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A STUDY OF THE NELDER AND MEAD MODIFIED SIMPLEX METHOD WITH THE SECOND-ORDER DESIGNS ON UNI- AND DUAL-RESPONSE SYSTEMS

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ABSTRACT

Modified simplex method (MSM) is a method for finding the optimal conditions of industrial processes. In general, this approach will search for the proper conditions under a consideration of a uni-response system, an average of process yields. However, the uni-response system may not be valid when the variance of yields is not constant. This research concerns a dual-response system, with both average and variance of responses. The objective of this work is to compare the efficiency of the MSM with the completion of the central composite and hexagon designs on various systems for determining the optimal values of a process in the presence of noise. On both uni- and dual-response systems, the average of actual responses and the average of distance between true optimum point and estimated optimum point are not significantly different when compared. However, the average of standard deviation of actual responses from the MSM with the central composite design seems to be worse. In summary, the optimisation strategy of the MSM based on hexagon design leads to the better condition with fewer experimental trials whilst searching for the maximum.

KEYWORDS: uni response, dual response; optimisation strategy; modified simplex method, hexagon design; central composite design

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1. INTRODUCTION

Response surface methodology (RSM), first proposed by Box and Wilson [1], is designed to explore an experimental region for finding the optimal settings of a set of variables that maximise the response. Usually the functional relationship between variables and the yield is unknown. In this situation the proper choices to optimise the response are search techniques. In RSM, 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. The process is normally extended to quadratic functions near optima.

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, 5] offer advice on this strategy. 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. Myers and Carter [8] proposed an algorithm associated with the exploration of a surface with dual responses. The approach is to search variable settings which optimise a primary response function of average responses subject to the condition that a constraint response function, the variance of responses, takes on some specified or preferable value. Vining and Myers [9] presented how the dual-response approach of optimising a primary (mean) response function while simultaneously satisfying conditions on a secondary response (variance) function can be applied to achieve the goal. Its significance is the use of statistical methods to achieve both criteria.

Castillo and Montgomery [10] expressed how the goals of a dual response optimisation approach can be achieved using standard Non-Linear Programming (NLP) technique, the generalised reduced gradient (GRG) algorithm. It has been claimed that the proposed method leads to be more flexible and easier to use than the original dual response approach. The dual response problem is nonlinear programming since the primary and secondary responses are quadratic (second order) function). Lin and Tu [11] proposed a more satisfying and substantially simpler optimisation procedure on a dual-response approach. Luangpaiboon [12] 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.

The rigid simplex method appears to have been first proposed by Spendley et al. [13]. The basic unit, called the simplex, of the simplex design in a problem with k predictor variables consists of $k+1$ equi-distance design points. The yield is measured for each of the $k+1$ design points. The vertex corresponding to the design point with the lowest yield is identified and reflected in the opposite hyperface, i.e. the vertex with the lowest yield is rejected. The next run is carried out with predictor variables set at values corresponding to this new point, and the algorithm can continue in this fashion. However, it is possible that the new design point leads to the least yield of the new simplex in which case the second lowest yield of the original simplex is rejected in an attempt to prevent the algorithm oscillating. Also, in order to avoid rotating about a spurious high yield, a replicate observation replaces the original if a vertex has been retained in $k+1$successive simplexes. The sequence of runs continues until the standard deviation of the estimated yields at the vertices of the simplex is less than some preset critical value, or the algorithm oscillates.

There are many variations on the rigid simplex algorithm, one of the best known being the modified simplex method (MSM) of Nelder and Mead [14]. In the MSM an expansion or contraction of the reflection is allowed at each step. Arnholt [15] compared the MSM with a steepest ascent algorithm, one of several algorithms we use in our comparison, and used a stopping rule for the MSM which was triggered by the ratio of the best to the worst yield in a simplex being less than some value close to unity.

This paper undertakes further investigation after a sequential movement accomplished with the MSM. Specifically, we compare the performance of the version of optimisation strategies based on the hexagon and central composite designs, in a process with measurement noises on the response.

2. METHODS

In this paper, we examine variations of the proposed optimisation strategy based on hexagon and central composite designs, considering both the mean and the standard deviation of the responses of interest, after a sequential movement of (MSM), regarding of 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 two process variables. Four measures of performances, followed [7], are implemented. The first and second measures are an average of actual response (y_{f1}) and an average linear distance from the estimate to the target (y_{f2}), respectively. The third is an average percentage of the estimate and the target response (y_{f3}). Finally, it is a standard deviation of the actual responses (y_{f4}). The objective of this paper is to investigate how the choice of best optimisation strategy for defining an optimal location depends on the amount of random variation in process yields when parameters are fixed.

2.1 Uni Response System

2.1.1 Modified Simplex Method

The simplex design is first applied at an arbitrary point within the safe region of operation. The response is measured for each of the design points. The vertex corresponding to the lowest yield is identified and reflected in the opposite hyperface. The new design point can be extended or contracted depending on the yield, in each vertex of the last simplex [14]. The next run is carried out with predictor variables set at values corresponding to this new point. This simplex algorithm stops, when either the standard deviation of the yields in the simplex is less than some preset critical value or the simplex is smaller than some preset minimum size.

2.1.2 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. 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 of the primary estimated response is fitted to the results from the CCD and the location of the maximum of this fitted surface is determined by calculus.

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.

2.1.3 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 (HEX) design, sixed equally spaced points on a circle of radius, ρ, augmented by n center points [9]. It is of interest to consider the important design moments for the hexagon. 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 Dual Response System

In order to achieve the objective of the dual-response system the experimenter can identify a primary estimated response, $\hat{y}_p$, as above to search for the appropriate location via

the method of steepest ascent. This optimisation strategy then adds a secondary estimated response, the standard deviation of responses ($\hat{y}_s$) for a first and second order design, written as,

$$\hat{y}_s = \hat{\gamma}_o + \sum_{i=1}^{k} \hat{\gamma}_i x_i + \sum_{i=1}^{k} \hat{\gamma}_{ii} x_i^{\,2} + \sum_{i<j} \sum_{j} \hat{\gamma}_{ij} x_i x_j \text{ , for a second order design.}$$

All other matrices are defined as above. Lin and Tu [11] proposed the dual response optimisation procedure focusing on the case "target value is best". This case means keeping the mean, μ, at a specified target value, μ_0, whilst minimising the standard deviation, σ, namely: Minimise $\hat{y}_s$

Subject to $\hat{y}_p = \mu_0$.

The procedures can be illustrated as follow,

1. Estimate the mean response ($\hat{y}_p$) and the standard deviation response ($\hat{y}_s$) and both are functions of **x**.
2. Find the optimal setting of conditions of **x** such that will be close to the target value, T, while the standard deviation, $\hat{y}_s$ is kept small. This condition minimises the mean square error, MSE,

$$MSE = (\hat{y}_p - T)^2 + \hat{y}_s^{\,2}$$

2.3 Response Surfaces

The optimisation strategies for noisy systems were compared for the case of two process variables, x_1 and x_2, on three response surfaces defined over a feasible region of 9 unit^2 area. The experimental region of the following response surfaces contains a single maximum that is $y^* = 100$ at (x_1, x_2) of (15, 15), (4, 4) and (5, 4) for *Surface 1*, *2* and *3* respectively. The response will be referred as yield, shown in Figures 1-3, and it would be generated by a computer simulation in this study throughout. The noise (ε) is taken to be independently and normally distributed with mean of zero and standard deviations (S.D) of 5 and 10 of the optimal response. The mathematical formulae of the yields are following.

Surface 1

$$y = 100 - 8[[\frac{(10-\frac{x_1}{1.5})^2}{7}]+[\frac{(10-\frac{x_2}{1.5})^2}{7}]] + \varepsilon$$

This response surface is a paraboloid.

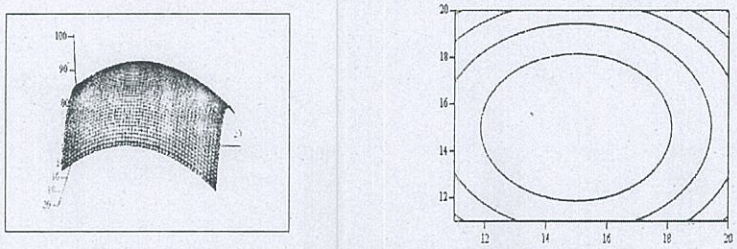


Figure 1 The Surface and Contour Plots for *Surface 1*

Surface 2

$$y = 80+10\mathrm{Exp}[-2(x_1-4)^2]+10\mathrm{Exp}[-2(x_2-4)^2]+$$
$$7\mathrm{Exp}[-9(x_1-8)^2]+7\mathrm{Exp}[-15(x_2-8)^2]+\varepsilon$$

This response surface is a curved ridge called a multi-peak hartman's family surface.

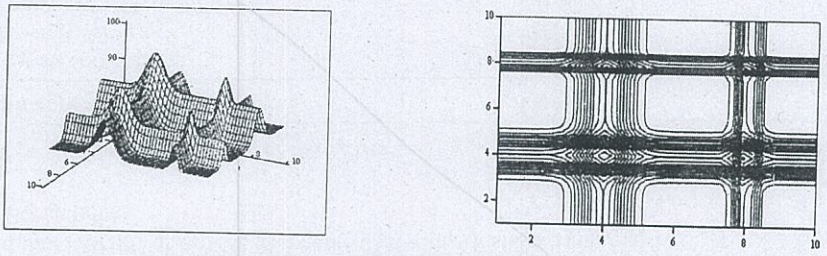


Figure 2 The Surface and Contour Plots for *Surface 2*

Surface 3

$$y = -(\frac{20}{17})[8(1-\frac{x_1}{5})^2+[(\frac{x_2}{5})-0.8(\frac{x_1}{5})^2]^2]+100+\varepsilon$$

This response surface is a curved ridge called a Rosenbrock curved ridge surface.

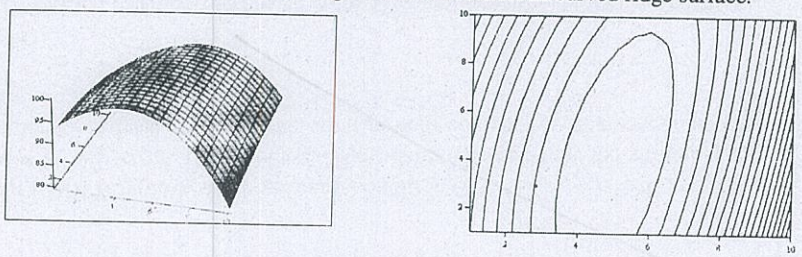


Figure 3 The Surface and Contour Plots for *Surface 3*

3. RESULTS AND DISCUSSIONS

Experimental results on the uni-response system were more equivocal [12]. 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 optimisation strategy based on the central composite design provided better results when the noise standard deviation was increased. The results obtained will be affected by the responses from ***Surface 3***, a modification of Rosenbrock curved ridge surface. On the dual response system Table 1 shows all performance measures based on 100 replicates for all scenario. The results of all hypothesised testings of the difference in means on both designs are also confirmed in Table 2. However, there was no significance on the first three performance measures of an average of actual response (y_{f1}); an average linear distance from the estimate to the target (y_{f2}) and an average percentage of the estimate and the target response (y_{f3}) [16].

Table 1 All performance measures categorised by surfaces

Surface	S.D	y_{f1}		y_{f2}		y_{f3}		y_{f4}	
		MSM CCD	MSM HEX	MSM CCD	MSM HEX	MSM CCD	MSM HEX	MSM CCD	MSM HEX
Paraboloid	5	98.86	98.89	1.33	1.32	-1.14	-1.11	2.94	2.34
	10	97.44	97.5	2.01	2.02	-2.56	-2.5	5.38	4.45
Hartman	5	99.12	99.01	2.77	2.92	-0.88	-0.99	2.82	2.16
	10	98.35	98.33	3.02	2.8	-1.65	-1.67	5.68	4.3
Rosenbrock	5	99.12	99.01	2.77	2.92	-0.88	-0.99	2.82	2.16
	10	98.35	98.33	3.02	2.8	-1.65	-1.67	5.68	4.3

Table 2 Hypothesised testings for all performance measures

Surface	S.D	*yf1*		*yf2*		*yf3*		*yf4*	
		P-Value	H0	P-Value	H0	P-Value	H0	P-Value	H0
Paraboloid	5	0.8414	Not Reject	0.8822	Not Reject	0.8414	Not Reject	0.0001	Reject
	10	0.8613	Not Reject	0.9814	Not Reject	0.8613	Not Reject	0.005	Reject
Hartman	5	0.6974	Not Reject	0.9487	Not Reject	0.6974	Not Reject	0.0017	Reject
	10	0.3312	Not Reject	0.9295	Not Reject	0.3312	Not Reject	0.0417	Reject
Rosenbrock	5	0.3366	Not Reject	0.5276	Not Reject	0.3366	Not Reject	0.0000	Reject
	10	0.9333	Not Reject	0.3543	Not Reject	0.9333	Not Reject	0.0000	Reject

For both concepts of the uni or dual response surface systems the average of actual responses and the average of distance between true optimum point and estimated optimum point are not significantly different when compared. The average of standard deviation of actual responses from the strategy with the central composite design seems to be worse though this version of the CCD seems to work well on the mean responses with higher noise levels. In summary, if there is no justification for any assumptions about the magnitude of the measurement noise of the response surface, the optimisation strategy based on the hexagon design leads to the better condition. The hexagon design also requires fewer experimental trials whilst searching for the maximum when compared.

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