UNIVERSITI PUTRA MALAYSIA

DUAL RESPONSE SURFACE AND ROBUST DESIGN OPTIMIZATION BASED ON PENALTY FUNCTION METHOD

ISHAQ ABDULLAHI BABA

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By

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Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Master of Science

May, 2015

DEDICATIONS

To my Late Mother Maryam Shuaibu Maikanwa
To my Late Father Alh. Abdullahi Baba

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Master of Science

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Chair: Professor Habshah Bt Midi, PhD
Faculty: Science

Despite all the existing optimization schemes for solving dual response surface problem, the tradeoffs between the mean and variance functions remain unsolved. It is now evident that selecting an appropriate optimization scheme in the determination of the optimal setting conditions is critical. Most of the existing optimization schemes do not take into account the measure on violation of constraint in the conversion of the constrained to an unconstrained optimization. The purpose of this thesis is to introduce a new optimization scheme based on the penalty function method. The penalty function method converts the constrained into unconstrained optimization problem by adding the constraint to the original objective function. The advantage of the new approach is that it takes into consideration the constraint by introducing a penalty constant. The performance of the new proposed technique is compared with three other existing techniques

Dual response surface optimization uses the ordinary least squares method OLS to determine the adequate process mean and variance response functions by assuming that the design data come from a normal distribution function and there is no outlier in the data set. Under this condition, the sample mean and sample variance are the most appropriate method to estimate the mean and variance of the response variables. However, the sample mean and the sample variance are duly affected by outlier in which may lead to producing inconsistent estimates of coefficient of the regression and sometime even change the sign of regression line. Robust methods are design to remedy this type of problems. Median and median absolute deviation MAD are robust substitute of mean and variance of response variables respectively. Nonetheless, they are known to be less efficient than mean in uncontaminated data. It is part of

our objective in this thesis, to propose using a highly efficient and resistant robust location and scale of the MM estimator for estimating the mean and variance of the response variables using the new proposed optimization scheme and also to propose MM estimator to estimate the parameters of response function for the process mean and variance.

Furthermore, the usual assumption of equal number of replications at each design point during an experiment is often impractical in real life industrial application of dual robust design optimization. In this case, applying the ordinary least squares method, OLS to determine the estimated response functions for mean and variance processes may be affected by the presence of heteroscedasticity problem. As our third objective in this thesis, we proposed using the weighted least squares method, WLS to estimate the parameters of the regression model and apply the new optimization scheme to find the optimal setting conditions for the estimation of the optimal mean response.

The overall results signify that the proposed optimization scheme PM is superior to other existing optimization schemes. The PM based on the proposed MM robust location and scale estimator also outperforms other methods. Finally, the proposed method based on WLS turned out to be the most efficient method in the presence of heteroscedasticity problem.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

DWI PERMUKAAN SAMBUTAN DAN PENGOPTIMUMAN REKABENTUK TEGUH BERDASARKAN KAEDAH FUNGSI PENALTI

Oleh

ISHAQ ABDULLAHI BABA

Mei, 2015

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Disamping semua skema pengoptimuman sedia ada bagi menyelesaikan masalah dua permukaan sambutan, pemilihan keutamaan antara fungsi min dan fungsi varians masih belum dapat diselesaikan sepenuhnya. Telah dibuktikan bahawa pemilihan skema pengoptimuman yang sesuai dalam menentukansituasi optimal setting adalah kritikal. Kebanyakan skema pengoptimuman sedia ada tidak mengambil peduli perlanggaran ukuran kekangan semasa penukaran pengoptimuman berkekangan kepada tidak berkekangan. Tujuan tesis ini ia lah untuk memperkenalkan suatu skema pengoptimuman berasaskan kaedah fungsi penalti. Kaedah fungsi penalti menukar fungsi pengoptimuman berkekangan kepada tak berkekangan dengan mencampurkan kekangan ke dalam fungsi objektif asal. Kebaikan pendekatan baru ini ialah ia mengambil kira ukuran perlanggaran kekangan dengan memperkenalkan pemalar penalti. Prestasi kaedah baru yang dicadangkan dibanding dengan tiga teknik sedia ada.

Pengoptimuman dua permukaan sambutan menggunakan kaedah kuasadua terkecil biasa (OLS) untuk menentukan kecukupan fungsi proses min dan fungsi proses varians dengan membuat anggapan bahawa data dipungut daripada fungsi taburan normal dan tiada titik terpencil di dalam set data. Di bawah situasi ini, min sampel dan varians sampel adalah kaedah paling sesuai digunakan bagi menganggarkan min dan varian bagi pembolehubah respond. Walau bagaimana pun, min sampel dan varians sampel mudah dipengaruhi titik terpencil dan ianya mungkin akan memberikan penganggar regresi yang tak konsisten dan ada kalanya tanda penganggar garis regresi berubah dari positif kepada negatif. Kaedah statistik teguh digunakan untuk mengatasi masalah ini. Median dan *Median Absolute Deviation* (MAD) masing-masing digunakan sebagai gantian kepada min dan varians sampel bagi pembolehubah re-

spond. Namun median di ketahui kurang efisien dibandingkan dengan min bagi data yang tidak tercemar. Ia adalah sebahagian daripada objektif di dalam tesis ini untuk mencadangkan penggunan penganggar teguh MM lokasi dan serakan yang sangat efisien dan resistan bagi menganggar min dan varian bagi pembolehubah respond menggunakan skema pengoptimuman baru yang dicadangkan dan juga mencadangkan penganggar MM bagi menganngar parameter bagi fungsi proses min dan proses varians.

Tambahan pula, andaian biasa bahawa bagi setiap titik rekabentuk semasa ujikaji dijalankan mempunyai bilangan replikasi yang sama, pada kebiasaannya tidak praktikal dalam aplikasi industri sebenar penggunaan dua pengoptimuman rekabentuk teguh. Dalam keadaan ini, menggunakan kaedah kuasadua terkecil (OLS) bagi menentukan penganggar fungsi respond bagi proses min dan proses varian akan terkesan dengan kehadiran masalah heteroskedastik. Objektif yang ketiga dalam tesis ini, kami mencadangkan penggunaan kaedah kuasadua terkecil berpemberat (WLS) untuk menganggar parameter model regresi dan mengaplikasi skema pengoptimuman (PM) baru untuk mencari situasi optimum bagi menganggar min respond yang optimum.

Keputusan keseluruhan menunjukkan bahawa Kaedah Pengoptimuman yang dicadangkan (PM) sangat mengatasi kaedah pengoptimuman lain yang sedia ada. Kaedah PM berasaskan penganggar teguh MM lokasi dan serakan yang di cadangkan juga mengatasi kaedah lain. Akhirnya, kaedah pengoptimuman yang di cadangkan (PM) berasaskan Kaedah Kuasadua

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I certify that a Thesis Examination Committee has met on **18th May 2015** to conduct the final examination of **Ishaq Abdullahi Baba** on his thesis entitled "**Dual response surface and robust design optimization based on the penalty function method**" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the **Master of Science**.

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LIST OF ABBREVIATIONS

T	Desired target for the mean response
x	Vector of control variables
y	Vector of the observed responses
s_u	Standard deviation of the observed responses
μ	Penalty constant
$\triangle$	Desired upper bound for the bias
$\hat{\mu}$	Estmated mean of the optimal response
$\bar{y}_u$	Average of the observed responses
$\hat{\omega}_\mu$	Fitted response surface for the mean function
$\hat{\omega}_\sigma$	Fitted response surface for the variance function
VM	Vining and Myers Vining and Myers (1990)
PM	Proposed method
LT	Lin and Tu (1995) or can be refered as MSE
WMSE	Ding et al Ding et al. (2004)
$\mathrm{OLS_{LT}}$	Least squares method with LT
$\mathrm{OLS_{PM}}$	Least squares method with PM
$\mathrm{WLS_{LT}}$	Weigted least squared method with LT
$\mathrm{WLS_{PM}}$	Weigted least squared method with PM
BFGS	Broyden-Fletcher-Goldfarb-Shanno
MSE($\hat{\mu}$)	Mean squared error of the estimated mean optimal response
$[MSE(\hat{\mu})]^{\frac{1}{2}}$	Root Mean squared error of the estimated mean optimal response

CHAPTER 1

INTRODUCTION

1.1 Background of the Study

Response surface methodology (RSM) which was introduced by Box and Wilson in 1951, involves the use of statistical and mathematical tools in the development of new products, enhancement of the existing designed products, as well as optimizing processes. The primary objective of the response surface methodology is to find the optimal setting conditions on a set of explanatory variables that minimizes or maximizes the fitted second order quadratic model. In dealing with RSM model, much attention is given to the response than the predictor variables because the predictor variables are kept fixed. Originally, RSM was designed to address only single response problems, but many real life industrial applications involve optimization of more than one response variable. In this situation, finding appropriate optimal setting solutions will demand taking all the responses into consideration simultaneously and this procedure is termed as multiple response problem (Khuri and Conlon (1981) and Kim and Lin (2006)). The multiple response procedure comprises of roughly four approaches including design of experiment, data collection, regression analysis and optimization of the build regression models. The commonly used regression estimation technique by practitioners of RSM is the ordinary least squares (OLS) approach. The aim of OLS is to find the estimates of the regression coefficients by minimizing the sum of the squared residuals of the regression model which represent the difference between the observed and estimated responses in a given data set. Design expert and researchers choose to use OLS because of its popularity and computational simplicity in solving linear regression models. Moreover, in RSM the observed response usually assumes to satisfy the assumptions of normality and constant variance which make it easier to apply OLS than any other procedures. However, the classical OLS estimates are easily affected by the violation of normality assumption and missing observations in the response variables and also when outliers are present in data. (see Leroy and Rousseeuw (1987), Wilcox (1998), Kutner et al. (2004) and Alma (2011)). According to most regression literature, outlier is defined as observation that behaves differently from the majority of the data (Rousseeuw and Leroy (2005)). Three types of outlying problem have been identified with regression approach: outlier in x plane, which is some times called leverage points, outlier in y plane and outlier in both x and y axis. Generally in RSM, outlier exists only in the y plane since the observations on x plane are fixed. Under this condition determination of the optimal solutions may be too expensive. Hence, selecting a suitable regression method is important toward achieving the global optimal solutions. Dual response surface approach introduced in Myers and Carter (1973) considered the primary and the secondary response as separate functions. The primary response function is the original optimization function to be optimized and the secondary response is the constraint function (Myers and Carter (1973)). The idea behind this approach is to identify the level of control factors that optimize the fitted primary response subject to the equality secondary response. The technique was introduced as a result of the failure of the single response surface optimization procedure known as ridge analysis Kim and Lin (1998), to identify the optimal condition accurately which mostly affect the estimates of the optimal mean response of the estimated regression function. Another motive behind the dual response is that it accommodate more than one response at a time whereas ridge analysis deal with only single response problem. In spite of the advantages of the dual response, the tradeoffs between the mean and variance remains the challenge of the design expert and practitioners until today. The Lagrangian multipliers approach is mostly used with fixed multiplier and target value. Other methods of solving multiple response problem includes the generalized distance method developed by Khuri and Conlon (1981), robust design parameter approach established by Taguchi and the desirability function method used in Derringer (1980), fuzzy modeling optimization and nonlinear programming used in Lai and Chang (1994) and Biles and Swain (1979) respectively. Most research in dual response robust design deal with balanced design data. Researchers in this area have not fully discussed in solving robust design problem when dealing with unequal design data. A balanced data has complete number of observations for each design point, that is the design points is the number of observations under each control factor settings corresponding to a specific number of response observations, while the unbalanced is when some data are missing from the sample sizes due to some uncontrolled factors. In this case, the mean and variance estimated functions may be affected which may cause heteroscedasticity problem in the response observations, indicating that the OLS procedure is not the best unbiased method. Other statistical inference such as standard error of the coefficient of the regression and analysis of variance may not hold correctly. To tackle this problem, weighetd least squares WLS approach is applied which is more proficient and suitable for estimating the model coefficients of regression when the designs have unequal number of observations. This can be achieved by setting appropriate amount of influence to each data point over the estimates of parameter, instead of giving more than what is required to some data point and give less to others. However, the aim is to apply a technique which considers all of the observation equally. In general RSM, dual response and robust design optimization has been an essential tool for product and quality improvement in industrial development, engineering, science, economics, chemistry and biotechnology to mention but a few. The main reasons behind this study will be explain in full in the next section.

1.2 Motivation of the Study

The widespread application of RSM in solving real life industrial problems make it necessary to find a more sophisticated and efficient approach that can achieve the needed results for a decision maker. To design a quality product that satisfies the interest of a customer, quality characteristics of interest must be well defined for that product. The quality characteristics of interest may include several factors such as cost of production, production dimensions, production time, and product quality and or any other important product characteristic specified by a customer or design expert. Most of the early research in RSM was based on the single response cases. This approach was introduced and developed in Box and Wilson (1951) and further study was presented by (Draper (1963), Khuri and Myers (1979)) among others. Graphical approach was used for solving RSM problems by representing the relationships between the response and control factors on a contour plot to locate the optimal condition. Obviously, this technique is impractical for more than two control factors. Continuous researches in this area lead to the development of dual response approach in Myers and Carter (1973), where they suggested the used of mean and variance function as separate functions in their effort to tackle the unequal variance problem. Many researchers have discussed the application of dual response in different areas such as robust parameter design, which was introduced by Genichi Taguchi for the purpose of reducing variation and improving process/product quality characteristics. Some characteristics of interest are most desirable at a target, while others are most desirable at the highest or lowest possible values. Despite its benefit, Taguchi approach faced a load of debate and queries form the scholars and practitioners about it statistical and optimization procedures see (Box and Wilson (1951), Nair et al. (1992) and Freeny and Nair (1992)). The extension of dual response surface was presented by Vining and Myers (1990) where they used the idea of Myers and Carter (1973) and Taguchi approach and considered both mean and variance functions as response of interest for the formulation of the objective function to be optimized. Further modifications and suggestions on how to improve the dual response method was studied by Myers (1991), Del Castillo and Montgomery (1993), and Copeland and Nelson (1996)). Lin and Tu (1995) pointed out that the Vining and Myers (1990) approach denoted by (VM) does not guarantee global optimal due to restriction of the constraint to a specific value. In this respect, they proposed an optimization scheme known as mean squared error objective function which allows a small bias and we referred this objective function as LT. The objective function consists of the bias and variance. The mean squared error formula is the most popular one used in solving dual response and multiple response problems. Nonetheless, this objective function does not take into account the measure of the violation of the constraint and it places no restriction on how large the estimated mean value might deviate from the target value (Kim and Lin (1998)). The modification of MSE method called the WMSE was introduce by Ding et al. (2004) to further reduce the influence of variance by introducing some weight on the MSE optimization scheme. The idea behind this approach is to determine the weight in such a way that it can reduce the effect of the bias and the variance in the determination of the optimal setting conditions. The major shortcoming of this approach as mentioned in Jeong et al. (2005) is that, it does not consider the interest of the decision maker in the determination of the weight functions. Later, Cho and Park (2005), Steenackers and Guillaume (2008), Shaibu and Cho (2009), Shin et al. (2011) and Chen (2004) discussed the optimization of robust design based on the mean squared error objective function as discussed by (Lin and Tu (1995)). The robust design approach is the method introduced in Taguchi and Wu (1979) for the purpose of reducing variation in the responses (Myers et al. (2009)). The work of the preceding researchers has motivated us to propose an alternative optimization scheme for use in the dual response, multiple response and robust design optimization. By proposing this alternative method, we hope to reduce the deviation from the target value while minimizing the variability in the response observations.

In addition, the assumption of normality, equal variance and independence in the residuals are commonly assumed to hold correctly in the observed responses.

The OLS method is often used to estimate the parameters of regression coefficients in multiple response regression problems. It is now evident that the OLS are easily affected by outliers (Rousseeuw and Leroy (2005),Wilcox (2012)). Hence in this thesis we propose to employ the MM estimator to estimate the parameters of mean and variance functions. When there are more than two response variables, the location and the scale of the response variable first need to be estimated. The sample mean and variance are often used to estimates these parameters. The mean and variance are duly affected by the presence outlier, which will further interrupt finding the optimal setting solution of the estimate mean response. Park and Park and Cho (2003) and Lee et al. (2007) suggested the used of median instead of mean, median absolute deviation MAD and inter quartile range instead of variance. The median is known to be ineffective than mean when the response data satisfy the normally assumptions and or there is no contamination (Maronna et al. (2006) and Bakar and Midi (2015)). The shortcoming of median as a location measure has inspired us to employ the MM estimates of location and scale to estimates the mean and variance of the response variable. We also apply our proposed optimization scheme denoted by PM to obtain the optimal settings that optimize the fitted mean and variance function simultaneously. The MM estimate of regression and MM estimates of location and spread are used to down weight the effect of the outliers in y axis.

In design of experiment some treatment combinations can be more difficult to obtain or more expensive to run than others. In this situation the experimenter may ends up collecting unbalanced data points which naturally violate the assumptions of balanced data. Thus, the classical regression method OLS may not be appropriate due to the presence of unequal variation in the response which may give raise to heteroscedasticity problem. This problem affects the estimates of standard error by making it large and some other inference like test of hypothesis and significance. To remedy the heteroscedasticity problem, Cho and Park (2005) employed the weighted least squares to estimates the parameter of the model.Cho and Park (2005) also used the mean squared error optimization function denoted as LT to find the optimal setting conditions that can achieve the target with small variance when there are unequal sample sizes in the response. Since the LT optimization function is less efficient than our proposed optimization scheme PM, this issue has inspired us to employ the weighted least squares with the proposed optimization scheme denoted as WLS_{PM} to obtain the optimal solutions. In the coming section, we enumerate the intending goals of this study.

1.3 Objectives of the Thesis

The primary aim of this thesis is to study and examine the behavior of the various optimization schemes for solving dual response surface problem and proposed a new objective function which can achieve better optimal solutions. To accomplish our objectives, we consider the following specific goals:

1. To derive a new optimization scheme based on the penalty function method for the implementation of dual response surface optimization

2. To propose using MM estimate of location and scale and MM estimate of regression for estimating the mean and variance response functions.

3. To propose using weighted least squares WLS and the new optimization scheme for response variables with heteroscedasticity problem.

4. To develope R programming codes for all the established techniques.

1.4 Organization of the Thesis

The thesis comprises of 6 Chapters. In Chapter 1, we introduced the concept of response surface methodology (RSM), dual response and robust design optimization technique. Research motivation and objectives are highlighted accordingly.

In Chapter 2, a brief review of linear regression with single response and second order response surface model are discussed. The review on ridge analysis and the modified ridge analysis method are also discussed. Some existing methods for solving dual response surface, robust design and multiple response variable optimization problem are reviewed and presented

In Chapter 3, we introduced an alternative approach of dual response surface optimization based on the penalty function method. Formulation of the newly objective function and the development of mean and variance models for more than two variables are discussed. Numerical examples and simulation study are presented to assess the performance of the proposed method. Finally, a brief conclusion is given at end of the Chapter.

In Chapter 4, we introduced a robust design optimization based on newly proposed objective function given in Chapter 3. Development of robust design optimization based upon the median, median absolute deviation (MAD), MM estimates of location and scale and MM estimates of regression with mean squared error optimization and the newly proposed method (PM) are established. Numerical example and simulation study are reported in tables and figures and discussed, and conclusions are established based on the computational results at the end of this Chapter.

In Chapter 5, robust design optimization with unequal sample sizes based on the OLS and WLS with mean squared error objective function and the OLS and WLS with the newly proposed objective function are discussed. Derivation of weighted least formula is given. Simulations and example are also given with conclusion remark at the end of the Chapter.

In Chapter 6, we provide the summary and the conclusion according to earlier cited objectives. A brief outline of the possible feature research related to our study is given with recommendations.

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