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Comparison of Stopping-Rule Methods in the Process Optimization Strategy Using Steepest Ascent or Descent in a Tension Measuring Machine

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Abstract: Nowadays, process improvement is already an essential competitive mechanism for companies around the world. Production processes require establishing improvement strategies to obtain greater productivity. In modern literature, there are a series of statistical experimentation schemes that allow the establishment of methodologies permitting such improvement to be carried out efficiently through a previously established analysis. The Steepest Ascent or Descent Method (SADM) is an example of this. SADM consists of the development of an experimental design that yields a linear model that follows a straight-line of ascent or descent path towards a target point within the process. Fundamentally, it is a procedure that builds a sequential experimentation model where two-level factorial designs are highlighted, in which a series of iterations are made to follow a line towards a region where optimization is feasible. These iterations or individual experimentations follow certain criteria called "Stopping rules". Series of rules to know when no more iterations are required because the desired region would have already been reached. This paper presents the implementation of the SADM in a case study based on a fitted linear obtained from a factorial design. The Myers-Khuri method and the Parabolic-Recursive method are applied to proceed with the stop. Both methodologies are intended to create a decisive and efficient stopping strategy. The objective is to make a comparison between both methods to show the predominant one in relation to a better use of resources. Results obtained and a conclusive analysis are disclosed at the end of this document.

Keywords: Statistical Experimentation, Linear Model, Stopping Rules, Response Variable, Optimization

1. Introduction

Nowadays, industries around the world have the need to continuously improve their processes to always guarantee a competitive advantage to succeed. Current literature has different methodologies used for this purpose. Most methods related to continuous improvement involve statistical and mathematical models oriented to optimization.

One of the strategies for a first approach to optimization is the one proposed by Biegler et al. (2002). As early as the turn of the millennium, these researchers harnessed the popularity of dynamic optimization to present an improved algorithm for simultaneous strategies, a nonlinear programming strategy, and a preconditioned conjugate gradient method. Almost in parallel, Syrcos (2003) analyzes several important process parameters of the die casting method of an aluminum alloy to obtain optimal settings of the die casting parameters, to obtain the optimum casting density of the alloy castings of this aluminum. Few years later, Tatjewski (2008) also already incorporates scenarios for the optimization of processes with advanced control algorithms and the optimization of the set point in line in the structures of control of processes in structures.

One of the most important and basic tools for process observing, analysis and improvement is the Design of Experiments (DOE). Several of professionals use DOE to understand better their processes and look for its optimization. As said by Montgomery (2019), an experiment can be defined as a test or series of runs where a set of variables take place. The intention in these experiments is the manipulation of the input variables of a process or system to observe possible changes in the output variable. This analysis allows the identification of the input variables that are responsible for the changes in the response, the development of a model relating the response to the important input variables, and the use of the model for improvement and decision-making.

In this context, an important tool for optimization is the one called Response Surface Methodology (RSM). According to Myers (2016), RSM is a collection of statistical techniques for process optimization. It also has applications in the design of new products and improvement of existing ones. It is ensured that the most extensive applications of RSM are related to the industrial world in cases where input variables potentially influence the performance of products or processes. The input variables are often called independent variables and they are into the control of the scientist for experimentation. Several symbols are recognized to manage the different varibales of this experiments. The two most important, the response varibale yield (y) and the independent, controllable or input variables, (ξ_k). The relationship between the the input variables and the response yield is proposed as follows:

$$y = f(\xi_1, \xi_2, \dots, \xi_k) + \varepsilon \tag{1}$$

In this equation, f is the unknown response function, and ε represents the implicit error that may be produced by any other unaccounted sources of variability.

Considering the RSM as a technique of optmization, Myers (2016) also contemplates a method where sequential experimentation is used to search for a region of improved reponse, the Steepest Ascent or Descent Method (SADM). This experimental design and model-building procedure, involves sequential movement from one region of the factors to another. This literature poproses a serie of steps for an ascent method where the most important assumption is the management of a first-order model or planar representation. SADM follows the next steps:

1. Assuring a first-order model using an orthogonal design.
2. Compute a path of steepest ascent (in the case of maximizing) or steepest descent (in case of minimizing).
3. Conduct experimental runs along the path to analyse the response value.A stopping decision proposes to stop after two concecutive drops in response values.

Myers & Khuri (1979) already had considered a stopping rule procedure for SADM into to the general area of RSM to find the maxima of a response function performing a sequence of sets of trials. Now known as Myers & Khuri Stopping Rule (MKSR). Each set of trials was obtained as a result of proceeding sequentially along the path of maximun increase in response. Nevertheless, when response values are subject to random error, the decision to stop can be premature due to a "false" drop in the observed response. Likewise, Miró-Quezada & Castillo (1997) presented Del Castillo´s Recursive Parabolic Rule (RPR). The authors studied the performance of rules including classical rules of stopping after 1, 2 or 3 consecutive drops in the response. For their procedure, the RPR fits a parabola to the sequence of observed responses.

A comparison of both, MKSR and RPR stopping methods, will be disclosed using steepest ascent or descent for a non-quadratic simulated response of a tension machine.

2. Method

A flow chart of the proposed method is presented in Figure 1 to easily visualize the progress. Firstly, the case study that is used to obtain data for the experiment. Then, the way the experiment is conducting with the form of the regression model that is used. After this, the statistical analysis of the experiment and the fitting of the linear model showing the factors and their levels. To continue, the implementation of the path for the steepest ascent or descent is shown. Only then, the application and comparison of stopping rules is possible. Finally, the identification of the maximum reached point is done.

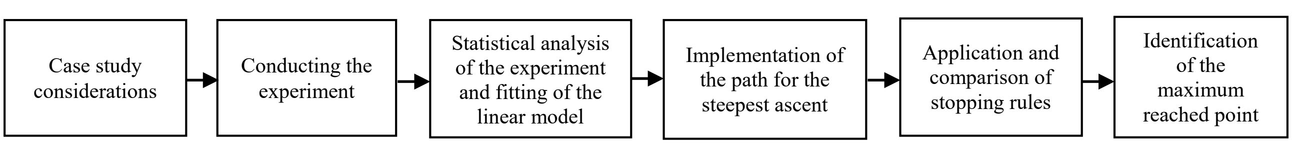

Figure 1. Flow diagram of the method

Case study considerations

A simulated response of a tension machine is used for this experiment. The machine measures the tension or pressure of saline water related to an intravenous drip therapy. The response variable is measured on mN/m. The factors involved are the temperature (degrees Fahrenheit) and the speed (meters per second) of the water. The response is the main piece of information to use into the DOE.

Conducting the experiment

The procedure initiated with a DOE. It is a 2^2 factorial analysis with three replicates. Each of the factors has two levels. The temperature goes from 80 to 115 °F and the speed goes from 3.4 to 6.0 m/s. Three replicates are implemented. The resulted value is the tension or pressure produced out from the combination of these two factors with their levels. A linear model is acquired out from that design. The full analysis of this factorial design is run using the software $\text{Minitab}^{\text{TM}}$.

Statistical analysis of the experiment and fitting of the linear model

A statistical analysis is started. The resulted ANOVA is one of the most important tool for the analysis. This is how the experiment reveals that both, the temperature and the speed are significant. Not the same way for the interaction. An important situation is the correct verification and appreciation of the ANOVA assumptions. These are shown in "the four-in-one graph" of the analysis. The three main assumptions for ANOVA residuals are: normality, common variance and independence. Once the verification of significance of the factors is done, the next step is fitting this linear model in the path building. The coefficients β_1 and β_2 in equation 2 are the main core for the increments in the path. The ecuation of the regression model has the form:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon . \tag{2}$$

Implementation of the path for the steepest ascent or descent

The model was used to obtain the steepest ascent or descent path (a fitted first-order response surface was obtained, only then, the visualization of the normal operation conditions is possible to determine the steepst ascent path). The development of the path needs the consideration of $\beta_i, i = 1,2$. According to Myers *et al.* (2016), it is necessary to determine Δx_i known as the size of steps, usually the variable that has the largest absolute regression coeffiecient $|\beta_i|$ is selected. Next, the step size in all of the variables need to be calculated with the formula:

$$\Delta x_j = \frac{\beta_j}{\beta_i / \Delta x_j}, \quad j = 1, 2, \dots, k, \quad i \neq j \tag{3}$$

After this, individual expermients are run according to the number of steps required or desired. A graph helped the observation of growth in data, the maximum point and its decline.

Application and comparison of stopping rules

Both, the MKSR and RPR stopping methods for this non-quadratic simulated response are applied to be compared. An observation of growth in data was possible for MKSR to stablish the necessary steps to the maximum point and its decline. Same dynamic for RPR. The purpose is to stage the behaviour of both strategies. Similities and differencies are presented and importants facts and observations are discussed.

Identification of the maximum reached point

Once the maxmium point was observed in the graph, it is considered to be in a region where an optimum value could be closed. Other DOE could be run near from the coditions of operations for factors where the maximum point is found. Other design could be developed because it may be necessary to experiment exaclty in the region of the maximum point where the optimum value was meant to be.

3. Development and results

The development starts with the measure of pressure (mN/m) of saline water for intravenous drip therapy. The pressure will depend on the temperature (°F) and the speed (m/s). The $\text{Minitab}^{\text{TM}}$ factorial regression analysis of the designed experiment establishes the Coded Coefficients shown in table 1. It ilustrates the Coefficients for the factors temperature and speed.

Table 1. Coded Coefficients for Factorial Regression: Y versus Temperature, Speed.

Term	Effect	Coef	SE Coef	T-Value	P-Value	VIF
Constant		1.7658	0.0130	136.16	0.000	
Temperature	1.5783	0.7892	0.0130	60.85	0.000	1.00
Speed	-1.4217	-0.7108	0.0130	-54.81	0.000	1.00
Temperature*Speed	-0.0550	-0.0275	0.0130	-2.12	0.058	1.00
Ct Pt		0.0342	0.0259	1.32	0.215	1.00

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It is always important to determine how well the model fits the data. The literature mentions the higher the R^2 value, the better the model fits the data. In this case, the 99.72% shown in table 2, assures the great fit of the model to the given data.

Table 2. Model Summary for Factorial Regression: Y versus Temperature, Speed.

S	R-sq	R-sq(adj)	R-sq(pred)
0.0449242	99.84%	99.78%	99.69%

As well, the ANOVA in table 3 shows the P-Values of the source. It explains that temperature and speed are significant factors in this designed experiment. Nevertheless, the P-Value of 0.058 from temperature*speed demonstrates that the interaction is not strongly significant.

Table 3. Analysis of Variance for Factorial Regression: Y versus Temperature, Speed.

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	4	13.5494	3.38735	1678.42	0.000
Linear	2	13.5368	6.76841	3353.72	0.000
Temperature	1	7.4734	7.47341	3703.04	0.000
Speed	1	6.0634	6.06341	3004.39	0.000
2-Way Interactions	1	0.0091	0.00908	4.50	0.058
Temperature*Speed	1	0.0091	0.00908	4.50	0.058
Curvature	1	0.0035	0.00350	1.74	0.215
Error	11	0.0222	0.00202		
Total	15	13.5716			

Consequently, the Regression Equation in Coded Units may be represented as shown in ecuation 4. The coefficient of 0.7892 in Temperature is explained as β_1 and the coefficient of -0.7108 in Speed is explained as $\beta_{2.}$ Both coefficients are used to observe the path of improvent in the SADM.

$$Y = 1.7658 + 0.7892\, Temperature - 0.7108\, Speed \tag{4}$$

According to this model, for each unit of change in $Temperature$ there will be a reason change of 0.7892 in the response variable if the speed remains constant. In the same way, for each unit of change in $Speed$ there will be a reason change of 0.7108 in the response if the temperature remains constant.

Next, the steps followed for the steepest ascent path in this experiment and the two stopping rule methods are shown:

1. A first-order model is obtained out from the factorial analysis. The identification of $\beta_1$and β_2 is crucial. According to (Myers, 2016) the step size for the path is commonly the largest absolute regression coefficient $|\beta_i|$. For this experiment, the coefficients are $\boldsymbol{\beta_1} = 0.7892$ and $\boldsymbol{\beta_2} = -0.7108$.
2. A conversion table is designed to diferentiate the coded units from the natural units (table 4). A relation of equivalence needs to be set. Also, equation 3 is applied to obtain the delta of the speed in coded units. Only then, delta of the speed in natural units can be obtained.

Table 4. Conversion chart from coded to natural units and a relation of equivalence.

	Step size	
	Δ --- T °F	Δ --- S m/s
Natural	1	-0.066906089
Coded	0.057142857	-0.051466223

Temperature	
Coded	Natural
1	17.5
0.057142857	1

	Temperature	Speed
Code	Natural	Natural
-1	80	3.4
0	17.5	1.3
1	115	6

3. The path is built obeying the increments (step zise) from table 4 in natural units. The center points declared in the facotrial analysis will be the step 0 in table 5. The response (Y) is obtained from actual individual runs.

Table 5. Steepest ascent path.

Steps	m --- T °F	m --- S m/s
0	97.5	4.7
1	98.5	4.633093911
2	99.5	4.566187821
3	100.5	4.499281732
4	101.5	4.432375643
5	102.5	4.365469553
6	103.5	4.298563464
7	104.5	4.231657375
8	105.5	4.164751285
9	106.5	4.097845196
10	107.5	4.030939107
11	108.5	3.964033017
12	109.5	3.897126928
13	110.5	3.830220838
14	111.5	3.763314749
15	112.5	3.69640866

4. Now, stopping rules can be applied. The decision to maximize, minimize or reach a certain objective value will be determined by the nature of the experiment. For illustrative purposes, the aim in this experiment will be to stop at a maximum response value given by the rule procedures. The first applied stopping rule is (Myers & Khuri, 1979). The hypothesis statement of the procedure is shown next in table 6.

Table 6. Hypothesis statement

Hypothesis	***i.e.***
$H0^i: \eta(t) \geq m_0^i$	The process mean is increasing
$H1^i: \eta(t) \leq m_1^i$	The process mean is decreasing

The procedure starts with equation 5 shown next:

$$a = -b = \Phi^{-1}\left(\frac{1}{2\kappa}\right) \hat{\sigma}_{\epsilon} (\sqrt{2}), \tag{5}$$

where Φ^{-1} represents the inverse cumulative standard normal distribution, κ in an initial guess of how many steps will be necessary to reach the maximum response, and $\hat{\sigma}_{\epsilon}$ is an estimation of the variance obtained from the MS of the factorial design. Basically, it considers these two variables to be compared. If $Y(n^i) - Y(n^i - 1) \geq b$ or $a < Y(n^i) - Y(n^i - 1) < b$; there is no rejection of $H0^i$ and experimentation continues. On the other hand, if $Y(n^i) - Y(n^i - 1) \leq a$ so, there is rejection of $H0^i$ and experimentation stops.

The variable Y is explained as the response variable of the experiment. It will be obtained individually over the steepest path. The stopping method will state where to stop according to $Y(n^i) - Y(n^i - 1)$ which represents the difference between the present value of the response and its previous value.

5. Following the criteria from table 6, a new table (table 7) is built to discover the moment where the individual experimentation over the path of the steepest ascent must stop.

Table 7. Decision test

Steps	m --- T °F	m --- S m/s	Y	$y(n_i) - y(n_i - 1)$	Condition		Decision
0	97.5	4.7	1.82	-	-	-	Starts
1	98.5	4.633093911	1.88	0.06	0.06	< b	Continues
2	99.5	4.566187821	1.96	0.08	0.08	≥ b > 0	Continues
3	100.5	4.499281732	1.97	0.01	0.01	< b	Continues
4	101.5	4.432375643	2.03	0.06	0.06	< b	Continues
5	102.5	4.365469553	2.06	0.03	0.03	< b	Continues
6	103.5	4.298563464	2.34	0.28	0.28	≥ b > 0	Continues
7	104.5	4.231657375	2.42	0.08	0.08	≥ b > 0	Continues
8	105.5	4.164751285	2.4	-0.02	-0.02	< b	Continues
9	106.5	4.097845196	2.45	0.05	0.05	< b	Continues
10	107.5	4.030939107	2.56	0.11	0.11	≥ b > 0	Continues
11	108.5	3.964033017	2.75	0.19	0.19	≥ b > 0	Continues
12	109.5	3.897126928	2.65	-0.1	-0.10	< b	Continues
13	110.5	3.830220838	2.73	0.08	0.08	< b	Continues
14	111.5	3.763314749	2.98	0.25	0.25	≥ b > 0	Continues
15	112.5	3.69640866	2.86	-0.12	-0.12	≤ a < 0	Stops

6. The second applied stopping rule is (Miró-Quezada & Castillo, 1997).
   a. The authors consider a model to be recursively fitted shown in equation 6.

$$Y(t) = \eta(t) + \epsilon_t = \theta_0 + \theta_1 t + \theta_2 t^2 + \epsilon_t \, , \tag{6}$$

   where $Y(t)$ are the observed values during the search and $\epsilon_t \sim N(0, \sigma_\epsilon^2)$ is a sequence of random variables.
   b. The rule proposes to estimate θ_0 from the arithmetic mean of the center points from the factorial. In this case, four center points were run and the estimate of θ_0 was obtained as $Y(0) = 1.8$.
   c. An estimate of θ_1 is needed (equation 7). This is the slope of the response function at the origin in the steepest direction.

$$\theta_1 = \left|\left|b\right|\right| = \sqrt{b_1^2 + b_2^2} \tag{7}$$

   In this case, the slope of the function is estimated following $\theta_1 = \sqrt{(0.7892)^2 + (-0.7108)^2} = 1.06211$
   d. The strategy to update the estimate $\theta_2^{(t)}$ goes as follows:

$$\theta_2^{(t)} = \theta_2^{(t-1)} + \frac{P_{t-1}t^2}{1+t^4 P_{t-1}}\left(Y(t) - Y(0) - \theta_1 t - \theta_2^{(t-1)} t^2\right) \tag{8}$$

   Nevertheless, it necessary to previously estimate $\theta_2^{(0)}$and its P_0 (the associated scaled variance when $t = 0$). For this purpose, it is necessary to use $\theta_2^{(0)} = -\theta_1 \, / \, 2t_{prior}$. In this case, t_{prior} is an initial guess about the number of steps needed to reach the optimim value. The value of P_0 is also an initial number determined by the experimenter. Although these values need to be specified by the experimenter. Its impact on the performance is not highly significant. The values of P_t decrease so rapidly that the value given to P_0 has practically no effect on the performace of the method.
   e. Next, an updating of P_t is required:

$$P_t = \left(1 - \frac{P_{t-1}t^4}{1+t^4 P_{t-1}}\right)(P_{t-1}) \tag{9}$$

   f. The procedure considers a samplig variability of $\theta_1 + 2\theta_2^{(t)} t$:

$$\sigma^2_{\left(\theta_1 + 2\theta_2^{(t)} t\right)} = \frac{120 t \sigma_\epsilon^2}{(t+1)(2t+1)(3t^2+3t-1)} \approx 4\sigma_\epsilon^2 t^2 P_t \tag{10}$$

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g. Finally, a comparison is needed to make a decision if the recursive procedure or method must stop or continue. If $\theta_1 + 2\theta_2^{(t)}t > -3\sqrt{\sigma^2_{\left(\theta_1+2\theta_2^{(t)}t\right)}}$, the experimentation continues. Otherwise, the experimentation stops when $\theta_1 + 2\theta_2^{(t)}t < -3\sqrt{\sigma^2_{\left(\theta_1+2\theta_2^{(t)}t\right)}}$.

7. The final table showing the procedure and the final decision (table 8) is shown next:

Table 8. Procedure and decision test

t	$Y(t)$	$\theta_2^{(t)}$	P_t	$\theta_1 + 2\theta_2^{(t)}t$	$\sigma^2_{\left(\theta_1+2\theta_2^{(t)}t\right)}$	$-3\sqrt{\sigma^2_{\left(\theta_1+2\theta_2^{(t)}t\right)}}$	**Decision**
0	1.80000	-0.053105286	10	1.062105728	0	0	Starts
1	1.88	-0.897651143	0.909090909	-0.733196557	0.007345455	0.257116882	Stops

4. Conclusions

After getting the steepest path, two different methods for a stopping rule were run. Firstly, the Myers & Khuri (1979) stopping rule. This procedure stopped in step 15 bringing a response value of 2.86 mN/m. On the other hand, Miró-Quezada & Castillo (1997) stopping rule stopped in the first step bringing a response value of 1.88 mN/m. The first applied procedure resulted in almost the double benefit than the second procedure. It does not necessarily mean that one method is better than the other one, it means that under certain circumstances and conditions both procedures act differently. In this scenario, the case study of a simulated response of a tension machine of saline water related to an intravenous drip therapy, resulted to have a better performance when the Myers & Khuri (1979) procedure is applied in a steepest path procedure. Additionally, RPR assumes a quadratic response function. Therefore, it seems like this method did not work properly under a non-quadratic response.

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