Effect of Size of the Step in the Response Surface Methodology using Nonlinear Test Functions

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Abstract—The response surface methodology (RSM) is a collection of mathematical and statistical techniques useful in the modeling and analysis of problems in which the dependent variable receives the influence of several independent variables, in order to determine which are the conditions under which should operate these variables to optimize a production process. The RSM estimated a regression model of first order, and sets the search direction using the method of maximum / minimum slope up / down MMS U/D. However, this method selects the step size intuitively, which can affect the efficiency of the RSM. This paper assesses how the step size affects the efficiency of this methodology. The numerical examples are carried out through Monte Carlo experiments, evaluating three response variables: efficiency gain function, the optimum distance and the number of iterations. The results in the simulation experiments showed that in response variables efficiency and gain function at the optimum distance were not affected by the step size, while the number of iterations is found that the efficiency if it is affected by the size of the step and function type of test used.

Keywords—RSM, dependent variable, independent variables, efficiency, simulation

I. INTRODUCTION

THE RSM is a collection of mathematical and statistical techniques used to determine the optimal levels of the independent variables of a production process, which involves estimating a regression model of first order by the method of least squares, with the coefficients of this model is set search direction by MMSD, subsequently, the step size on the ascent route is chosen until there is no further increase in the response, this method stops [1]-[2].

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Then we fit a new linear regression model, a new path of upward slope is determined and the procedure continues until it fits the regression model of first order. Finally, we start in the region where it was not possible to adjust the regression model of first order, a more detailed design is posed, as the central composite design (CCD), which is the kind of classic design to fit models of second order and find the optimal values of the independent variables analyzed, using methods of differential calculus. [3]-[7]

This paper will focus on the early stages of the RSM, specifically in the MMSD, which is an iterative method that determines the optimum search direction, with the estimated regression coefficients of first-order model. Generally, a simple procedure to determine the coordinates of a point on the trajectory of MMSD, assuming that the point $x_1 = x_2 = \ldots = x_k = 0$ is the base or point of origin. Then, we choose the step size in one of the independent variables of the process called Δx_i. Usually, you would select the independent variable which has more information or would select the variable that has the largest absolute regression coefficient $\left|\hat{\beta}_i\right|$. The step size of the other variables is shown as (1):

$$\Delta x_j = \hat{\beta}_j / (\hat{\beta}_i / \Delta x_i), \ \text{j=1,2,...,k, i} \neq \text{j} \qquad (1)$$

Subsequently, the Δx_j are converted from encoded variables into natural variables. [2],[7]-[8]. The contribution of this research is to determine if the efficiency of the RSM depends on the size of the step, where step sizes to be evaluated are: $\Delta x_i = 0.01, 0.02, 0.03$. The efficiency of the RSM is defined by three variables of response, efficiency in the gain function, represents the percentage of improvement is achieved in the process yield from the starting conditions until the actual optimum conditions, the optimum distance represents the optimum distance between the optimal conditions generated by the RSM and the optimal actual conditions of a process; [9] and the number of iterations obtained by the MMSD within the RSM [10]; the functions that are used to build the simulation model (test function) are the functions of two variables used for numerical comparison of experimental techniques [11]. These functions are designed to hinder the determination of their minimum values with the implementation of experimental techniques. Furthermore, the use of these functions allows us to estimate the usefulness of experimental techniques in the optimization of production processes [12]. Therefore, the test functions that are used in this work represent the functional relationship between the

controllable factors $x_1, x_2,..., x_k$ and the performance of a y_i process. The following is an algebraic description of the test functions that are used in this simulation to calculate the response variable y_i. The Rosenbrock´s parabolic valley function (RPVF), The Rosenbrock´s cubic function (RCF), and The Beale Function (BF) are given by (2), (3) and (4) respectively:

$$f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \qquad (2)$$

$$f(x_1, x_2) = 100(x_2 - x_1^3)^2 + (1 - x_1)^2 \qquad (3)$$

$$f(x_1, x_2) = [1.5 - x_1(1 - x_2)]^2 + [2.25 - x_1(1 - x_2^2)]^2 + [2.625 - x_1(1 - x_2^3)]^2 \qquad (4)$$

This paper is organized as follows. Section 2 summarizes the materials and method used for the development of this research. Section 3 presents the results to determine if the efficiency of the RSM depends on the step size and type of test function used. Section 4 presents the conclusions and future research.

II. METHODOLOGICAL FORMULATION

A. Materials

The materials used for the development and validation of this research project are: a Laptop Computer Intel Core i5, processor, 2.4 GHz and 4.00 GB of RAM. The software for statistical analysis of data is: MINITAB®15, STATISTICA, MATLAB® and Microsoft® Office Excel 2007.

B. Methods

Next, it is described the method used to obtain the required information in assessing the effect of the step size in the efficiency of the RSM [2]. How was carried out to generate the samples, the experimental errors ε, the 2^k factorial designs, construction designs of response surfaces, estimating the coefficients of the first order model set, the search for a new design region of the first order and obtaining the stationary point.

First, are determined randomly thirty-three pairs of focal points for the independent variables $x_1, x_2,..., x_k$, so that x_k continue independent uniform distributions in the range from 0 to 5 units, which will be used as representative of current operating conditions of a process. These pairs of focal points generated with the software MINITAB ® 15.

Second, in each of these points is carried out a run of the methodology comprising: a) Each pair of points (x_1, x_2) is used as the central design point repeated five times. These central values are encoded in (0.0). b) Building the design 2^2 whose levels are equidistant in a value Δ natural units from the central point encoded as $(\pm 1, \pm 1)$.

Third, once the design surface of the first order is posed, are calculated the values of the response variable $y_i = f(x_k) + \varepsilon_i$. Where: $f(x_k)$ represents the test function of the response variable, and the ε_i represents the experimental error of each run i of the design 2^k, where $i = 1, 2,..., 9$; the error is generated at random with a normal distribution $(\mu = 0, \sigma = 5)$ [13], using the random number generator software MINITAB® 15.

Fourth, the response variables calculated with the test function $f(x_k)$, serve to estimate the coefficients corresponding to the adjusted first-order model with the form:

$$\hat{y}_i = \hat{\beta}_0 + \sum_{j=1}^{k} \hat{\beta}_j x_j \qquad (5)$$

The surface design outlined above, is estimated by the least squares method, therefore, to estimate the model coefficients, (6) and (7), are usually used:

$$\hat{\beta}_k = \sum_{k=1}^{2} \sum_{i=1}^{9} x_{ki} \hat{y}_i \qquad (6)$$

$$\hat{\beta}_0 = \sum_{i=1}^{9} \hat{y}_i / 9 \qquad (7)$$

Where: x_{ki} represents the encoded value of the variable k in the column i the surface design of the First Order. $\hat{y}_i$ represents the value of the response i.

Fifth, it is verified the suitability of first-order model set, it is important to know if the order of the fitted model is correct. The lack of fit test establishes the following hypothesis: H_0: The model adequately fit the data. H_1: The model does not fit the data. The lack of fit test can be introduced in the analysis of variance (ANOVA) addressed the significance of the regression. For this study the significance level was 5% $(\alpha = 0.05)$. If the null hypothesis of the adequacy of the model is rejected, the model does not adequately represent the behavior of the system and one that is appropriate must be found.

Sixth, once the adjusted first-order model is not rejected, begins with the MMSD, to accept the model occurs when the regression is significant and the interaction and the quadratic term are not significant according to ANOVA done on the fifth step. The vector formed by the regression coefficients $\beta' = (\hat{\beta}_1,..., \hat{\beta}_k)'$ of the fitted model, determines the direction of maximum decrease in the response variable, we choose the step size $(\Delta x_i = 0.01, 0.02, 0.03)$ in any of the variables of the process. The MMSD is stopped when; in the path there is a change in the response variable, that point is the center of a new surface design of the first order. The new values obtained in this new couple (x_1, x_2) apply again from the second step. Obtain measurements of the response variable with the test function $f(x_k)$ to set a new first-order model, repeating this process until the model does not fit, the regression was not

significant or the interaction or the quadratic term are meaningful.

Seventh at the time that the first-order model shows a lack of adjustment, the MMSD ends and we proceed to make the design of surfaces of second order. The Central Composite Design (CCD), this is the most popular class of designs used to fit these models. Overall, the CCD has a 2^k factorial design (or a fractional factorial design of resolution V) with n_f runs, 2^k axial or star runs and runs central n_c. Where n_f is the number of points in the 2^k design and n_c is the number of repetitions of the central or initial focus of the design 2^k. That is, to the points (x_1, x_2) of the surface design of the first order model point the last region of interest found in the MMSD of the sixth step that did not adjust, add four axial points which encoded as $(\pm\sqrt{2}, 0)$ and $(0, \pm\sqrt{2})$, once posed the CCD, are obtained the values of the response variable of the test function $f(x_k)$ at each point of the design, to which result we add the experimental error ε_i where $i = 1, 2, ..., 13$.

Eighth, once the CCD is posed, are obtained the regression coefficients of the model of second order, with the method of least squares regression using the software module STATISTICA. To find the stationary point of the second order model adjusted, [7] we use (8):

$$\hat{y}_i = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i + \sum_{i=1}^{k} \hat{\beta}_{ii} x_i^2 + \sum \sum_{i<j=2}^{k} \hat{\beta}_{ij} x_i x_j + \varepsilon \quad (8)$$

Where: $i = 1, 2$, and $j = 1, 2$.

The general mathematical solution to locate the optimal point for a second order model with two independent variables arises in matrix form as shown in (9):

$$\hat{y}_i = \hat{\beta}_0 + (\hat{\beta}_1, \hat{\beta}_2) * \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + (x_1, x_2) + \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 \\ \hat{\beta}_{21}/2 & \hat{\beta}_{22} \end{bmatrix} * \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad (9)$$

Find the stationary point by solving (10):

$$x_0 = -1/2 \begin{bmatrix} \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 \\ \hat{\beta}_{21}/2 & \hat{\beta}_{22} \end{bmatrix}^{-1} * \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} \end{bmatrix} \quad (10)$$

Ninth, after obtaining the optimum operating conditions (x_1^*, x_2^*) by analyzing the stationary point using the RSM using MATLAB® simulation, are carried out the calculations for the thirty-three pairs of central point, considering the three step sizes $(\Delta = 0.01, 0.02, 0.03)$, and the three test functions used in this study.

Tenth, once obtained the values of the runs consistent in the experiments performed to obtain the stationary point using the RSM through simulation, for the thirty-three replicas or central points (blocks) are performed considering the step

sizes as a factor of fixed effects. This factor determines the value of the response variable of the process and the effect on the resulting number of steps to arrive to the stationary point. In each replica (block) are tested the three step sizes randomly one at a time, leaving the observations of each replica [1] as shown in Table I:

TABLE I
FORMAT USED IN THE ANALYSIS OF VARIANCE FOR MMSD EFFICIENCY IN THE RSM

Delta	Normal Distribution
0.01	$\hat{y}_{0.01j}$
0.02	$\hat{y}_{0.02j}$
0.03	$\hat{y}_{0.03j}$

Where:

$\hat{y}_{ij}$: represents the response variable when the step size is i $(i = 0.01, 0.02, 0.03)$, corresponding to the replica j.

It is desired that the experimental error be as small as possible by subtracting from the experimental error the variability caused by the blocks. The design to be considered for the analysis of variance is the randomized design by complete blocks. The statistical model for this design is (11):

$$\hat{y}_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij} \quad (11)$$

Where:

$\hat{y}_{ij}$: Represents the corresponding observation to the replica j with step sizes i.

μ: Represents the overall mean of the data.

τ_i: Represents the effect of the i-th step size $i = 1, 2, 3$

β_j: Represents the effect of the j-th replica (block). $(j = 1, 2, ..., 33)$

ε_{ij}: Represents the random error.

The effects of treatment and block are considered as deviations from the overall average, so you want to test the equality of the means of treatment. The null hypothesis is:

$H_0: \tau_1 = \tau_2 = \tau_3 = 0$

$H_1: \tau_i \neq 0$ at least for an i

III. RESULTS

The results obtained during the development of this research are presented in four stages. The first involves the analysis performed in approach on the design of the first order response surface. The second stage is the search for optimal region by the MMSD. Part three covers the approach of the second model of the first order response surface, based on that optimal result obtained by the MMSD. Finally, the fourth stage shows the analysis of models of second order response surface, as well as stationary points and response surface

graphs for each test function. Example is shown of a run on simulation, which was conducted with the test function RCF, which has its minimum value at the (1,1) $f(x_k)$ min $= 0$. We set a 2^k factorial design with 5 central repetitions as the design response surface of first-order, where the point $(x_1 = 3.7915, x_2 = 3.7128)$ is the focal point of design and the design points separated by a distance 2^k of ± 0.03 units. The values of the response variable are obtained by evaluating the test function in the natural variables and adding this result to the experimental error randomly generated by software MINITAB®15. By the method of least squares, we obtain the following values $(\hat{\beta}_1 = 22023, \hat{\beta}_2 = -9182)'$, is the vector of the regression coefficients of the first order model set, where the analysis of variance showed that the data fit well with a significance level of 5% ($\alpha = 0.05$). The direction provided by this vector is in Fig. 1 using the step size of 0.03 natural units on x_2, since this variable has the lowest coefficient, indicating the search line to where should be moved the levels of the factors to select the new center point of the next design surface of the first order.

To make the process of decline, we choose the step size of 0.03, (1 code), then there are the points obtained in the path indicated by the vector, which are equidistant a unit from the axis and a distance of (22,023 / - 9182) relative to the axis, get the values of the response variable to evaluate the test function on the points of minimum slope, obtaining the minimum value of the response variable at (1.6329, 4.6128). This point is considered the centerpiece of a new surface design of the first order and that point is taken as the current operating status of the process, from which is repeated from step 2 explained in the previous section of methods. According to MMSD search in the new region found with the couple of the center point (1.6329, 4.6128), a new search direction with the vector of regression coefficients (-10.4, -2.9). The new design shows a first order analysis of variance that the second regression model obtained does not fit the data with a significance level of 5% ($\alpha = 0.05$). Once it is observed that the first order model does not fit in some new region given, the next step of the methodology is to fit a model of second order in the region indicated by the MMSD. Applying the least squares method, we obtain the regression coefficients of the second order model, as shown in Fig. 2 of the surface of response obtained for this point:

$(\hat{\beta}_1 = 9527.2487,\ \hat{\beta}_2 = 25.7884,\ \beta_{11} = 10882.9986,$

$\beta_{12} = 1.6244,\ \beta_{22} = -3559.0475)'$

using Matlab® was reached the optimal points of the natural variables in the region of the second order design, resulting in the following values: $(x_1^* = 1.6259, x_2^* = 4.6190)$. It is calculated the efficiency of the gain function of the value of the first pair of randomly generated central points $(x_1 = 3.7915, x_2 = 3.7128)$ regarding the result obtained of the optimum point $(x_1^* = 1.6259, x_2^* = 4.6190)$ with the result

that the efficiency gain function for this pair of center points and optimal points obtained would be of 99.9959% which is the percentage of improvement which is achieved in the process yield. With regard to the optimum distance (D^*) for the first couple of optimal points obtained $(x_1^* = 1.6259, x_2^* = 4.6190)$ is calculated using the Euclidean distance replacing the initial values of the pair of center points and the results of the pair of optimal points, thus obtaining the optimal distance generated RSM to the true optimum test function resulting in 3.6727 units. Finally, we obtain the number of iterations performed in the first phase of the methodology within the MMSD, resulting for the first couple of central points 30 iterations to the optimum of the independent variables.

The process described in this example was performed to the replica two, with delta 0.03 for the test function RCF. Was subsequently carried out the method described in the previous section for the 33 pairs of randomly generated central points and with the three step sizes (0.01, 0.02, and 0.03) and the three test functions.

For example, Table II shows the average values of the response variables for The Rosenbrock´s parabolic valley function (RPVF) test function, where the response variable efficiency in the gain function the highest percentage of improvement that gets this function is 99.91% with a size of step of 0.02, whereas the lowest value is 99.24% with a step size of 0.03. It is also shown that the maximum distance of separation between the optimal generated by the methodology and the true optimum function test is 2.26, which belongs to the step size of 0.01 and the minimum distance is 1.56 with a step size 0.02. Finally, for the variable number of iterations, the smallest amount was obtained with the step size of 0.03 to 27.5 and the highest was with the step size of 0.02. The same interpretation held for the test functions RCF and BF, which are shown in Table III and IV respectively.

TABLE II
AVERAGE VALUES OF THE RESPONSE VARIABLES FOR RPVF

Dependent Variable	Step sizes		
	0.01	0.02	0.03
Efficiency (%)	99.29	99.91	99.24
Distance to optimum	2.26	1.56	1.69
Number of iterations	49.18	49.42	27.5

TABLE III
AVERAGE VALUES OF THE RESPONSE VARIABLES FOR RCF

Dependent Variable	Step sizes		
	0.01	0.02	0.03
Efficiency (%)	99.01	99.09	99.70
Distance to optimum	1.95	2.27	2.31
Number of iterations	4.3	6.05	11.07

TABLE IV
AVERAGE VALUES OF THE RESPONSE VARIABLES FOR BF

Dependent Variable	Step sizes		
	0.01	0.02	0.03
Efficiency (%)	75.89	80.86	84.69
Distance to optimum	2.98	2.97	2.95
Number of iterations	66.33	29.06	18.96
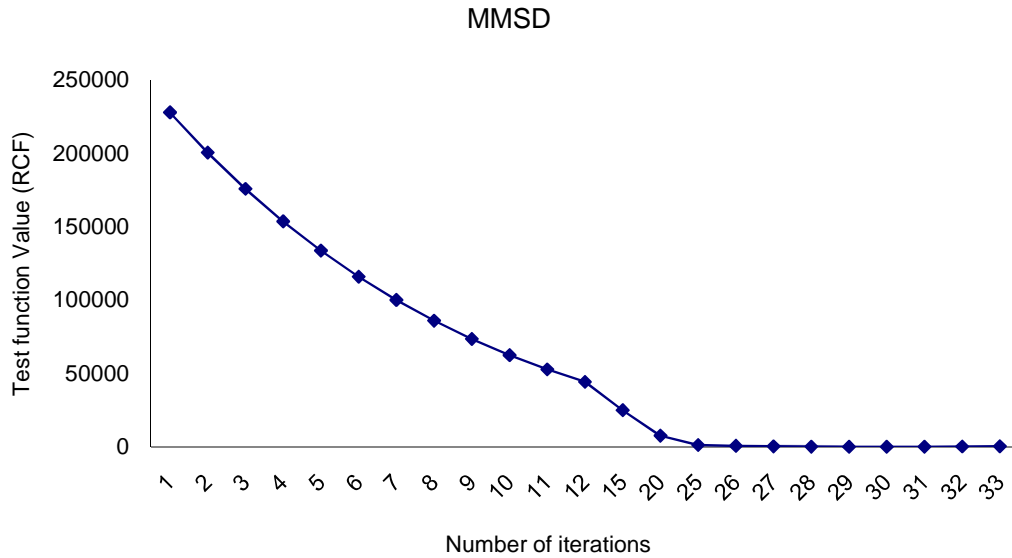
MMSD

Fig. 1 Path of the MMSD of the first pair of central points $(x_1 = 3.7915, x_2 = 3.7128)$

3D Surface Plot (pto1 10v*13c)
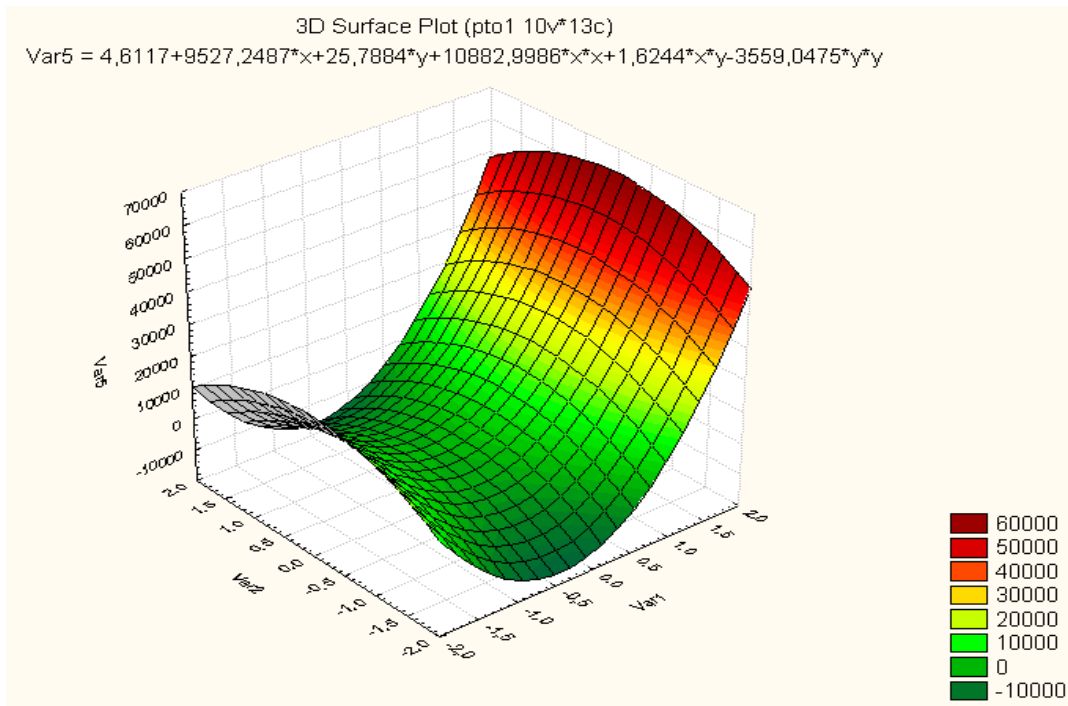Var5 = 4,6117+9527,2487*x+25,7884*y+10882,9986*x*x+1,6244*x*y−3559,0475*y*y

Fig. 2 Response surface of the second order model.

IV. CONCLUSION

In this article has been posed the problem of assessing the effect of the step size in the efficiency of the RSM. This methodology was evaluated at different steps outlined in section 2 of this article, with the initial test conditions, such as: the 3 step sizes, the 33 pairs of focal points and the 3 types of test function. Based on this, the results obtained in the analysis of variance of the randomized complete block designs for each of the variables evaluated, it is concluded that: the efficiency of the RSM is not affected by the step size, with a significance level of 5% $(\alpha = 0.05)$ since the improvement achieved in the response variable efficiency in the gain function, showed approximately equal values, therefore, we conclude that the methodology is robust to the step size used in the MMSD for the test functions used for this response variable. The response variable to the optimum distance indicates that the efficiency of the RSM is neither affected by the step size, with a significance level of 5% $(\alpha = 0.05)$. Finally, in the response

variable number of iterations indicates that the efficiency of the RSM is affected by the step size and the type of test function used, with a significance level of 5% $(\alpha = 0.05)$ since in each function test values were obtained that on average differed from the type of test function and the step size, as shown in Tables 1, 2 and 3 of Section 3. Therefore, these results assert that comparing the performance of the RSM with three step sizes and the 3 test functions, the methodology is a useful tool in the continuous improvement of processes.

In future research, a) is recommended that to the regression coefficients of first-order models were not significant within the RSM, a transformation is applied to that model and evaluate if must be continued the next phase of the RSM. b) Compare the performance of the study system before various improvement techniques such as design and analysis of classical experiments, methods of operational evolution, Taguchi method, simplex method of Nelder and Mead, genetic algorithms, among others, and to determine which of these is more efficient in the response variables outlined in this article. c) Experiment with different step sizes and test function from those used in this investigation to see if there is an improvement or effect within the RSM with the independent variables analyzed. d) Determine the optimum step size in the RSM for the optimization of resources in production systems.

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