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Research Article

APPLICATION OF RESPONSE SURFACE METHODOLOGY: DESIGN OF EXPERIMENTS AND OPTIMIZATION: A MINI REVIEW

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ABSTRACT
The concept of response surface methodology can be used to establish an approximate explicit functional relationship between input random variables and output response through regression analysis and probabilistic analysis can be performed. Response Surface Methodology (RSM) is a collection of mathematical and statistical techniques useful for the modeling and analysis of problems. By careful design of *experiments*, the objective is to optimize a *response* (output variable) which is influenced by several *independent variables* (input variables). An experiment is a series of tests, called *runs*, in which changes are made in the input variables in order to identify the reasons for changes in the output response. It is the process of identifying and fitting an approximate response surface model from input and output data obtained from experimental studies or from the numerical analysis where each run can be regarded as an experiment.

Keywords: *Response Surface Methodology, Optimization, Design of Experiments*

INTRODUCTION
Response surface method (RSM) is a set of techniques used in the empirical study of relationships (Cornell, 1990). RSM is a collection of mathematical and statistical techniques for empirical model building, in which a response of interest is influenced by several variables and the objective is to optimize this response (Montgomery 2005). RSM is useful in three different techniques or methods (Myers and Montgomery, 2002): (i) statistical experimental design, in particular two level factorial or fractional factorial design, (ii) regression modeling techniques, and (iii) optimization methods. The most common applications of RSM are in Industrial, Biological and Clinical Science, Social Science, Food Science, and Physical and Engineering Sciences. The first goal for Response Surface Method is to find the optimum response. When there is more than one response then it is important to find the compromise optimum that does not optimize only one response (Oehlert 2000). When there are constraints on the design data, then the experimental design has to meet requirements of the constraints. The second goal is to understand how the response changes in a given direction by adjusting the design variables. In the probabilistic analysis, an explicit or implicit functional relationship between input parameters and output response is required, which is normally difficult to establish except for simple cases and even the established functional relationship is sometimes too complicated to perform the conventional probabilistic analysis through integration or through first or second order derivatives. In such circumstances, authors propose to use the concept of response surface methodology to establish an approximate explicit functional relationship [Eq. (1)] between input variables (x1, x2, x3 …) and output response (y) through regression analysis for the range of expected variation in the input parameters.

$$Y = f(x_1, x_2, x_3 \ldots) + e \qquad (1)$$

The above relationship can be simple linear or factorial model, or more complex quadratic or cubic model. ‘e’ represents other sources of uncertainty not accounted for in ‘f’’, such as measurement error on the output response, other sources of variation inherent in the process or the system, effect of other variables and so on. Myers and Montgomery (2002) presented an excellent literature on Response surface methodology and can be referred to for more details on RSM analysis. In brief, 2n factorial design is often used to fit linear and non-linear (second order) response surface models for n number of input variables. These set of input variables are also termed as natural variables as they are given in their respective units.

In the RSM analysis, natural variables (x1, x2, x3,….xn) are converted into coded variables using the following relationship;

$$\xi_i = \frac{x_i - [\max(x_i) + \min(x_i)]/2}{[\max(x_i) - \min(x_i)]/2}$$

The maximum and minimum values of x, cover the range of variation in the input parameters. The procedure involves determination of output response (y) for the combination of input parameters (sample points) and regression analysis is performed based on least square error approach to fit a linear or non-linear regression model. The output response corresponding to each combination of input parameters can be obtained either from the established functional relationship between input and output or through numerical analysis. The adequacy of the fitted model is examined to ensure that it provides an adequate approximation of the true system and none of the least square assumptions are violated. For that, the normal probability plot should be approximately along a straight line (Sivakumar and Srivastavav, 2007). To examine the adequacy of the fitted model and to ensure that it provides a good approximation of the true system, a normal probability plot should be approximately along a straight line. In addition, computed values of coefficients of multiple determinations (R2) and adjusted R2 also give information on the adequacy of the fitted model.

$$R^2 = \frac{\sum_{i=1}^{n}\left(\hat{y}_i - \bar{y}\right)^2}{\sum_{i=1}^{n}\left(y_i - \bar{y}\right)^2}$$

Where $\bar{y}$, y_i and y^ are estimated mean value, actual and predicted values of output response (y) respectively. The value of R^2 lies between 0 and 1 and a value close to 1 indicates that most of the variability in y is explained by regression model. It should be noted that it is always possible to increase the value of R^2 by adding more regressor variables. Therefore, adjusted R^2 value is calculated using following Eq.

$$R^2_{adj} = 1 - \frac{k-1}{k-p}\left(1 - R^2\right)$$

Where k is total number of observations and p is number of regression coefficients. For a good model, values of R^2 and adjusted R^2 should be close to each other and also they should be close to 1 (Sivakumar and Srivastavav, 2007). In general, the response surface can be visualized graphically. The graph is helpful to see the shape of a response surface; hills, valleys, and ridge lines. Hence, the function f (x1, x2) can be plotted versus the levels of x1 and x2 as shown as Figure 1.

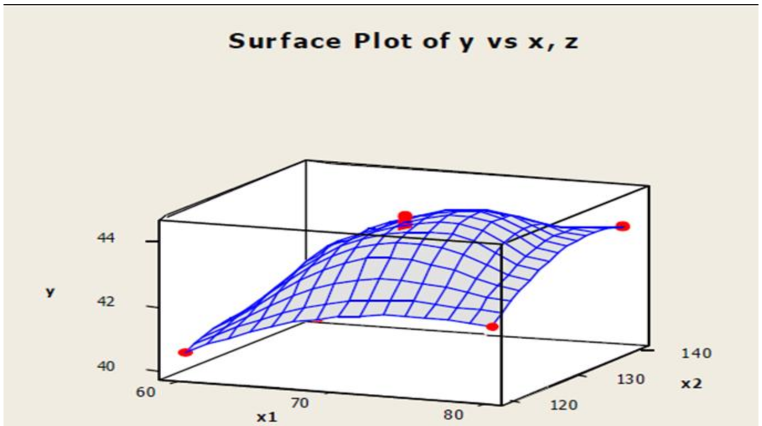

Figure 1: Response surface plot (Nuran 2007)

In this graph, each value of x1 and x2 generates a y-value. This three-dimensional graph shows the response surface from the side and it is called a response surface plot. Sometimes, it is less complicated to view the response surface in two-dimensional graphs. The contour plots can show contour lines of x1 and x2 pairs that have the same response value y. An example of contour plot is as shown in Figure 2 (Nuran 2007).

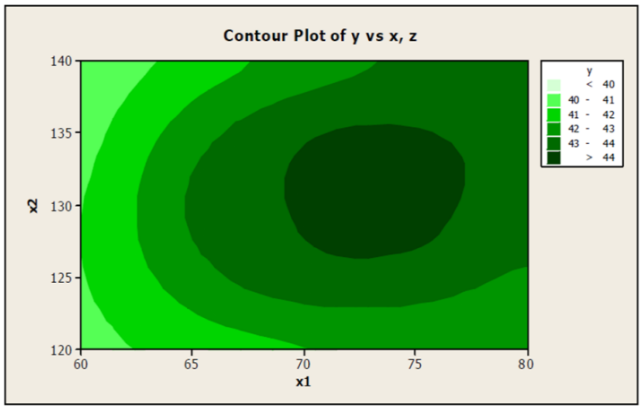

Figure 2: Contour plot (Nuran 2007)

In order to understand the surface of a response, graphs are helpful tools. But, when there are more than two independent variables, graphs are difficult or almost impossible to use to illustrate the response surface, since it is beyond 3-dimension. For this reason, response surface models are essential for analyzing the unknown function f (Nuran, 2007).
Cornell (1990) discussed the response surface methodology as follows:
a) If the system response is rather well-understood, RSM techniques are used to quantify the set of sensitive parameters for obtaining the optimum value of the system response.
b) If identifying the best value is beyond the available resources of the experiment, then RSM techniques are used to at least gain a better understanding of the overall response system.
c) If obtaining the system response necessitates a very complicated analysis that requires hours of run-time and advanced computational resources then a simplified equivalent response surface may be obtained by a few numbers of runs to replace the complicated analysis. When treatments are from a continuous range of values, then a Response Surface Methodology is useful for developing, improving, and optimizing the response variable. For example, the plant growth *y* is the response variable, and it is a function of water and sunshine. It can be expressed as:
y = *f* (*x1*, *x2*) + *e*
The variables *x1* and *x2* are independent variables where the response *y* depends on them. The dependent variable *y* is a function of *x1*, *x2*, and the experimental error term, denoted as *e*. 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

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

A first-order model uses low-order polynomial terms to describe some part of the response surface. This model is appropriate for describing a flat surface with or without tilted surfaces. Usually a first-order model fits the data by least squares. Once the estimated equation is obtained, an experimenter can examine the normal plot, the main effects, the contour plot, and ANOVA statistics (F-test, t-test, R2, the adjusted R2, and lack of fit) to determine adequacy of the fitted model (Nuran 2007). If there is a curvature in the response surface, then a higher degree polynomial should be used. The approximating function with 2 variables is called a **second-order model**:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_{11}^2 + \beta_{22} x_{22}^2 + \beta_{12} x_1 x_2 + \varepsilon$$

Lack of fit of the first-order model happens when the response surface is not a plane. If there is a significant lack of fit of the first-order model, then a more highly structured model, such as second-order model, may be studied in order to locate the optimum. There are many designs available for fitting a second-order model. The most popular one is the central composite design (CCD). It consists of factorial point s (from a 2q design and 2q-k fractional factorial design), central points, and axial points (Nuran 2007). When a first-order model shows an evidence of lack of fit, axial points can be added to the quadratic terms with more center points to develop CCD. The number of center points nc at the origin and the distance *a* of the axial runs from the design center are two parameters in the CCD design. The center runs contain information about the curvature of the surface, if the curvature is significant, the additional axial points allow for the experimenter to obtain an efficient estimation of the quadratic terms. When the first-order model shows a significant lack of fit, then an experimenter can use a second-order model to describe the response surface. There are many designs available to conduct a second-order design. The central composite design is one of the most popular ones. An experimenter can start with 2*q* factorial point, and then add center and axial points to get central composite design. Adding the axial points will allow quadratic terms to be included into the model. Second-order model describes quadratic surfaces, and this kind of surface can take many shapes. Therefore, response surface can represent maximum, minimum, ridge or saddle point. Contour plot is a helpful visualization of the surface when the factors are no more than three. When there are more than three design variables, it is almost impossible to visualize the surface. For that reason, in order to locate the optimum value, one can find the stationary point. Once the stationary point is located, either an experimenter can draw a conclusion about the result or continue in further studying of the surface. The factorial designs are widely used in experiments when the curvature in the response surface is concerned. All treatment factors have 3- levels in the three- level factorial design. This design requires many runs, as a result, the confounding in blocks can be used. Also, the fractional factorial design can be an alternative approach when the number of factors gets large. The three- level fractional factorial design partitions the full 3*q* runs into blocks, but it only runs one of the blocks. This design is more efficient, it allows collecting information on the main effects and on the low-order interactions. The one problem with three- level fractional factorial is that when number of factors is large, it becomes very complicated to separate the aliased effects and to interpret their significance. For this reason, when *q* is large, most of the time this kind of design is used for screening designs. After an appropriate design is conducted, the response surface analysis can be done by any statistical computer software and then statistical analyses can be applied to draw the appropriate conclusions (Nuran, 2007).

Design of Experiments (DoE)

The choice of the design of experiments can have a large influence on the accuracy of the approximation and the cost of constructing the response surface. An important aspect of RSM is the design of experiments (Box and Draper, 1987), usually abbreviated as DoE. These strategies were originally developed for the model fitting of physical experiments, but can also be applied to numerical experiments. The objective of DoE is the selection of the points where the response should be evaluated. Most of the criteria for optimal design of experiments are associated with the mathematical model of the process. Generally, these mathematical models are polynomials with an unknown structure, so the corresponding experiments are designed only for every particular problem. In a traditional DoE, screening experiments are performed in the early stages of the process, when it is likely that many of the design variables initially considered have little or no effect on the response. The purpose is to identify the design variables that have large effects for further investigation. A detailed description of the design of experiments theory can be found in Box and Draper (1987), Myers and Montgomery (1995), among many others. Schoofs (1987) has reviewed the application of experimental design to structural optimization, Unal *et al.*, (1996) discussed the use of several designs for response surface methodology and multidisciplinary design optimization and Simpson *et al.*, (1997) presented a complete review of the use of statistics in design. A particular combination of runs defines an experimental design. The possible settings of each independent variable in the N dimensional space are called levels. Different methodologies is used such as Full factorial design, Central composite design, D-optimal designs, Taguchi's contribution to experimental design, Latin hypercube design, Audze-Eglais' approach, Van Keulen's approach.

Determination of Optimum Conditions

One of the main objectives of RSM is the determination of the optimum settings of the control variables that result in a maximum (or a minimum) response over a certain region of interest, R. This requires having a 'good' fitting model that provides an adequate representation of the mean response because such a model is to be utilized to determine the value of the optimum. Optimization techniques used in RSM depend on the nature of the fitted model.

For first-degree models, the method of steepest ascent (or descent) is a viable technique for sequentially moving toward the optimum response. Myers and Khuri (1979) developed certain improvements regarding the stopping rule used in the execution of this method. The first-degree model is usually used at the preliminary stage of a response surface investigation. Second-degree models are used after a series of experiments have been sequentially carried out leading up to a region that is believed to contain the location of the optimum response (Andre and Khuri 2010).

Response Surface Methodology in Agriculture

The field of RSM is well-researched and established within the industrial context and researchers in agriculture and related disciplines could well draw with advantage on the broad framework provided by this methodology in order to design and analyze their experiments. It has long been perceived that the RSM approach, having as it does an intrinsically sequential nature, is not particularly appropriate in the agricultural setting. Many agricultural experiments involve responses to the explanatory variables which are binary or count in nature and which can thus be modelled within the generalized linear model framework. For example, a researcher may be interested in the potency of the combination of two insecticides and, specifically, in their synergistic or antagonistic action. Response surface techniques are eminently suitable to such situations but this area of application has only recently attracted attention in the RSM literature (Myers, 1999).

Mead and Pike (1975) review the role of RSM in agriculture but, in so doing, emphasize the use of nonlinear models to accommodate biological data rather than of the empirical models traditionally used in RSM. Khuri and Cornell (1987) analyze an experiment on snap bean yield conducted using a central composite design. However such papers are rare and there is surprisingly little interest in RSM in agricultural applications within the mainstream statistical literature. On balance it is clear that while certain approaches within RSM are not appropriate for an agricultural setting, there is nevertheless a wealth of knowledge embedded within the broad field of RSM which can be drawn upon with advantage by agriculturalists.

The dependence of the yield of sugar cane on varying amounts of the nutrients, nitrogen, phosphorus and potassium, can be modelled empirically using a second-order polynomial model (Mapham, 1975) and this scenario is considered here. Edmondson (1991) provides an interesting application of RSM to greenhouse experiments and, in addition, presents some valuable insights into the use of RSM within an agricultural as opposed to an industrial setting. Designs taken from the RSM paradigm can be used to good effect in a traditional agricultural setting and this point is further underscored by the work of Khuri and Cornell (1987) and of Edmondson (1991).

CONCLUSION

Response Surface Methodology (RSM) is a collection of statistical and mathematical techniques useful for developing, improving and optimizing processes. The most extensive applications of RSM are in the particular situations where several input variables potentially influence some performance measure or quality characteristic of the process. RSM can be used for the approximation of both experimental and numerical responses. Two steps are necessary, the definition of an approximation function and the design of the plan of experiments. A desirable design of experiments should provide a distribution of points throughout the region of interest, which means to provide as much information as possible on the problem.

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