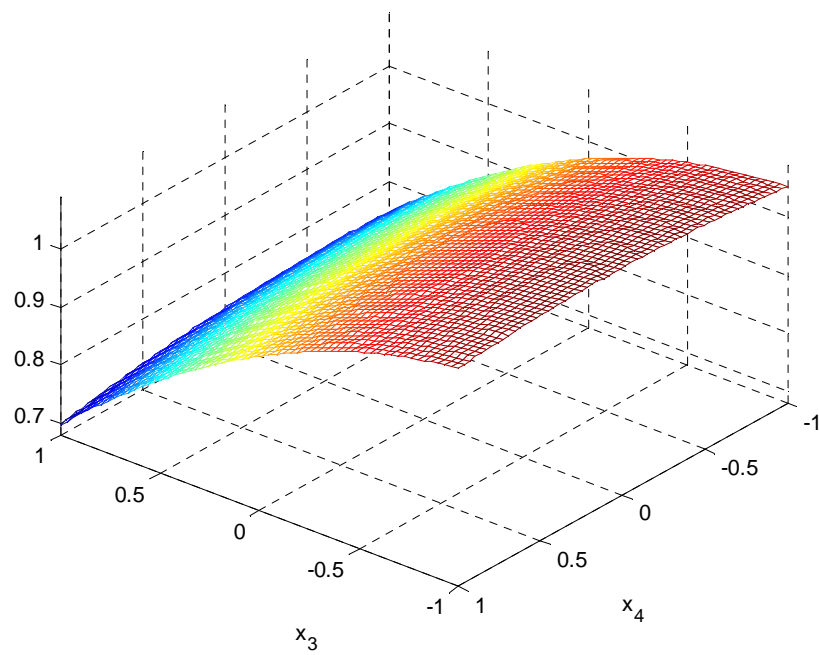


Figure 5; Plot of S and K against response Y

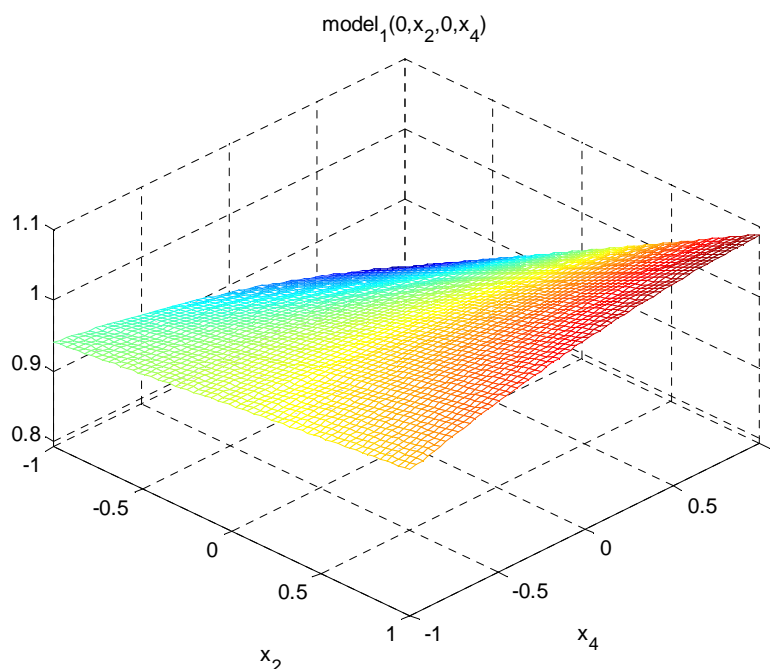


Figure 6: Plot of S and K against response Y

DISCUSSION

This section interprets the application of the steepest ascent for the optimization of multivariate experimental process. In the initial iteration. The equations and procedures explained above are all translated into excel spreadsheet as presented in the table attached .

Since the various combinations of the factors can be plotted in a single figure, the various interactions based on the aspect of the optimal data obtained, six combination mesh grids are plotted as presented in figures 1 – 6 below.

Figure 1 clearly shows the response Y against N and P. The optimum point is at N = 0.5 and P = 0.5 also. From figure 2 the combination of N and S shows that they have an optimal response at N = 0.5 and S = 0.5 with the response at 1.0.

Figure 3 clearly depicts the optimum points of the response at 0.90 at the combination of N at 0.45 and K at also 0.5. While, figure 4 displays the combination of P and S. These combinations displayed a good and optimum response at the point 1.2 with a value of 1.0 for factor P and 0.5 for factor S respectively. Figures 5 and 6 displayed the optimum level of response at 1.0 and 1.1 respectively due to various combinations of S and K, and P and K at points 1.0 each.

CONCLUSION

From the result of the analyses conducted based on the attached table and as presented in the six figures 1 – 6, we can clearly see that optimum level is obtained for the response at the various combinations of the factors at points ranging from 1.02 ± 0.05 .

The optimal response for all the various combinations of N,P,S and K settings are within the values of 0.48 ± 0.05 , 0.83 ± 0.17 , 0.67 ± 0.17 and 0.83 ± 0.17 respectively.

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