Proposed Finishing Strategies Based on Experimental Designs for Process Optimisation

Pongchanun Luangpaiboon
Department of Industrial Engineering, Faculty of Engineering,
Thammasat University, Pathumthani 12121 Thailand

Abstract

The objective of this work is to compare the efficiency of the second order experimental designs for determining the optimal values of a process after a sequential movement accomplished with the first order designs and a path of steepest ascent, in the presence of noise. Widely used second order designs such as a hexagon design and a central composite design in a new aspect, finishing strategies, are implemented on response surfaces with various levels of signal noise, in this study. The relationships between variables and responses of a process are restricted to three dimensional uni-modal functions. Performance measures considered are a response and a linear distance achieved by each design. The results suggest that the hexagon design is the most efficient on all the response surfaces at the lower level of noise whereas this version of the central composite design seems to be the most suitable on the response surfaces with higher noise levels. However, the hexagon design requires fewer experimental trials whilst searching for the maximum.

Key words: Response surface; orthogonal hexagon design; finishing strategies; central composite design

1. Introduction

The goal of this study is to compare two strategies for determining an optimal (maximal) response. The variables that determine the yield or response of the process are usually measured in their natural units. Usually the functional relationship between variables and the yield is unknown. In this situation the proper choices to optimise the response are search techniques. Response surface methodology is of interest among them. In response surface methodology, it is convenient to transform these variables to corresponding coded variables $x_1, x_2, \ldots, x_k$, referred as process variables. The coding is chosen so that changes of one unit are practical when searching for optimum conditions. In terms of coded variables, the relationship has a general form,

$$y = f(x_1, x_2, \ldots, x_k) + \varepsilon,$$

in which f is the unknown response surface function of x's and the ε is the error. In geometric terms, this equation can be represented by a surface in k+1 dimensions. The procedures rely on local linear approximations, which are normally extended to quadratic functions near optima.

Box and Wilson [1] proposed a procedure for seeking the optimum using the method of steepest ascent. The procedure begins with a factorial experiment around the prevailing operating conditions. A plane is fitted to the results and a sequence of runs is carried out by moving in the direction of steepest ascent. When curvature is detected, another factorial experiment is conducted. This is used either to estimate the position of the optimum or to specify a new direction of steepest ascent.

Box [2] suggested a sequence of 2^k factorial experiments; each displaced in the direction of steepest ascent from the preceding experiment. He described this as evolutionary operation, and stated that the objective of evolutionary operation is to move a full scale process towards optimum efficiency as quickly as possible. Many textbooks, for example, [3,4] offer advice on this strategy.

Brooks [5] investigated the performance of various methods such as the steepest ascent, univariate, factorial and random methods, for seeking maximum on responses with and without noise. Brooks and Mickey [6] gave a theoretical argument that the minimal number of trials to estimate the direction of steepest ascent, from noisy observations, is just one more than the number of influential variables, that is a simplex design. For a planar surface, the best design in terms of expected improvement per unit effort is a triangular design.

However, these papers investigated the applications of first order designs through computer simulation models. Montgomery and Evans [7] later considered and discussed the use of various second order approximating polynomials on six response surfaces with the presence of noises. They found that a hexagon design emerged as the best design on the average in all situations investigated. A central composite class of designs, more widely used, also gave good results.

Most papers on response surface methodology discuss the use of second order designs to improve the estimate of the optimum after a sequential movement accomplished with the first order design. Many textbooks, for example, [3,4] also offer advice on this procedure. However, despite the form of second order designs widely applied in this manner, the purpose of the experimental design is one that should allow the experimenter to seek other appropriate ways.

Luangpaiboon [8] introduced *a finishing strategy* based on the second order central composite design in a new aspect for finding the maximum on a hypersurface after the use of the first order investigation of response surfaces with various levels of measurement noises. For the finishing strategy the final estimate of the optimal values of the process variables were found by interpolation, within a further experiment, rather than by taking the optimum as the last design point.

This paper undertakes further investigation after a sequential movement accomplished with the first order design. Specifically, we compare the performance of the version of finishing strategies based on the hexagon and central composite designs, in a process with measurement noises on the response. Section 2 gives a brief overview of finishing strategies and response surfaces investigated. Section 3 contains the numerical results and discussions.

2. Methods

In this paper, we examine variations of the proposed finishing strategies based on hexagon and central composite designs, after a sequential movement of first order designs with the path of steepest ascent, regarding different error standard deviations. These classes of designs were constructed and applied to surfaces typically generated by computer simulation models. One hundred replicates were implemented at each value of the error standard deviation. The centre points of designs were chosen randomly on a square feasible region of operation for all response surfaces. The numerical comparisons are limited to a hypothetical process with uni-modal and two process variables. Two measures of performances, followed [7], are implemented. The first measure is an achieved response (observed at the estimated optimum variable combination) and the latter is a linear distance from the stationary point (the predicted optimum levels for the independent variables to the point corresponding to the actual optimum levels of the independent variables). The objective of this paper is to investigate how the choice of best strategy for defining an optimal location depends on the amount of random variation in process yields when parameters are fixed.

2.1 Finishing Strategies Investigated

2.1.1 Central Composite Design

This is the variation on the sequential use of factorial designs augmented with star designs to estimate curvature when appropriate. For k variables the basic factorial will be a 2^k design. The star design consists of $2k$ axial points together with centre points, the combination of the 2^k and star design giving a central composite design (Figure 1). The following variations all start from a single 2^k design at some convenient point in the safe region of operation.

The finishing strategy is to carry out a central composite design (CCD), centred on the design point with the greatest observed yield. A quadratic polynomial,

$$\hat{y} = \hat{\beta}_o + \sum_{i=1}^{k} \hat{\beta}_k x_i + \sum_{i=1}^{k} \hat{\beta}_{ii} x_i^2 + \sum_{i}\sum_{j, i<j} \hat{\beta}_{ij} x_i x_j ,$$

is fitted to the results from the CCD and the location of the maximum of this fitted surface is determined by calculus. In matrix notation, the quadratic surface is

$$\hat{y} = \hat{\beta}_o + \mathbf{x}^T\mathbf{b} + \mathbf{x}^T\mathbf{B}\mathbf{x}, \text{ where}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \mathbf{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} \text{ and}$$

$$\mathbf{B} = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \dots & \hat{\beta}_{1k}/2 \\ \hat{\beta}_{12}/2 & \hat{\beta}_{22} & \dots & \hat{\beta}_{2k}/2 \\ . & . & & . \\ . & . & & . \\ \hat{\beta}_{1k}/2 & \hat{\beta}_{2k}/2 & \dots & \hat{\beta}_{kk} \end{bmatrix}$$

Partial derivatives of $\hat{y}$ with respect to $\mathbf{x}$ are equated to the zero vector, i.e.

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = \mathbf{0}$$

and the stationary point, $\mathbf{x}_0$, is given by:

$$\mathbf{x}_0 = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b}.$$

If this maximum is within the hypercube which just contains the CCD, it is taken as the optimum operating point. If the maximum is outside the hypercube then a second CCD is carried out, centred on the design point of the preceding CCD, which had the greatest yield. A quadratic surface is then fitted to the results of both CCDs, and the maximum is determined by calculus. If this maximum is inside the union of the hypercubes, which just contain the CCDs, it is taken as the optimum operating point. If the maximum is outside the hypercubes then the optimum operating point is taken as the point on the edge of the union of the hypercubes which corresponds to the greatest value of the fitted polynomial. This is referred as a finishing strategy rather than a stopping rule because the final estimate of the optimum values of the variables are found by interpolation, within further experiment, rather than by assuming the optimum is at the design point with the highest recorded yield.

2.1.2 Hexagon Design

There are other classes of second order designs, excluding some of the most often used designs today. An equiradial design is very useful. The special case is the hexagon design (Figure 2), sixed equally spaced points on a circle of radius ρ, augmented by n center points. If the first design point makes an angle θ with the real axis, then the portion of the design matrix involving all the points on the axis can be written, for example, the two variable case:

x_1	x_2
$\{\rho\cos[\theta + (2\pi u)/6]\}$	$\{\rho\sin[\theta + (2\pi u)/6]\}$

; u = 0, 1, 2, 3, 4, 5

[9]. It is of interest to consider the important design moments for the hexagon. This makes a hexagon design to be indeed rotatable. From the design matrix of a hexagon design it can be constructed to be a rotatable and orthogonal experimental design; one starts with a set of 6 equally spaced and augmented with 6 centre points.

From this second order design we implement the same fitted model procedure as the finishing strategy does to determine the estimated optimum variable levels as the stationary point.

2.2 Response Surfaces

The finishing strategies for noisy systems were compared for the case of two process variables, x_1 and x_2, on six three-dimensional uni-modal response surfaces defined over a square feasible region of operation ranging from 0 to 200. The experimental region of the following response surfaces contains a single maximum that is $y^* = 100$ at $x_1 = 100$ and $x_2 = 100$. The response will be referred to as yield and it would be generated by a computer simulation in this study. The comparisons are made for three different levels of measurement noises on the response. The noise is taken to be independently and normally distributed with mean of zero and standard deviations of 0, 5 and 10. The mathematical formulae of the yields were as follows.

Surface 1

$$y=100\sum_{j=1}^{2}[(1-x_j/100)^2]+\varepsilon$$

This response surface is a paraboloid.

Surface 2

$$y=100[1-\{(100[(x_2/100)-(x_1/100)^2]^2)+[1-(x_1/100)]^2\}]+\varepsilon$$

This response surface is a curved ridge called a Rosenbrock banana shaped surface [10].

Surface 3

$$y=100\{(0.5+0.5(x_1/100))^4(x_2/100)^4\exp[2-(0.5+0.5\,(x_1/100))^4-(x_2/100)^4]\}+\varepsilon$$

This response surface can be called independent since the relative effect of one factor is independent of the level of the other factor.

Surface 4

$$y=100\{(0.3+0.4(x_1/100)+0.3(x_2/100))^4(0.8-0.6(x_1/100)+0.8(x_2/100))^4\exp[2-(0.3+0.4(x_1/100)+0.3(x_2/100))^4-(0.8-0.6(x_1/100)+0.8(x_2/100))^4]\}+\varepsilon$$

This response surface is the same as ***Surface 3*** rotated approximately 37 degrees [5].

Surface 5

$$y=100\{(x_1/100)^2\exp[1-(x_1/100)^2-20.25((x_1/100)-(x_2/100))^2]\}+\varepsilon$$

This response surface is a sharp, narrow ridge with large area of low flat response.

Surface 6

$$y=100\{(0.3(x_1/100)^2+0.7(x_2/100)^2)^3\exp[1-0.6((x_1/100)-(x_2/100))^2-(0.3(x_1/100)^2+0.7(x_2/100)^2)^3]\}+\varepsilon$$

This response surface is a relatively flat curvilinear ridge [7].

3. Results and discussions

Table 1 shows performance measures, an achieved yield and a linear distance, based on 100 replicates. The detailed results of two designs for the achieved yield in each surface are shown in Table 2-7. In general, the finishing strategy based on the hexagon design gave both performance measures better than the strategy based on the central composite design when there was no measurement noise. However, the finishing strategy based on the central composite design provided better results when the noise standard deviation was increased. This may be significant although 26 experimental trials, on the average, were required. The results obtained will be affected by the responses from ***Surface 2***, a modification of Rosenbrock banana shaped surface. This surface has a steep curving ridge with negative response values, further from the optimum. Thus this deducted the average values of responses in each design compared.

On the basis of the experiments and the results obtained it may be difficult to assuredly draw a conclusion. There is a hierarchy of errors involved in computer simulations of processes. If randomisation is included, then different realisations will lead to different results. This can be allowed for by replicate realisations and the error can be reduced to any desired level, given sufficient computing resources. A second source of error, as with any mathematical model, is that the performance of the computer simulation will not be identical to that of the plant or the process [11]. As mentioned, the numerical comparisons are limited to a hypothetical process with uni-modal and two process variables. The results obtained may not be practical to extend to response surfaces with more than three dimensional multi peaks.

4. References

[1] Box, G.E.P. and Wilson, K.B., On the Experimental Attainment of Optimum Conditions, Journal of the Royal Statistical Society, Series. B, Vol.13, pp.1-45, 1951.

[2] Box, G.E.P., Evolutionary Operation: a Method for Increasing Industrial Productivity, Applied Statistics, Vol.6, pp. 81-101, 1957.

[3] Box, G.E.P. and Draper, N.R., Evolutionary Operation A Statistical Method for Process Improvement, John Wiley, New York, 1969.

[4] Montgomery, D.C., Design and Analysis of Experiment (5th ed.), John Wiley, New York, 2001.

[5] Brooks, S.H., A Comparison of Maximum-Seeking Methods, Operations Research, Vol.7, pp.430-457, 1959.

[6] Brooks, S.H. and Mickey, M.R., Optimum Estimation of Gradient Direction in Steepest Ascent Experiments, Biometrics, Vol.46, pp.48-56, 1961.

[7] Montgomery, D.C. and Evans, D.M., Jr., Second-order Response Surface Designs in Computer Simulation. Simulation, Vol.25, No.6, pp.169-178, 1975.

[8] Luangpaiboon, P., A Comparison of Algorithms for Automatic Process Optimisation, Ph.D. Thesis, Newcastle upon Tyne, UK, 2000.

[9] Myers, R.H. and Montgomery, D.C., Response Surface Methodology: Process and Product Optimisation Using Designed Experiments, John Wiley, New York, 1995.

[10] Gill, P.E., Murray, W. and Wright, M.H., Practical Optimisation, Academic Press, New York, 1981.

[11] Luangpaiboon, P., Metcalfe, A.V., Rowlands, R.J., Tham M.T. and Willis M.J., Comparison of the Modified Simplex Method and a Genetic Algorithm for Optimising a Chemical Process, Proceedings of the 1st International Conference on Industrial Statistics in Action 2000, Newcastle upon Tyne, UK, 2000.

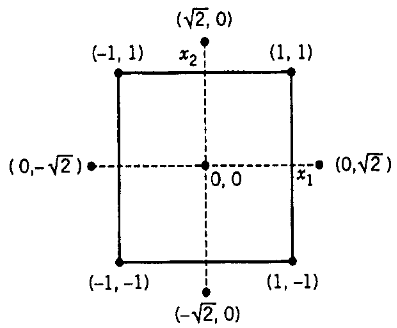

Figure 1. Central composite design for a two-variable case

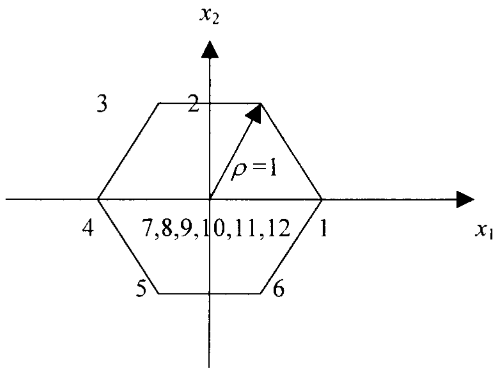

Figure 2 Hexagon design for a two-variable case

Table 1 Average and standard deviation of responses by designs for all surfaces

Performance	Measure	Central Composite Design			Hexagon Design		
		Stdev. of Noise			Stdev. of Noise		
		0	5	10	0	5	10
Achieved Yield	Average	89.5623	56.7828	69.513	90.553	1.2191	15.123
	Stdev.	9.8433	46.0233	61.2113	10.8362	108.6373	132.1671
Linear Distance	Average	10.2315	11.2005	10.5447	9.2384	19.9271	19.4377
	Stdev.	5.8144	8.5332	6.5118	4.6596	11.293	12.1727

Table 2 Performance measure of the achieved yield for *Surface 1*

Design	Stdev. of Noise			Average
	0	5	10	
Central Composite Design	100	97.8963	97.2564	98.38423
Hexagon Design	100	98.0174	97.9275	98.6483

Table 3 Performance measure of the achieved yield for *Surface 2*

Design	Stdev. of Noise			Average
	0	5	10	
Central Composite Design	99	-165.235	-297.626	-121.287
Hexagon Design	99	-400.418	-348.134	-216.518

Table 4 Performance measure of the achieved yield for *Surface 3*

Design	Stdev. of Noise			Average
	0	5	10	
Central Composite Design	99.1016	92.2982	90.6452	94.015
Hexagon Design	99.2659	89.1417	90.8202	93.07593

Table 5 Performance measure of the achieved yield for *Surface 4*

Design	Stdev. of Noise			Average
	0	5	10	
Central Composite Design	98.2315	84.0568	66.8325	83.04027
Hexagon Design	98.397	67.4326	91.413	85.74753

Table 6 Performance measure of the achieved yield for *Surface 5*

Design	Stdev. of Noise			Average
	0	5	10	
Central Composite Design	78.8965	75.7386	50.8916	68.5089
Hexagon Design	50.1949	66.3121	69.9417	62.14957

Table 7 Performance measure of the achieved yield for *Surface 6*

Design	Stdev. of Noise			Average
	0	5	10	
Central Composite Design	98.2307	89.1156	90.1258	92.4907
Hexagon Design	96.4602	86.8292	88.7699	90.68643