A computer-based educational tool for simulating multifactorial experiments of physical processes

Abstract

In this article, challenges in designing example problems of multifactorial experiments for an academic purpose are identified, and an algorithm for simulating multifactorial experiments is presented. It is based on a proposed mathematical function, which mimics a physical system, can be employed for any number of finite factors, and contains a unique peak, with which a unique optimal solution for an experiment is guaranteed. The proposed algorithm is implemented on an application developed with JavaScript, HTML, and CSS, which has been tested in the classroom for highlighting all characteristics of experimental design.

Keywords

Experimental design, educational tool, generating examples, problem-based learning, multifactorial model.

1. Introduction

Almost all the fields involving experimentation use experimental design [1]–[4]. It is part of various undergraduate and graduate curriculum, ranging from engineering to biological sciences. The objective of experimental design is to minimize cost and time of experiments and maximize its yield. As an example, it can be used to find the values of factors such as pH, oxygen concentration, sugar concentration, with which the enzyme production is maximized. Different optimization techniques can be employed to minimize number of experiments, with which the objective of experimental design is achieved [5] . On the other hand, an improper experimental design may lead to inaccurate or false conclusions, as well as a loss of money, material, and time [6].

Solving numerical examples helps students to learn statistics or mathematics [7] , or to develop insight into a particular topic [8] . Moreover, students obtain good learning experience using visual numerical examples of experiments [9] . On the other hand, finding the most accurate mathematical model for a process in experimental design involves performing various experiments with different combinations of factors. Usually, conducting experiments on a real system is not feasible due to any of the following limitations: 1) experiments on a real system can be costly, 2) a considerable amount of time may take each experiment, and 3) a great variety of experiments is difficult to be carried out. Hence, a computer program, that generates responses for some specific factors, is an excellent alternative to mimic physical systems, and to develop experimental design.

In this article, a computer-based educational tool for simulating experiments is proposed, which takes into account factor limits selected by the user. Teachers may adopt this educational tool in order to generate numerical examples, and to highlight all characteristics of experimental design. Moreover, the proposed educational tool allows teachers to evaluate the knowledge acquired by students during a course, and to implement problem-based learning. In this pedagogy, a student learns the topic while solving a problem given by the teacher. The core of the educational tool is a novel mathematical function that is designed to have a unique peak, thus providing a unique optimal solution of an experiment subjected to a number of finite factors. Moreover, this function has the quality that its gradient is not proportional to the distance from the optimal solution.

The paper has the following structure. Section 2 describes a multi-response model. The proposed mathematical function, employed by the computer-education tool, is presented in Section 3. The implementation of the proposed function is mentioned in Section 4. Section 5 describes the algorithm that generates an experiment of a multi-factorial process. Section 6 shows an application used to implement this algorithm. The paper ends with some concluding remarks.

1. Multi-response mathematical model

A numerical example for an experimental design is generated through a multi-response mathematical model that represents the physical process. This model consist of a set of static functions that map the factors to the responses, and it is given by



where ,  are responses, ,  are factors, ,  are nonlinear functions mapping the  factors to the  responses, and ,  are zero mean random noise. All factors, , are constrained by upper and lower limits. Numerical examples should produce unique optimal responses, , for the set of factors.

The algorithm developed in this paper uses a single response mathematical model, which is described by a proposed function presented in the next section. Several functions of this kind are used to mimic a multi-response system, since a set of  singe response systems can represent a multi-response system.

1. Proposed mathematical function

A static mathematical function with a single peak is achieved by any of the following functions:







Functions  and are a quadratic polynomial and a multivariable Gaussian function, respectively. Function is obtained by replacing the multiplication operator with a summation one. Figures 1, 2 and 3 respectively represent functions, , and  depending of two variables and. In addition, these figures include quiver plots, which represent the gradient’s direction and amplitude. The dotted lines in these figures indicate and .

Functions , , and have the following limitations:

1. Function  has a property that its slope increases linearly as it moves far away from the optimal point, i.e., its gradient at any point is directly proportional to the distance from the optimal point, which is not always true in physical systems. This fact is illustrated in Figure 1, where the lengths of the arrows of the quiver plot increase as a point moves far away from the intersection of the dotted lines.
2. Response surface methodology uses a second order fit algorithm. Hence, reaching an optimal solution for a system based on  requires very less effort, which is not recommended as a practical problem.
3. The solutions of , , and  do not contain the terms of other factors where . Multi factorial example problems based on these functions are easy to solve, because the optimization of a factor is independent of the optimization of the other factors. Figures 1, 2 and 3 show this property, which means that some arrows of the quiver plots coincide with the dotted lines.

Multiplying function  by  and making a change of variable produce the following proposed

mathematical function:



where ,,  and  are, respectively, the rows of some matrices  and  such that . Moreover, and.

Figures 4 and 5 depict  with ,  and ,  , respectively. The transpose of the gradient of  is given by



where  is a positive definite matrix. If  and are non-singular, then matrices  and are positive definite, respectively [10]. Moreover,  and are positive semidefinite when  and  are singular. Therefore, if either, or both are non-singular, then matrix in is positive definite, and as a consequence a unique peek at,  is guaranteed.

Unlike function, the gradient of function in is not directly proportional to the distance from its optimum point. Moreover, in contrast to functions ,  and, the solution  contains terms of other factors, where. These two facts can be observed by comparing Figures 1, 2, 3 with Figures 4, 5. Unlike Figures 1, 2 and 3, the arrows of the red quiver plots of Figures 4 and 5 do not coincide with the dotted lines.

In the next section, a method is presented to adapt the function, defined at , in order to generate random experiments.

1. Implementation of the proposed function

A scaled version of the proposed function  in is given by

























where ,  ,  is a random variable such that  and , with  the expected value notation. Moreover,  is a random variable with the properties  and. On the other hand  is the function range, and is a factor that introduces noise into the system. Parameter is a difficulty factor; the higher its value, the harder it is to reach the optimum value. In addition,  are the optimal factors where function reaches its maximum value,  and  are lower and upper limits of the  factor respectively,  and  are padding constants that limit the maximum value of the function  within the desired region.

It is worth mentioning that function, shown in , preserves all the mathematical properties of function. Moreover, multiplying function  in by a negative number inverts the peak of function.

Next section presents an algorithm that implements the proposed procedure.

5. Algorithm

The objective of the algorithm is to generate experimental results by simulating a multi-factorial process. Teacher gives the parameters required by the multi-factorial process such as upper and lower limits of the factors, and students perform experiments at different factors. The algorithm generates responses for the given,  factors using the equations and inequalities shown in equations to .

Figure 6 shows the flowchart of the proposed algorithm. The teacher should define the values of  and , where  and  should be less than 0.5. Based on our experience, It is recommended to use, and . It is important to mention that this algorithm can be implemented in any programming language.

6. Application

The triad of JavaScript (JS), Hypertext markup language (HTML) and Cascading Style Sheets (CSS) is used to create the application presented at the web page [11]. JS is used to implement the algorithm discussed in the previous section.

Master students of the Biological Sciences Faculty, Universidad Autónoma de Coahuila, are instructed to use this application. Figure 7 shows the screenshot of the application. It is employed by students in the classroom, at homework, and in projects related to the learning of Response Surface Methodology (RSM). Students are asked to perform experiments on this application by opening it in the web browser with the objective of maximizing the response of a biological process with  factors. The graphic user interface allows performing multiple experiments at once, where a student can paste factorial information and copy the model response to the clipboard. The factors computed by the students, are compared with the optimal ones in order to evaluate the student's performance. It is worth mentioning that the optimal values are not shown in the graphic user interface. The application contains a distance tool, which measures the distance between the estimated values to the optimal ones, thus students can use this tool in order to verify if their computed values are correct or not.

As an example of an experiment, consider a biological process with two factors, which are pH and temperature that takes values between 1 to 13 and 0 to 100° Celsius, respectively. Letand the factors pH and temperature, respectively, and let  the enzyme production that will be maximized. The lower and upper limits of these factors are,, , and as shown in Fig. 7. The scaled version of function , described in equations (7) to (18), uses the parameters:, , , , , , , , , and , , , , , , , , and . Figure 8 shows the surface plot of. Moreover, Figures 9 and 10 show, respectively, the contour and surface plots of the function  when it is not corrupted by the noise term, i.e.,. In this experiment, the Response Surface Methodology estimates the optimal values of and, and the results of each iteration are superimposed over these plots.

7. Conclusions

This article presented a computed educational tool, designed in HTML, CSS, and JavaScript, in order to generate random processes with factors provided by a teacher. It is based on a novel single response, unique peak multivariable mathematical function, denoted as. This function mimics a multi response physical process designed for experiments, it is adapted to generate experimental data for a selected range of factors, and its gradient is not proportional to the distance from the optimal point. Students that learn the topic of Response Surface Methodology use the proposed education tool in order to perform experiments with the objective of maximizing the response of a biological process with factors. This educational tool can be used for showing the performance of other optimization algorithms that can maximize the response of a process, such as the Taguchi methods.

Acknowledgments

The authors thank the anonymous reviewers for their helpful comments.

References

[1] R. A. Fisher, *The design of experiments*. Oliver And Boyd; Edinburgh; London, 1937.

[2] G. P. Quinn and M. J. Keough, *Experimental Design and Data Analysis for Biologists*. Cambridge University Press, 2002.

[3] D. C. Montgomery, *Design and Analysis of Experiments*. John Wiley & Sons, 2008.

[4] J. Antony, *Design of Experiments for Engineers and Scientists*. Elsevier Science, 2014.

[5] A. M. Sarotti, R. A. Spanevello, and A. G. Suarez, “An efficient microwave-assisted green transformation of cellulose into levoglucosenone. Advantages of the use of an experimental design approach,” *Green Chem.*, vol. 9, no. 10, pp. 1137–1140, 2007.

[6] M. F. W. Festing, “Principles: The need for better experimental design,” *Trends Pharmacol. Sci.*, vol. 24, no. 7, pp. 341–345, 2003.

[7] X. Zhu and H. A. Simon, “Learning mathematics from examples and by doing,” *Cogn. Instr.*, vol. 4, no. 3, pp. 137–166, 1987.

[8] A. Renkl, “Learning from worked-out examples: A study on individual differences,” *Cogn. Sci.*, vol. 21, no. 1, pp. 1–29, 1997.

[9] J. Hattie and G. C. R. Yates, *Visible Learning and the Science of How We Learn*. Taylor & Francis, 2013.

[10] A. S. Poznyak, *Advanced mathematical tools for automatic control engineers. Volume 1, Deterministic techniques*. Elsevier, 2008.

[11] S. K. Gadi, “Multifactorial experiment simulator - Suresh Kumar Gadi,” 2017. [Online]. Available: https://skgadi.com/tools/multifactorial-experiment-simulator/. [Accessed: 27-Aug-2017].