AN INTERACTIVE APPROACH TO TWO-RESPONSE PRODUCT AND PROCESS DESIGN OPTIMIZATION WITH STATISTICAL INFERENCES

A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF
MIDDLE EAST TECHNICAL UNIVERSITY

BY

MELİS ÖZATEŞ

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR
THE DEGREE OF MASTER OF SCIENCE
IN
INDUSTRIAL ENGINEERING

JULY 2015

Approval of the thesis:

AN INTERACTIVE APPROACH TO TWO-RESPONSE PRODUCT AND PROCESS DESIGN OPTIMIZATION WITH STATISTICAL INFERENCES

submitted by **MELİS ÖZATEŞ** in partial fulfillment of the requirements for the degree of **Master of Science in Industrial Engineering Department, Middle East Technical University** by,

Prof. Dr. Gülbin Dural Ünver
Dean, Graduate School of **Natural and Applied Sciences** _____

Prof. Dr. Murat Köksalan
Head of Department, **Industrial Engineering** _____

Prof. Dr. Gülser Köksal
Supervisor, **Industrial Engineering Dept., METU** _____

Prof. Dr. Murat Köksalan
Co-supervisor, **Industrial Engineering Dept., METU** _____

Examining Committee Members:

Assoc. Prof. Dr. Sinan Gürel
Industrial Engineering Department, METU _____

Prof. Dr. Gülser Köksal
Industrial Engineering Department, METU _____

Prof. Dr. Murat Köksalan
Industrial Engineering Department, METU _____

Assoc. Prof. Dr. Cem İyigün
Industrial Engineering Department, METU _____

Assoc. Prof. Dr. Ferda Can Çetinkaya
Industrial Engineering Department, Çankaya University _____

Date: **July 30, 2015**

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Name, Last Name: MELİS ÖZATEŞ

Signature :

ABSTRACT

AN INTERACTIVE APPROACH TO TWO-RESPONSE PRODUCT AND PROCESS DESIGN OPTIMIZATION WITH STATISTICAL INFERENCES

Özateş, Melis

M.S., Department of Industrial Engineering

Supervisor : Prof. Dr. Gülser Köksal

Co-Supervisor : Prof. Dr. Murat Köksalan

July 2015, 74 pages

In this study, an interactive approach has been developed for two-response product and process design optimization problems treating the single response problems as a special case. This approach considers preferences of the decision maker explicitly and the correlation between the responses. It uses a predefined set of objectives that are commonly encountered in the literature and industrial applications. However, instead of presenting all objective values at each iteration, a set of performance measures are used to represent the objectives in a way to communicate with the decision maker better. A significant part of this communication utilizes visual aids such as specification and prediction regions of a solution. Thus, the decision maker is able to decide better which objective can be sacrificed by how much in order to improve an unsatisfactory objective in the next iteration. The developed approach is demonstrated on two examples; one exemplifies binary response problem and the other is on single response problem. The advantages and disadvantages of the developed approach and issues

for covering more than two responses are discussed.

Keywords: Multiresponse problems, robust product and process design optimization, multi response surface optimization, interactive approaches

ÖZ

İKİ YANITLI ÜRÜN VE SÜREÇ TASARIM OPTİMİZASYONU İÇİN İSTATİSTİKSEL ÇIKARIMLI ETKİLEŞİMLİ BİR YAKLAŞIM

Özateş, Melis
Yüksek Lisans, Endüstri Mühendisliği Bölümü
Tez Yöneticisi : Prof. Dr. Gülser Köksal
Ortak Tez Yöneticisi : Prof. Dr. Murat Köksalan

Temmuz 2015 , 74 sayfa

Bu çalışmada, iki yanıtlı ürün ve süreç tasarım optimizasyonu problemleri için etkileşimli bir yaklaşım geliştirildi. Buna ek olarak, tek yanıtlı problemler geliştirilen yöntemin özel durumu olarak incelendi. Bu yaklaşım, karar vericinin tercihlerini açık bir şekilde dikkate almakta ve yanıtlar arasındaki korelasyonu gözetmektedir. Problemin çözümünde literatür ve endüstriyel uygulamalar temel alınarak oluşturulmuş amaç fonksiyonları kullanılmaktadır. Karar vericiye her iterasyonda tüm amaç değerlerini sunmak yerine, bu amaçları yansıtacak ve karar verici ile daha iyi iletişim kurulmasını sağlayacak bir grup performans ölçüsü belirlenmiştir. Karar verici ile iletişimin önemli bir bölümü, çözümün spesifikasyon ve tahmin bölgelerinin görselleriyle desteklenmektedir. Böylece karar verici yetersiz gördüğü amacı iyileştirmek için bir sonraki iterasyonda hangi amaçtan ne kadar fedakarlık edeceğine daha rahat karar verebilmektedir. Geliştirilen yaklaşım iki uygulamayla örneklendirilmiştir. Örneklerden bir iki yanıtlı

problemlerin diğeri ise tek yanıtlı problemlerin çözümünü örneklendirmektedir. Yöntemin avantaj ve dezavantajları ve ikiden fazla yanıt olan durumlarda ne gibi çözüm önerileri sunulabileceği tartışılmıştır.

Anahtar Kelimeler: Çok yanıtlı problemler, robust ürün ve süreç tasarım optimizasyonu, çok yanıtlı yüzey optimizasyonu, etkileşimli yaklaşımlar

To my mother, my father, my fiancé

and

my aunt Selma Özateş...

ACKNOWLEDGMENTS

I inform that there have been many people around me during my graduate studies and these are the people who all make it happen for me to present a thesis study I am comfortable with. Unfortunately, only few of them can be mentioned here due to lack of space.

First and foremost, I would like to express my sincere thanks to my supervisors Prof. Dr. Gülser Köksal and Prof. Dr. Murat Köksalan for their constant support and patience. Their wisdom has guided me to new research areas that otherwise I would be unaware. I have always felt privileged to be a graduate student of such brilliant people.

Secondly, I would like to thank to all my colleagues for their kind collaboration during teaching and other departmental stuff. I thank to Derya Dinler for being a kind companion during the teaching assistant works we have conducted together. I also thank to Gülten Göğayaz for sharing her know-how with me for my studies whenever I need. Together with them, I would like to thank Begün Efeoğlu, Ece Sancı, Yasemin Limon for the heard to heard talks that we had with a cup of Turkish coffee. I also want to thank to Emrecan Batı for always asking me if I need help and help me whenever I need without thinking twice. In addition, I thank to Ece Selin Böncü for her nice touches to our English.

Most importantly, I offer my greatest and sincere thanks to love of my life, Yeti Ziya Gürbüz, for his support. He has been with me all the time with patience and love. Especially, when I was stuck, his support and encouragement triggered my enthusiasm to move on towards finishing my studies. I cannot express his support and contributions to both my personal and academic life within two lines. He has been always a shoulder to put head on. There is no doubt that without him I would not be where I am today.

Last but not least, no thank would be enough for my family's support. My parents, Mediha-Selim Özateş, have made everything all possible with their endless support. They have put their ultimate effort into my personal and academic life since my very first day in life. They make me rise to my feet every time I fall by believing me so much like nobody ever does. I cannot imagine how my life would be without such gorgeous parents.

TABLE OF CONTENTS

LIST OF TABLES

TABLES

LIST OF FIGURES

FIGURES

LIST OF ABBREVIATIONS

ANOVA	Analysis of variance
CI	Confidence interval
DM	Decision maker
GDA	Generalized distance approach
GLS	Generalized least squares
LNTL	Lower natural tolerance limit
MOO	Multi objective optimization
MRO	Multi response optimization
MRSO	Multi response surface optimization
MSE	Mean square error
MVR	Multivariate regression
NTL	Natural tolerance limit
OLS	Ordinary least squares
PI	Prediction interval
RPD	Robust parameter design
RSM	Response surface methodology
STEM	STEP method
SUR	Seemingly unrelated regression
S/N	Signal-to-noise
UNTL	Upper natural tolerance limit
WLS	Weighted least squares

CHAPTER 1

INTRODUCTION

In recent years, achieving high quality in products and processes through off-line quality engineering methods [89] has been of an ever-increasing interest due to the competitive market conditions. The purpose of off-line quality engineering, also known as robust engineering [89], is to increase the competitiveness of the new products and processes by reducing their cost and improving their quality via research and development at the design stage. There are several design parameters affecting the quality (or performance) of the products and processes to be considered simultaneously. As a part of off-line quality engineering, robust parameter design aims to increase the quality and reliability of a product or process by finding the optimal setting of the input variables (parameters) that makes the product or process insensitive to the uncontrollable variations in the system. On the other hand, quality is typically multidimensional [13]. In other words, quality of a product is defined by multiple quality characteristics of a product or process. In addition, in most cases, an optimal design setting for a response (or quality characteristic) is not optimal for some other responses. This problem is referred to as a *multi response product and process design* or *multi response problem* [36]. In most of the multi response product and process design problems, considering each response separately causes incompatible solutions in practice due to the conflicting nature of the responses. Therefore, in order to find a compromising solution, the multiple responses should be taken into account simultaneously. In this regard, there have been several approaches to these problems. Most of the approaches in the literature use *multi-response surface optimization (MRSO)* techniques. These approaches first design experi-

ments to gather data to build empirical relationship functions as models of the relationships between responses (or performance measures) of interest and several controllable design variables, and then treat these functions as objectives or constraints in an optimization model.

Even though, there are different opinions about the classification of MRSO approaches such as [75,97], they are viewed as multi objective optimization (MOO) problems by many researchers such as Park and Kim [71], Lee et al. [50]. Thus, the MRSO approaches are analysed under three categories of MOO literature according to the timing of articulation of the decision maker's (DM) preference information as prior, progressive (or interactive) and posterior preference articulation methods. Prior preference articulation approaches require all necessary information about preferences of the DM prior to the solution procedure. Interactive approaches take preferences of the DM progressively during the solution procedure. Finally, posterior approaches do not require any information on the DM's preferences before or during the problem solving procedure. DM's preferences are incorporated after a representative set of solutions are identified.

Most of the existing approaches in the MRSO literature are prior approaches requiring all preference information before problem solving, which is very difficult in practice. These approaches tend to combine the multiple responses into a single function to optimize them simultaneously such as desirability function approaches [19,26,35,40,74] and loss function approaches [42,73,92]. In addition, some approaches utilize MOO methods such as goal programming [34, 75] and goal attainment [96]. Yet, in many cases, such aggregations fail to satisfactorily represent the decision makers' preferences.

Moreover, in multi response problems, responses may statistically and preferentially depend on each other. However, some approaches such as desirability function based methods do not take into account the possible correlations between responses. Furthermore, some studies such as [92] consider the variances of the responses as constant over the experimental region, which contradicts with the aim of the robust parameter design.

Additionally, modelling and estimation difficulties are encountered in MRSO

problems due to limiting assumptions of the modelling approaches such as normality of the errors of a model with zero mean and constant variance. In some cases, data transformations are required to satisfy those assumptions. For instance, logarithmic transformation of the data is performed in several cases where the response variable follows log-normal distribution [84]. However, those transformations are usually used erroneously which affects the solution of the problem [7, 47, 68].

In this study, to overcome many of the aforementioned deficiencies, we develop an interactive approach for two-response product and process design optimization problems as well as addressing the single response problem as a special case. We assume that properly collected data is available prior to the implementation of the developed method, since data collection is out of the scope of this thesis. At the model building stage, we use ordinary least squares (OLS) regression which is a commonly used approach [23] for building the functional relationship models between responses and the controllable input variables. We fit separate models to means and variances of the responses and that of the correlation coefficient between the responses. At the optimization stage, our method follows an interactive procedure that explicitly considers the preferences of the DM. It is based on some concepts of the STEP method (STEM) proposed in [5]. Moreover, we define a set of performance measures that are commonly encountered in the literature and industrial applications. At each iteration, instead of presenting all objective values, we use those performance measures to represent the objectives in a way to facilitate the communication with the DM. In addition, we consider the possible correlations between the responses by these performance measures. Furthermore, we support this communication by visual aids such as presentation of specification and prediction regions of the solution at each iteration. In this way, the DM can decide better which objective can be sacrificed by how much in order to improve an unsatisfactory objective in the proceeding iteration.

In Chapter 2, we review the studies that are related to our work. We provide background information on response surface methodology (RSM), Taguchi's robust parameter design (RPD) and multi objective optimization. We give details on STEP Method concepts of which are exploited in this study. Finally, we sum-

marize MRSO approaches and we address their contributions and limitations.

In Chapter 3, we explain the development of the method in detail. First we briefly explain data collection procedure commonly used in the literature and industrial applications. Then, we present the model building stage and the performance measures that are functions of the mean, variance and correlation coefficient models. In addition, the estimation difficulties encountered due to the limiting assumptions of the modelling methods are addressed and ways of handling these difficulties are proposed. Lastly, we introduce the developed interactive procedure and how the aforementioned visual aids are exploited at each step of this procedure. We discuss convergence issues and nonlinearity of the method.

In Chapter 4, we illustrate the developed approach on two examples. First example is polymer experiment which is used in the literature [42,64,92]. Second example is generated for illustrating how the developed method is applied to a single response problem in which the response variable is log normally distributed.

In Chapter 5, we summarize our method for two response product and process design problems. We discuss the strengths and the limitations of our method when comparing the existing methods in the literature. Finally, we address issues for covering more than two responses and handling further problems on modelling and estimation as future research directions.

CHAPTER 2

LITERATURE REVIEW

In this chapter, studies in the literature that are most relevant to this thesis are presented. These studies are grouped into four sections as response surface methodology, robust parameter design, multi objective optimization and multi response surface optimization.

2.1 Response Surface Methodology

Response surface methodology (RSM) is a set of statistical and mathematical techniques used to build a functional relationship between response of interest and a number of inputs presumed to affect the response. The foundations of RSM date back to the studies in the early 1930s or even earlier [37]. Nevertheless, G.E.P. Box and K.B. Wilson have been known as the pioneers of RSM since their work in 1951 [37,64,80]. Believing that their method is to be of value in the other fields, their aim is to find out the optimum conditions in chemical investigations to attain maximum yield [12]. As predicted, RSM has been used and applied in various areas after their development [12,37].

The main objectives of RSM are

1. To explore and quantify the relationship between the value of a response and the settings of a group of factors that can be used to predict the value of response for a given setting of factors and
2. To discover the settings of the factors where the best value of the response

of interest is achieved [10,37,38].

The statistical and mathematical techniques used in RSM covers (1) designing a set of experiments to gather measurements of the response of interest, (2) building a mathematical model by using the data collected in the experiments and test the model via hypotheses and (3) determining the optimal settings of experimental factors by using statistical experimentation techniques, regression modeling and elementary optimization methods respectively [37,64].

Let us define the response variable, y, as a quantity for measuring quality (performance measure or quality characteristic). Its value is assumed to be influenced by the changes in the levels of processing conditions or input variables, which are called factors usually to be formed by transforming natural variables to coded variables. The values of the factors denoted by $x_1, x_2, \cdots, x_k$ can be controlled by the experimenter.

The relationship between y and $\boldsymbol{x}$ is generally approximated by building a low-order polynomial in the form of the following model [38]:

$$y = f'(\boldsymbol{x})\,\boldsymbol{\beta} + \epsilon \tag{2.1}$$

where $\boldsymbol{x} = (x_1, x_2, \cdots, x_k)$, $f(\boldsymbol{x})$ is a vector function containing p elements of powers and cross-products of powers of factors (up to a specific degree, $d \geqslant 1$), $\boldsymbol{\beta}$ denotes a vector of p unknown constant coefficients and ϵ is a random experimental error often assumed to be normally distributed with zero mean and variance σ^2. ϵ contains measurement error on the response, some sources of variation inherent in the process such as background noise, the effect of other unknown variables, and so on [64]. With this formulation, expected value of y (mean response, $\mu(\boldsymbol{x})$) becomes by $f'(\boldsymbol{x})\,\boldsymbol{\beta}$.

To build such a relationship given by (2.1), first-order and second-order models are commonly used in most of the cases. If the true response surface of interest is approximated over a small region of the input variables (factors) where there is a little curvature in true response function, then the first-order model given

by (2.2) is considered to be appropriate:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i \, x_i + \epsilon \, . \tag{2.2}$$

The degree of curvature in the true response function is usually high and hence, the first-order model is not adequate. In such cases, second-order model provided in (2.3) is used:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i \, x_i + \sum \sum_{i<j} \beta_{ij} \, x_i \, x_j + \sum_{i=1}^{k} \beta_i \, x_i^2 + \epsilon \, . \tag{2.3}$$

Moreover, since second order models can take various functional forms and estimating βs are easy by the method of least squares, these models are widely used in RSM [64].

In addition to the modelling issues, designing the experiments to gather data on response and optimization of the models to find the optimal setting of the input variables are important parts of response surface methodology. Experiments are usually conducted sequentially on the purpose of searching a smaller region of factors containing optimum and approximating relationship model more accurately in that region. In that framework, different experimental designs are used to obtain the first and the second degree models. These designs are called first-order designs and second-order designs, respectively. The most common first order designs are $2k$ factorial (k is the number of control variables), Plackett-Burman and simplex designs. The most frequently used second order designs are the $3k$ factorial, central composite, and the Box-Behnken designs [38]. Optimization methods employed to find the optimum settings of factors also change depending on the nature of the fitted model. The method of steepest ascent (or descent) is a proper technique for first degree models to move toward the optimum response sequentially. For second degree models, the most common approach is ridge analysis. It is basically the method of steepest ascent applied to second-order surfaces as constrained optimization [10, 38].

In order to have a detailed understanding on the methods involved in response surface methodology, the books [10, 37, 64] can be referred. Additionally, [28, 38, 66] provide reviews on RSM techniques.

2.2 Taguchi's Robust Parameter Design

Robust parameter design (RPD) is a method that is a part of quality engineering introduced by Genichi Taguchi during 1950s in Japan and 1980s in the United States [89]. The aim of RPD is to increase the quality and reliability of a product or process by finding the optimal setting of the input variables (referred to as parameters by Taguchi [88]) that make the response of the system (product or process) under consideration insensitive to the uncontrollable variations in the system. Taguchi introduces that all factors are not controllable in a designed experiment [38,80]. There exist some other factors so called *noise factors* which are hard (i.e., costly) or impossible to control. There are mainly three types of noise factors, which are external noise such as environmental conditions indisposing the product or process, internal noise owing to the changes occurring after production (during warehousing or usage) and unit-to-unit noise which is the difference seen from product to product [88].

Taguchi relates quality to cost and defines robust design as the design that minimizes the average loss not only to producer, but also to the customer and society [72]. He introduces a quadratic loss function as:

$$L(y) = k\,(y-t)^2\,, \tag{2.4}$$

where y is the response of interest, k is the constant defining loss and t is the target value. The expected value of $L(y)$ is

$$Q = E[L(y)] = k\,\left(\sigma^2 + (\mu - t)^2\right)\,, \tag{2.5}$$

where μ and σ^2 are the mean and variance of y. As seen in (2.4) and (2.5), when the response deviates from its target value, a loss is arisen. Following from the aforementioned fact, that variation from the desired target performance defines quality. Thus, to find the setting of control factors minimizing the average loss, Taguchi defines performance criteria, which is derived from average loss, known as signal-to-noise (S/N) ratios considering both the process mean and variance. S/N ratios are formulated according to the goal of the experiment (Table 2.1) which might be either smaller the better or larger the better or target is best, where the target value is either zero or infinity or a specified value t respectively.

All of these S/N ratios are formed to be maximized independent of the goal of the experiment and each experimental run is to be replicated to calculate S/N ratio. For further details on those derivations, [72] can be referred.

Table2.1: S/N rations and optimization models according to the goals of the experiment

Problem Type	**Signal to Noise Ratio (S/N Ratio)**	**Optimization Model**
Larger the better (y is positive)	$-10\log\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{y^2}\right)$ $-10\log\left(\frac{1}{y^2}\left(1+3\frac{s^2}{y^2}\right)\right)$	Max $E(Y)=f_1(x_1,x_2,\cdots,x_k)$ Min $V(Y)=f_2(x_1,x_2,\cdots,x_k)$ $\underline{s.t.}$ $l_i \leqslant x_i \leqslant u_i$ $E(Y)\geqslant 0$ $V(Y)\geqslant 0$
Smaller the better (y is positive or zero)	$-10\log\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{y^2}\right)$ $-10\log(\bar{y}^2+s^2)$	Max $E(Y)=f_1(x_1,x_2,\cdots,x_k)$ Min $V(Y)=f_2(x_1,x_2,\cdots,x_k)$ $\underline{s.t.}$ $l_i \leqslant x_i \leqslant u_i$ $E(Y)\geqslant 0$ $V(Y)\geqslant 0$
Nominal the best, Type 1 (y is proportional to s^2, $y\geqslant 0$, target is finite and positive) *Nominal the best, Type 2* (y is independent from s^2, y is free, target is zero)	$-10\log\left(\frac{\bar{y}^2}{s^2}\right)$ or $-10\log\left(\frac{\bar{y}^2-\frac{s^2}{n}}{s^2}\right)$ $-10\log s^2$	Min $(E(Y)-Target)$ Min $V(Y)$ $\underline{s.t.}$ $l_i \leqslant x_i \leqslant u_i$ $E(Y)=f_1(x_1,x_2,\cdots,x_k)\geqslant 0$ $V(Y)=f_2(x_1,x_2,\cdots,x_k)\geqslant 0$

In Taguchi's RPD, orthogonal arrays, which are simple experimental matrices developed by Rao in 1946 [27], are used to assign the controllable and uncontrollable input variables to an experimental layout. Mostly, the smallest size of an orthogonal array is selected according to the number of controllable input variables and the number of levels [72]. In an experimental layout, orthogonal array of controllable input variables are called inner array and orthogonal array of noise variables having multiple combinations of experiments for a row of inner array are called outer array [27, 52, 72]. In Figure 2.1, an experimental layout is represented and in that figure, inner array and outer array variables are coloured by red and blue respectively.

Once the S/N ratios are calculated for each run (row of inner array) as illustrated in Figure 2.1 by using the measured response values, analysis of variance (ANOVA) is widely used in order to determine the significant factors (and factor

Controllable Input Variables (Parameters) \ Uncontrollable Input (Noise) Variables							H	1	2	2	1			
							I	1	2	1	2			
							J	1	1	2	2			
Runs	**A**	**B**	**C**	**D**	**E**	**F**	**G**	y_1	y_2	y_3	y_4	$\bar{y}$	s^2	**S/N ratio**
1	1	1	1	1	1	1	1							
2	1	1	1	2	2	2	2							
3	1	2	2	1	1	2	2							
4	1	2	2	2	2	1	1							
5	2	1	2	1	2	1	2							
6	2	1	2	2	1	2	1							
7	2	2	1	1	2	2	1							
8	2	2	1	2	1	1	2							

Figure 2.1: Illustration of an experimental layout of robust parameter design

interactions) [81]. The decision of whether a factor is significant or not is also supported by the main effect plots for means of S/N ratios. After finding the significant factors (and factor interactions), the optimum setting of the factors (controllable inputs) is defined by selecting the levels where the mean S/N ratio is highest on the main effect plots. Yet, in the presence of significant interactions, it is not easy to identify them via orthogonal arrays. The specified setting should be tested through confirmation experiments. To conduct these experiments, one way of obtaining variations may be the utilization of outer array. For a detailed understanding of Taguchi's quality engineering and robust parameter design, [72, 81, 88, 89] and some overview studies such as [33, 70, 80] are useful references.

Although the Taguchi method has been used in various fields because of its simple procedures [8, 16, 68, 88], the statistical techniques used by his method have been the matter of much debate since its introduction [68]. It has been shown that his method cannot estimate the interactions between controllable inputs and a great number of experimental runs are needed. Moreover, S/N ratios are not capable of distinguishing the inputs affecting the mean and the ones affecting the variance. The studies [8, 64, 68] provide some criticisms on Taguchi's parameter design techniques. As the results of these criticisms, the response surface approach has been suggested to be utilized to have an approach which statistically sound more and which is more efficient for analysis within the concept of Taguchi's RPD [64].

To consider the variance of the response within the concept of Taguchi's RPD, RSM approaches basically propose modelling the variance in addition to the mean model. Variance modelling is first studied by Bartlett and Kendall in 1946 [4]. The variance model is formulated as:

$$\log(s_i^2) = \boldsymbol{x}_i' \boldsymbol{\gamma} + \epsilon_i^* \,, \tag{2.6}$$

where s_i^2 is the sample variance of n replications at design setting x_i and $\boldsymbol{\gamma}$ is a k dimensional vector of dispersion effects. Assuming the independence of the errors in the mean model and normality with $\log(\sigma^2) = \boldsymbol{x}_i' \gamma$, they point out that the errors in the variance model are normal with constant variance. Thus, under these assumptions the maximum likelihood estimation of the dispersion effects simply becomes the ordinary least squares estimation. Finally, the model for the mean is assumed to be:

$$y_{ij} = \boldsymbol{x}_i' \boldsymbol{\beta} + \epsilon_{ij}\, \sigma_i \,, \tag{2.7}$$

where $\boldsymbol{\beta}$ is the k dimensional vector of location effects.

Box and Meyer [11] are the first to introduce the variance modelling in the concept of RPD. Their motivation is based on the fact that the formulation of S/N ratios require replications which may be impractical when many controllable input variables exist. Hence, they make the use of mean and variance models to separate the location and dispersion effects.

After Taguchi's introduction of his methods, many researchers have studied uncoupling the mean and the variance of the response of interest and suggested the use of separate models to achieve a better understanding of the process in terms of mean and variance. In that manner, the robust design problem can be handled through utilizing response surface methodology [64] and that makes the separate modelling of the mean and the variance attractive to the robust design problems.

Mainly, two response surface approaches which are *dual response* and *single model* approach are developed for robust parameter design in 1990s [38,80]. The dual response approach proposed by Vining and Myers [93] in 1990 [38, 70, 80] is based on the dual response problem introduced by Myers and Carter [65] as

stated in [80]. In that approach, two separate models are fitted to the mean and the variance of the response of interest in order to satisfy the objectives related with them simultaneously. Thus, the problem becomes a multi objective optimization problem as shown in Table 2.1.

If $\hat{\mu}_y$ and $\hat{\sigma}_y^2$ are denoted as the models obtained by approximating separate response surface for the mean and the variance, respectively, then $\hat{\sigma}_y^2$ is minimized subject to the equality constraint, $\hat{\mu}_y = t$, where t denotes the target value, when the problem is target is best type problem. To solve a similar optimization problem, Del Castillo and Montgomery [17] suggest the use of inequality constraints instead of equality constraints due to the fact that equality constraints do not always produce a local optima. They have proposed a nonlinear programming procedure to solve these problems. Later, Lin and Tu [55] have come up with a procedure aiming to minimize mean square error (MSE) including bias (deviation of the response mean from the target value) and variance. Similarly, various extensions of dual response approach have been studied by many researchers and some example studies are [21,32,39,49,56,90].

In single model approach, by using combined array design suggested by [94], the mean and the variance functions of the response are estimated by taking unconditional expectation and finding unconditional variance of a model containing both noise and controllable input variables [67].

Additionally, there are some other approaches that consider the problems consisting of separate mean and variance models as a multi objective optimization problems and study robust optimization based on optimization techniques such as weighted sum method, compromise decision support problem and physical programming [70]. Those approaches ensure that the problems can be solved in a continuous space of input parameters contrary to the Taguchi method. For further understanding on those approaches, the study [70] and the references it provides can be referred.

2.3 Multi Objective Optimization

Multi objective optimization (MOO), also known as multi criteria optimization, is a field of multiple criteria decision making, which is one of the sub-disciplines of operations research and aims to solve more than one mathematical optimization problem simultaneously [87]. MOO methods are widely used techniques in many real life problems due to the multiple criteria concern nature of the most of the optimization problems in real life.

In MOO problems, it is always assumed that the decision maker (DM) is involved in the solution procedure at some stage [44]. Those procedures are classified into prior, interactive and posterior preference articulation approaches according to the stages that the DM's preferences are involved during the problem solving.

Prior preference articulation approaches assume that all necessary information about preferences of the DM can be obtained prior to the solution procedure. Those procedures are widely used in practice. However, it is very difficult or impossible to obtain all information about the DM's preferences prior to the problem solving. Even the DM may not be aware of her/his preferences. Thus, these approaches may result in solutions that do not satisfy the DM when the preference parameters are not well-estimated.

Posterior approaches do not require any information about the DM's preferences before or during the problem solving procedure. When the problem is solved, the resulting alternatives are presented to the DM to take her/his preference. In most cases, a large number of solution alternatives are presented to the DM which makes difficult to select the satisfactory solution among all.

Interactive approaches extract preferences of the DM progressively during the solution procedure. Steuer [87] states that "The future of multiple objective programming is in its interactive application". These approaches ensure feedback between the DM and the model which helps the DM to learn more about her/his problem and eventually to reach a preferred solution [71, 87]. Some examples of interactive procedures are STEM [5], GDF [24], Z-W method [99] and visual interactive approach [45]. The multi objective optimization approaches are

reviewed in detail in the studies [22, 29, 44, 59, 87]. Particularly for interactive approaches [60, 85] can be referred.

In this study, we utilize some concepts of the STEP method and use in multi response surface optimization problem. The STEP method is briefly explained in the following sub section.

2.3.1 STEP Method

The STEP method (STEM) is one of the first interactive approaches to multi objective optimization problems. It is introduced by Benayoun and others in 1971 for maximization of multi objective linear problems [5]. In addition, STEM has been modified to be used for multi objective nonlinear problems as stated in [59].

STEM proposes that the DM can indicate the responses that have acceptable values and those whose values are unacceptable (too high) in each iteration of the solution procedure. Then, the DM can tolerate the values of some objective function values to increase in order to improve unacceptable function values due to the fact that the solutions are searched in Pareto optimal set (the set of feasible solutions for which it is not possible to improve any objective without sacrificing from at least one other objective). In the below formulation all objectives are of minimization type. To generate new solutions, the following weighted Tchebycheff problem given by (2.8) is used:

$$\begin{gathered} \min \ max[w_i \, |z_i(\boldsymbol{x}) - z_i^*|] \\ subject\,to \\ \boldsymbol{x} \in \boldsymbol{S} \end{gathered} \tag{2.8}$$

In (2.8), the objective functions are assumed to be bounded over a feasible region $\boldsymbol{S}$. A vector called ideal objective vector, $\boldsymbol{z}^*$, is used as a reference point in the calculations. The reference points are determined by separately minimizing each objective function subject to the feasible region $\boldsymbol{S}$. The results determined by minimizing each response form the corresponding row of payoff table illustrated in Figure 2.2. The ranges of non-dominated solutions are required to obtain

weighting vector, w. The idea is to bring all objective functions into a similar scale by the help of the weighting vector. The nadir objective vector, $\boldsymbol{z}^{nad}$, is approximated from the payoff table by choosing the maximum element of each column.

$$\boldsymbol{P} = \begin{matrix} z_1 & z_2 \\ \left[\begin{matrix} z_1^* & z_{12} \\ z_{21} & z_2^* \end{matrix}\right] & \begin{matrix} \Leftarrow \min z_1(\boldsymbol{x}) \\ \Leftarrow \min z_2(\boldsymbol{x}) \end{matrix} \end{matrix}$$

Figure 2.2: Illustration of payoff table

The weighting vector is calculated by the formula:

$$w_i = \frac{e_i}{\sum_{j=1}^{k} e_j}, \; i = 1, \cdots, k, \tag{2.9}$$

where for every $i = 1, \cdots, k$

$$e_i = \frac{1}{z_i^*} \frac{z_i^{nad} - z_i^*}{z_i^{nad}} \tag{2.10}$$

or

$$e_i = \frac{z_i^{nad} - z_i^*}{max\left(\mid z_i^{nad} \mid, \mid z_i^* \mid\right)} \tag{2.11}$$

where the denominator cannot take zero value [59]. According to these formulas, for the objective functions that are farther from their ideal objective vector component, the weight becomes larger.

After DM states classification of objective functions and allowable values from the acceptable objective values, it is ensured that unsatisfactory objective values do not get worse. The procedure ends when the DM does not desire to change any of the objective function values or continues until DM is not satisfied with any of the components. In the latter case, STEM algorithm fails at finding a satisfactory solution. It should be noted that it is not possible to comment on convergence of STEM according to a value function since it does not assume an underlying value function.

STEM has many advantages such as the simplicity of the underlying ideas, ease of handling preference information and less complicatedness of the concepts

presented to the DM. On the other hand, it may be difficult to estimate the appropriate amount of increment for the DM. For further extensions of STEM algorithm, [59,87] and the references provided within those can be reviewed.

2.4 Multi Response Surface Design Optimization

Previous sections introduces that there are several factors affecting the quality of a product and those factors are defined as controllable and uncontrollable input variables. The factors are to be considered to determine the optimal settings of controllable design variables to consistently produce high quality of products and processes. Taguchi's methodology and RSM approaches to these design problems focus on one response of interest. However, quality of a product is typically defined by multiple responses of a product or process where optimal design solution for a response may not be optimal with regard to some other responses. This problem is referred to as a *multi response optimization (MRO) problem* [36] or *multi response product and process design*. In these problems, analysing each response separately results in incompatible solutions in practice. Thus, in order to find a compromising solution, the multiple responses should be considered simultaneously. In this regard, there have been several approaches to these problems.

As stated in [36], although there are some multi response experiments there has not been much attention on multi response experiments until the studies [9,98] pointing out parameter estimation problem in multi response models. These works have been followed by various studies.

Most of the approaches in the literature use *multi response surface optimization (MRSO)* techniques. MRSO can be formally defined as:

$$\begin{aligned} &optimize\,\{\hat{y}_1, \hat{y}_2, \cdots, \hat{y}_k\} \\ &subject\,to\,\boldsymbol{x} \in \boldsymbol{\Omega} \end{aligned} \tag{2.12}$$

where $\hat{y}_i(\boldsymbol{x})$s are the estimated response models for $y = (y_1, y_2, \cdots, y_k)$ denoting k response variables which are determined by the controllable design variables $\boldsymbol{x}$ and $\boldsymbol{\Omega}$ is the experimental region [31]. These approaches commonly suggest

a three stage solution procedure involving data collection via experimental design, model building and optimization. Each of these three stages carries high importance due to the fact that the success of the optimization depends on the accuracy of the fitted model and designed experiments used for building models. In the first stage, experiments are designed to collect response data and to identify statistically significant controllable factors. In the second stage, empirical relationship models are built as functions of the relationships between responses (or performance measures) of interest and several controllable design variables (i.e., multiple regression). In the last stage, the empirical models are treated as objectives or constraints in an optimization model to determine the setting of input variables (controllable factors) satisfying certain system requirements.

Even though, MRSO problems have been considered as MOO problems recently, there are still several different opinions on the categorization of the existing approaches. [97] supports that all existing MRO approaches can be classified into dual response approach, desirability function and loss function-based optimization. According to [75] MRSO approaches are divided into two categories which are loss function approach and MOO approaches, on the other hand; [71] supports that all MRSO approaches can regarded as special cases of MOO approaches so that MRSO approaches can be classified into the same three categories of MOO methods. In this study, the latter idea has been followed and the MRSO approaches are analysed under three categories of MOO literature: prior, interactive and posterior preference articulation methods, which are determined with respect to the stage where the DM's preferences are articulated.

2.4.1 Prior Methods

Desirability function, generalized distance and loss function approaches are well-known conventional approaches in the MRSO literature. These approaches aggregate the objectives into a single one to optimize them simultaneously. Since, this is a very similar approach to assuming a utility function to be optimized, they are a part of prior methods. Moreover, there are some studies utilizing goal programming to solve MRSO problems such as [34, 75]. In addition, approaches

such as weighted p-norm, displaced ideal, weighting, neutral compromise and global criterion methods reviewed in [2] are considered as prior methods. Furthermore, there are some other approaches which can be counted as prior methods. The study in [13] proposes an approach to determine the optimal setting of controllable input variables by maximizing the probability of meeting specifications for all responses simultaneously. In [54], a process capability index based desirability function approach is proposed. In [3], location and dispersion effects are considered simultaneously. [6] uses principle component based multivariate capability index as an objective function.

2.4.1.1 Desirability Function Approach

Desirability function approach is first introduced in [26] and it has become the most popular approach for multi response surface optimization problems due to its simplicity and flexibility [53]. Desirability function transforms an estimated response $y_i(\boldsymbol{x})$ (where $\boldsymbol{x}$ denotes vector of input variables) into a scale free value, d_i, called desirability which is assigned to a value from 0, where one or more unacceptable characteristics exist, to 1, where all response values are acceptable. By combining the individual desirability values, the overall desirability, D, is defined which turns the MRSO problem into a single response problem to reach an optimal solution which ensures that none of the responses lie outside of the acceptable limits.

The study [19] modifies overall desirability, introduced as the geometric mean of the individual desirability values in [26], to add robustness. It proposes different forms of individual desirability functions for nominal-the-best (target is best), smaller-the-better and larger-the-better type responses. Then, using weighted geometric mean is considered in [20] in order to consider relative importance of the responses while aggregating the individual desirability values. In [18], desirability functions that are differentiable everywhere are introduced and the problems are to be solved with gradient based optimization procedures. [74] proposes different models that can be divided into two groups which are minimizing the deviation of responses from their targets and centring the responses between

their upper and lower bounds set. Later, a function form is suggested by using exponential functions in [40]. These functions can generate various shapes when their parameters are adjusted. Desirability function approaches have been preferred by many researchers such as in the studies [41,46,95] and so on. For further extensions of desirability functions, useful references are provided in [14, 71].

2.4.1.2 Generalized Distance Function and Loss Function Approaches

Several MRSO methods have been proposed based on generalized distance function and loss function extending Taguchi's quadratic loss function. These techniques consider both mean and variance-covariance effects. By using this information from several responses, they construct a single function to represent the expected loss to be minimized. Uncertainty and the correlation structure are addressed through the use of variance-covariance matrices for the responses [71].

The study in [35] introduces generalized distance approach (GDA) which is basically minimizing the Mahalanobis distance between responses and their individual ideal optimum found over the experimental region. The correlations among the responses and the quality of predictions are taken into account. However, preferences of the DM are not considered and all response variables depend on the same input variables [15].

A loss function for MRO is proposed in [73] by extending Taguchi's single response quadratic loss function to a multi response one. Then, a new loss function is presented in [92]. That function includes the predicted response, $\hat{y}(\boldsymbol{x})$ instead of $y(\boldsymbol{x})$ in expected multi response squared error loss suggested in [73]. In [1] weight parameters are used to penalize the loss incurred when the response value is off the target. The study in [42] introduces predicted responses in the loss function. The definition has three desired properties of small bias, high robustness and high quality of predictions. It is desired that deviation of expected responses from their targets and variances of the true and predicted responses to be small at the compromise optimal [42]. It is indicated in [42] that [1,35,92] assume that variance of responses ($\Sigma_y(\boldsymbol{x})$) is constant over the experimental space (equal robustness), unlike [73].

2.4.2 Interactive Approaches

Some studies utilize interactive MOO approaches for optimization stage of MRSO problems. In those studies, an iterative solution procedure is followed. The DM is provided with a solution and s/he adjusts the preference parameters (directly or indirectly) at each iteration. Then, the optimization problem is solved by using the adjusted preference parameters and a new solution is obtained. These iterations continue until the DM is satisfied.

In [77], an interactive method which combines goal programming and RSM is proposed to meet user specified goals. Instead of solving a complete goal programming model, RSM is used to achieve a single highest ranked goal. Once it is achieved, the same procedure is repeated for the next highest ranked goal without violating the previous achievements. The DM may accept the solution for a goal under consideration or s/he may want to continue through more investigation which requires another experimental design that brings additional cost in practice. The DM's preferences are based on the point estimations and hence, the prediction variance is not considered. As stated by the authors, the method proposed in [77] does not address the cases where the error variance is not constant and/or the errors are correlated.

In [62] and [71], interactive approaches to MRSO problems are proposed based on GDF algorithm [25]. In these methods, trade-off weights are specified by the DM. In [62], response surface models are built only for the means of the responses. Thus, uncertainty is not considered and that may result in unrealistic solutions. In [71], prediction variance is taken into consideration during the solution procedure. However, the DM is presented directly with desirability and prediction variance values which may not be easy to be interpreted by the DM. No additional performance metrics are used to ease the interpretation.

An interactive approach using univariate capability indices as performance measures is developed in [43]. This approach is based on parametric achievement scalarizing program proposed in [45]. At each iteration the DM chooses a desirable point in objective space (by observing the C_{pk} values of the responses)

and the direction or weight parameters are adjusted based on that point. Those C_{pk} estimations are point estimations thus uncertainty in the predictions are not considered. In addition C_{pk} values may not be sufficient to represent the preferences of the DM satisfactorily.

In [51], the approach assumes a general monotone utility function which covers a wide variety of preference structures. During the solution procedure, series of pairwise comparisons are performed. Estimated utility functions such as weighted desirability functions are constructed. At each iteration, utility functions are updated according to the preference information provided by the DM and a new solution is obtained to be compared with the previous solution. In this approach, the uncertainty in the response surface models and the variances of the responses which may not be constant over the experimental region are not taken into account. This may lead to unrealistic solutions in practice.

Furthermore, some STEM based approaches exist in the MRSO literature. In [61], the DM needs to provide least satisfactory performance measure at a given solution. Differently from STEM, he does not need to identify the amount to be sacrificed from a satisfactory performance measure. Then a new solution where the provided least satisfactory performance measure is improved at the expense of other performance measures by gradient search is generated. Since the allowable values of the satisfactory performance measures are not satisfied by the DM, it may be difficult to reach a satisfactory solution.

In [30, 31], at each iteration the DM is allowed to adjust the shape of the desirability function by adjusting the bounds or the target values of responses. However, to adjust the preference parameter values directly may be difficult for the DM. In addition, using desirability functions as only performance measures may not represent the preferences of the DM properly.

2.4.3 Posterior Approaches

Posterior articulation approaches are not commonly utilized to solve MRSO problems. There are a few studies under this group.

An ϵ-constraint method based approach for dual response optimization problems is introduced in [49]. In this approach, after finding the non-dominated solutions without any preference information, alternative intervals are defined and they are presented to DM graphically to facilitate DM's decision making. When the number of objectives, which is two in dual response problems, is more than two, this graphical representation may not be helpful.

For multi response surface optimization problems, a posterior preference articulation approach is proposed in [50]. This approach initially finds the set of non-dominated solutions without taking the preferences of DM. Then, DM selects the best solution from the non-dominated solutions presented. At this stage, an interactive selection method based on pairwise comparisons is utilized to ease the DM's decision making.

CHAPTER 3

DEVELOPMENT OF THE METHOD

Most of the approaches mentioned in the previous chapter aggregate the objectives into a single one to optimize them simultaneously. However, in many cases, such aggregations fail to satisfactorily represent the decision makers' preferences. Moreover, in multi response robust product and process parameter design problems, responses may statistically and preferentially depend on each other. In addition, modelling and estimation difficulties are encountered in these problems due to reasons including limiting assumptions of the modelling approaches, insufficiency of data, representation of results in appropriate scales and multiple dimensions.

In this study, to overcome many of those deficiencies, an interactive approach has been developed for binary response product and process design optimization problems with an emphasis on the single response special case. This approach addresses three stages of MRSO, which are data collection (via experimental design), building empirical relationship functions, and optimization. Yet, data collection is not a primary concern in this study. It is assumed that data are collected properly prior to the implementation of the developed method.

At the model building stage, we utilize ordinary least squares (OLS) regression, a commonly used approach [23] for building the functional relationship models of means and variances of the responses of interest and that of the correlation coefficient between the responses. By using these models, we formulate a set of performance measures that can be of use in the design optimization process.

At the optimization stage, our method follows an interactive procedure explicitly considering preferences of the DM, similar to the STEM algorithm. At each iteration of the optimization procedure, instead of presenting all objective function values to the DM, the aforementioned set of performance measures that facilitates communication with the DM is presented. Moreover, this communication is supported by visual aids such as presentation of specification and prediction regions of the solution at each iteration. Thus, the decision maker is able to decide better which objective can be sacrificed by how much in order to improve an unsatisfactory objective in the next iteration. Differently from STEM, the DM can turn back to the solutions s/he is presented in the previous iterations, which means that s/he can use this method to learn the limitations of the current technology and how the objectives behave according to the changes in each other by searching the space.

This chapter is organized as follows. Common data collection procedure used in the literature and industrial applications is briefly summarized. Then, the model building stage is explained and the performance measures formed by using the mean, variance and correlation coefficient models are introduced. Thereafter, the estimation difficulties encountered due to the limiting assumptions of the modelling methods are addressed and ways of handling these difficulties are proposed. In addition, the interactive approach followed in the optimization stage and how the aforementioned visual aids are used at each step of this procedure are presented. Finally, convergence of the interactive procedure and nonlinearity of the objective functions are discussed.

3.1 Data Collection

Experiments are designed in order to collect response values for different settings of controllable input variables (design parameters). There are several different experimental designs in the literature (as those presented in [38, 80]). A commonly used experimental layout for collecting data through experimental design is illustrated in Figure 3.1, where y_{ij} denotes j^{th} replication for i^{th} response in the corresponding experimental run; A, B, C, D, E, F and G are controllable

Controllable Input Variables (Parameters) \ Uncontrollable Input (Noise) Variables																
							H	1	2	2	1					
							I	1	2	1	2					
							J	1	1	2	2					
Run	**A**	**B**	**C**	**D**	**E**	**F**	**G**	y_{11}, y_{21}	y_{12}, y_{22}	y_{13}, y_{23}	y_{14}, y_{24}	$\bar{y}_1$	s_1^2	$\bar{y}_2$	s_2^2	ρ
1	1	1	1	1	1	1	1									
2	1	1	1	2	2	2	2									
3	1	2	2	1	1	2	2									
4	1	2	2	2	2	1	1									
5	2	1	2	1	2	1	2									
6	2	1	2	2	1	2	1									
7	2	2	1	1	2	2	1									
8	2	2	1	2	1	1	2									

Figure 3.1: Illustration of an experimental layout where each run is replicated four times according to an experimental design

input variables forming the inner array, and H, I and J are uncontrollable input variables forming the outer array. Each of the factors is assumed to have two levels denoted by "1" and "2", in this layout. However, more or mixed levels can also be used in other cases.

In general, each experimental run is replicated r times in order to calculate sample means and sample variances of the response variables and the correlation coefficient for the run. The number of replications can be determined according to the design of the outer array. When it is not possible to control noise factors during the experiments, runs can be replicated in a random manner. Some researchers discuss disadvantages of the methods using designed experiments requiring replications [11]. They state that it is usually impractical to replicate the runs of an experiment which leads to an extensive number of runs. Even though there exists methods to model the variances without replicating the experiments, replicated experiments provide a better insight to approximate response surface models especially when the separate models for variances of the responses are utilized [47].

3.2 Empirical Model Building

We fit models for means and variances of the response variables separately. Besides, we fit a model for the correlation coefficient to be used for calculating

the performance measures explained in the following parts of this section. In order to estimate those models, we use ordinary least squares (OLS) regression which is a widely used approach for this purpose [23]. The model for each response is built in the following form:

$$\boldsymbol{y}_i = \boldsymbol{X}_i \boldsymbol{\beta}_i + \boldsymbol{\epsilon}_i \,, \;\; i = 1, 2 \quad , \tag{3.1}$$

where $\boldsymbol{y}_i = [y_{i1}, y_{i2}, \cdots, y_{in}]^T$ is a vector of observations for the i^{th} response variable,

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ 1 & x_{21} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{bmatrix} \tag{3.2}$$

is an $n \times (p+1)$ design matrix specifying values of the regressors (i.e. controllable input variables or their functions) at each and every observation (if certain regressors are not included in the model their columns are chosen as zero vectors, and categorical variables are treated as binary dummy variables), $\boldsymbol{\beta}_i = [\beta_{i1}, \beta_{i2}, \cdots, \beta_{in}]^T$ is a vector of coefficients of the model for the i^{th} response variable, and $\boldsymbol{\epsilon}_i = [\epsilon_{i1}, \epsilon_{i2}, \cdots, \epsilon_{in}]^T$ is the random error vector. The elements of $\boldsymbol{\epsilon}_i$ are assumed to be independent across time, and have the following properties:

1. $E(\boldsymbol{\epsilon}_i) = \boldsymbol{0}$ which implies that $E(\epsilon_{ij}) = 0$ for $j = 1, \cdots, n$,
2. $Cov(\boldsymbol{\epsilon}_i) = \sigma^2 \boldsymbol{I}$ or equivalently $Var(\epsilon_{ij}) = \sigma^2$ (constant) and $Cov(\epsilon_{ij}, \epsilon_{il}) = 0$, $\forall (j, l), j \neq l$.

Furthermore, $\boldsymbol{\epsilon}_i$ is assumed to follow a normal distribution to be able to make confidence statements and test hypotheses [79]. In order to satisfy these properties, the response variables may need to be transformed to another scale using logarithm or power transformation functions [47, 58, 63]. Some difficulties associated with these transformations are finding an appropriate one, interpreting the results in the transformed scale and estimating the response in the original scale.

In addition to OLS regression, there are other regression methods such as generalized least squares (GLS) regression, weighted least squares (WLS) regression,

seemingly unrelated regression (SUR) and multivariate regression (MVR) that are used in MRSO problems to develop empirical models [23, 78]. These methods differ from each other with respect to their assumptions. Yet, all these methods assume that the error terms are distributed normally.

If the variance of a response is constant over the experimental region (homoscedasticity, or homogeneity of variance), and each response surface model has potentially a different set of regressors and correlations exist between the responses, then SUR is an appropriate method to use [83, 98].

MVR, on the other hand, can be viewed as a special case of SUR when the same set of regressors is used to estimate the models of all responses. In that case, MVR provides the same set of coefficients ($\boldsymbol{\beta}$) whether the correlations between responses are ignored (the case of OLS) or taken into consideration (the case of MVR or SUR). Yet, prediction variance (variance of $\boldsymbol{\beta}$) estimates of SUR are smaller than those of MVR or OLS when responses are correlated and different set of regressors are used [23]. MVR may yield a large set of regressors, that is; fitted models include insignificant factors which lead to high prediction variance [42]. This is a disadvantage of the MVR method. The same disadvantage applies to an equivalent approach to MVR: using OLS regression for all responses separately with the same set of regressors.

If variances of a response at different design variable settings are non-homogeneous (heteroscedastic errors) and there exists correlation between the response variances at different design variable settings (serial correlation or autocorrelation), then GLS can be used to build an empirical model of that response. A special case of GLS is WLS when there is heteroscedasticity but no serial correlation. In the latter case, it may also be possible to transform the response data to stabilize the variance and then apply OLS regression. In the case of multiple correlated responses, SUR and GLS regression approaches can be combined [57, 86]. However, estimation approaches used might not be efficient especially for small and medium size data. Furthermore, variance-covariance matrix estimation and construction of confidence regions of the estimated parameters using such an approach need further investigation.

In this study, variances of responses cannot be considered as constant at different settings of the controllable design parameters due to the nature of the robust design problem and we aim to consider possible correlations between the responses. In this general case, none of the parametric regression approaches discussed above dominates the others when their disadvantages are considered besides advantages. We prefer to use OLS regression with data transformation whenever necessary due to its common use in the literature, well-known properties and consistent and efficient estimators under specific conditions.

In OLS regression, in order to satisfy that errors of a model has normal distribution with zero mean and constant variance σ^2, data transformations are commonly used. Especially log-normal linear models are postulated to build empirical models for variance of a response and correlation between two responses as functions of the controllable design variables. To illustrate, $\log \hat{\sigma}^2$ and $tanh^{-1}\hat{\rho}$ (equivalently $\frac{1}{2}\log\frac{1+\rho}{1-\rho}$) are approximately normally distributed with zero mean and constant variance [4, 76]. In addition, in [84] log-normality is stated to have been observed in various applications. Thus, in this study we consider such log transformations of data to satisfy the assumptions of OLS regression.

We observe that these transformations are generally used erroneously and those errors affect the solution of the problem [7, 48, 69]. In most of the applications, after obtaining the log-normal model of a mean response (or performance measure), to find its equivalent in the original scale, direct back transformation of the predicted mean value to the original scale is used. This leads to find the median (instead of the mean) of the response (or performance measure) in the original scale. In order to minimize such back transformation errors, we follow the approach proposed in [84].

They propose two estimators one minimizing mean squared error (MSE), the other minimizing bias. Their simulation results indicate that the estimator which minimizes MSE is more appropriate for this study. Details about this estimator are provided below.

A log-normal linear model assumes that

$$\log(\boldsymbol{z}) = \boldsymbol{X}\,\boldsymbol{\beta} + \boldsymbol{\epsilon} \tag{3.3}$$

where $\boldsymbol{X}$ is the design matrix, $\boldsymbol{\beta}$ is the vector of regression coefficients and $\boldsymbol{\epsilon}$ is the vector of random errors with $\epsilon_j \sim N(0, \sigma^2)$ and $\boldsymbol{z}$ is the vector of observations on the response, z, (or performance measure) which is typically mean or variance or correlation coefficient in our case. The conditional mean of response variable given $\boldsymbol{x}_0$ can be written in the original scale as follows:

$$E\left(z \mid \boldsymbol{x}_0\right) = \exp\left(\boldsymbol{x}_0^T\,\boldsymbol{\beta} + \frac{1}{2}\sigma^2\right) \tag{3.4}$$

where $\boldsymbol{x}_0$ is the given set of regressors. The estimator minimizing MSE is defined as

$$\hat{\mu}_{MM} = \exp\left[\boldsymbol{x}_0^T\,\hat{\boldsymbol{\beta}} + \frac{m\,RSS}{2\left(n - p + 1 + 3\,n\,v_0\right)m + 3\,RSS}\right] \tag{3.5}$$

where $\hat{\boldsymbol{\beta}}$ is the vector of OLS estimators for coefficients, n is the number of observations, p is the number of regressors and $m = n - (p+1)$. RSS is residual sum of squares calculated as

$$\log(\boldsymbol{z})^T\,\left[\boldsymbol{I} - \boldsymbol{X}\,\left(\boldsymbol{X}^T\,\boldsymbol{X}\right)^{-1}\,\boldsymbol{X}^T\right]\,\log(\boldsymbol{z}) \tag{3.6}$$

and

$$v_0 = \boldsymbol{x}_0^T\,\left(\boldsymbol{X}^T\,\boldsymbol{X}\right)^{-1}\,\boldsymbol{x}_0\,. \tag{3.7}$$

3.2.1 Performance Measures (Objectives)

We determine a set of performance measures to obtain a solution for the problem. These measures are designed to ease interaction with the decision maker and to support the optimization process. The measures take into account uncertainties lying in the estimated functions.

Suppose that there are two responses with certain target values to be considered in an MRSO problem. Then the performance measures are defined as follows:

1. *Distance to target*

   Distance to target is a typical performance measure commonly used in

the literature and industrial applications [78]. We define this as L1-norm of the difference between estimated mean model and its target value as follows:

$$| \hat{\mu}_i(\boldsymbol{x}) - t_i | , \quad i \in \{1, 2\} \tag{3.8}$$

where $\hat{\mu}_i(\boldsymbol{x})$ is the model for the mean of the response i, estimated by OLS regression, $\boldsymbol{x}$ is the design solution under consideration and t_i is the target value for response i.

If the means of the responses do not satisfy the assumptions of OLS regression and logarithmic transformation is appropriate for satisfying those assumptions, then $\hat{\mu}_i(\boldsymbol{x})$ represents the estimated mean model in the original scale obtained by Equation (3.5).

2. *Response variance*

   Estimating models for variances of the responses, $\hat{\sigma}_i^2(\boldsymbol{x})$, has been commonly used to reach robust design solutions since Taguchi's introduction of RPD. As stated in [4], log-normal linear model of variance approximately satisfies the assumptions of OLS regression. Thus, we define estimated model for variance of response i as follows:

$$\log \hat{\sigma}_i^2(\boldsymbol{x}) , \quad i \in \{1, 2\} \tag{3.9}$$

   where $\boldsymbol{x}$ is the vector of controllable design variable values under consideration. These models are estimated by fitting models to the logarithm of sample variances calculated for each run (as illustrated in Figure 3.1 by s_i^2) using OLS regression. Then, we find the estimated model in the original scale by using the Equation (3.5) when it is required.

3. *Area of the* 99.73% *prediction region*

   In order to consider possible correlations between responses we use a performance measure, area of the prediction region, which provides information on both the means and variances of the responses. 99.73% corresponding to middle 99.73% of the distribution corresponds to natural tolerance limits (NTLs) which are referred to as three sigma limits for a normally distributed process. If those limits are within the specifications it typically

means that the process is capable of meeting the specifications. Thus we prefer to use 99.73% prediction region in this study.

First, we form the prediction region as a function of controllable input variables. We cannot assume variances of the responses to be constant at different settings of the parameters due to the nature of the considered robust design problem and we aim to consider possible correlations between the responses. None of the parametric regression approaches are appropriate for that type of problem. A combination of SUR and GLS regressions can be used [86]. However, developing these models is beyond the scope of this thesis. Thus, for illustrative purposes we apply OLS regression separately for means and variances of each response and correlation coefficient then, we predict $\boldsymbol{\Sigma}$ by using empirical models, $\hat{\sigma}_1^2(\boldsymbol{x})$, $\hat{\sigma}_1^2(\boldsymbol{x})$ and $\hat{\rho}$.

$$\hat{\boldsymbol{\Sigma}}(\boldsymbol{x}) = \begin{bmatrix} \hat{\sigma}_1^2(\boldsymbol{x}) & \hat{\rho}\,\hat{\sigma}_1(\boldsymbol{x})\,\hat{\sigma}_2(\boldsymbol{x}) \\ \hat{\rho}\,\hat{\sigma}_1(\boldsymbol{x})\,\hat{\sigma}_2(\boldsymbol{x}) & \hat{\sigma}_2^2(\boldsymbol{x}) \end{bmatrix} \tag{3.10}$$

$\hat{\sigma}_1^2(\boldsymbol{x})$, $\hat{\sigma}_1^2(\boldsymbol{x})$ and $\hat{\rho}$ are the estimated models for variances of the responses and correlation coefficient in the original scale, respectively. They are formulated according to equations (3.5) - (3.7) as:

$$\begin{aligned} \hat{\sigma}_1^2(\boldsymbol{x}) &= \mathrm{e}^{\left(\boldsymbol{x}^T\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_1^2(\boldsymbol{x})} + \dfrac{m\,RSS_{\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_1^2(\boldsymbol{x})}}}{2\,m\,(n-p+1+3\,n\,v_0)+3\,RSS_{\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_1^2(\boldsymbol{x})}}}\right)} \\ \hat{\sigma}_2^2(\boldsymbol{x}) &= \mathrm{e}^{\left(\boldsymbol{x}^T\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_2^2(\boldsymbol{x})} + \dfrac{m\,RSS_{\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_2^2(\boldsymbol{x})}}}{2\,m\,(n-p+1+3\,n\,v_0)+3\,RSS_{\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_2^2(\boldsymbol{x})}}}\right)} \end{aligned} \tag{3.11}$$

and

$$\hat{\rho} = \frac{\mathrm{e}^{\left(\boldsymbol{x}^T\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}} + \dfrac{m\,RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}{2\,m\,(n-p+1+3\,n\,v_0)+3\,RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}\right)} - 1}{\mathrm{e}^{\left(\boldsymbol{x}^T\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}} + \dfrac{m\,RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}{2\,m\,(n-p+1+3\,n\,v_0)+3\,RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}\right)} + 1} \tag{3.12}$$

where n is the number of observations, p is the number of regressors and $m = n-(p+1)$; $\boldsymbol{x}^T\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_1^2(\boldsymbol{x})}$, $\boldsymbol{x}^T\hat{\boldsymbol{\beta}}_{\log\hat{\sigma}_2^2(\boldsymbol{x})}$ and $\boldsymbol{x}^T\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}$ denote estimated models for $\log\hat{\sigma}_1^2(\boldsymbol{x})$, $\log\hat{\sigma}_2^2(\boldsymbol{x})$ and $tanh^{-1}\hat{\rho} = \dfrac{1}{2}\log\dfrac{1+\rho}{1-\rho}$. RSS values and v_0 are determined by equations (3.6) and (3.7).

Furthermore, we calculate the prediction ellipsoids (prediction regions when the number of responses is two) by using the equation of MVR given in Equation (3.13) below. Since the assumptions of MVR (constant $\boldsymbol{\Sigma}$ and common set of regressors) are not satisfied, the prediction ellipsoids calculated from this formula can be considered as a rough estimate. As a future study one can develop more appropriate empirical models and prediction ellipsoid for this case combining SUR and GLS or using non parametric regression and prediction region estimation methods.

The $100\,(1-\alpha)\%$ prediction ellipsoid used in this study is

$$\begin{aligned} &\left(\boldsymbol{\beta}^T\,\boldsymbol{x}_0 - \hat{\boldsymbol{\mu}}(\boldsymbol{x})\right)^T \left(\frac{n}{n-r-1}\,\hat{\boldsymbol{\Sigma}}(\boldsymbol{x})\right)^{-1} \left(\boldsymbol{\beta}^T\,\boldsymbol{x}_0 - \hat{\boldsymbol{\mu}}(\boldsymbol{x})\right) \\ &\leqslant \left(1 + \boldsymbol{x}_0^T\,\left(\boldsymbol{X}^T\,\boldsymbol{X}\right)^{-1}\,\boldsymbol{x}_0\,\left[\frac{M\,(n-r-1)}{n-r-M}\,F_{M,n-r-M}(\alpha)\right]\right) \end{aligned} \tag{3.13}$$

where $\boldsymbol{x}_0$ is the given set of regressors, $\hat{\boldsymbol{\mu}}(\boldsymbol{x}) = [\hat{\mu}_1(\boldsymbol{x}), \hat{\mu}_2(\boldsymbol{x})]^T$ is the vector estimated models of response means, $\boldsymbol{X}$ is the design matrix specifying values of regressors, $\hat{\boldsymbol{\Sigma}}(\boldsymbol{x})$ is the variance-covariance matrix given by Equation (3.10), $\boldsymbol{\beta}$ is the true vector of coefficients which is unknown, n is the number of observations, r is the number of regressors and M is the number of responses [79].

The area of an ellipse defined in Equation (3.13) is found as follows:

$$A(\boldsymbol{x}) = k_2 \left|\frac{n}{n-r-1}\,\hat{\boldsymbol{\Sigma}}(\boldsymbol{x})\right|^{\frac{1}{2}}\,c^2 \tag{3.14}$$

where

$$c^2 = \left(1 + \boldsymbol{x}_0^T\,\left(\boldsymbol{X}^T\,\boldsymbol{X}\right)^{-1}\,\boldsymbol{x}_0\,\left[\frac{M\,(n-r-1)}{n-r-M}\,F_{M,n-r-M}(\alpha)\right]\right) \tag{3.15}$$

and k_2 is a constant term calculated by using gamma function [79]. Since the constant term is same for all settings of parameters, it does not affect the preferences of the DM. Thus, it is removed from the function and hence

$$A(\boldsymbol{x}) = \left|\frac{n}{n-r-1}\,\hat{\boldsymbol{\Sigma}}(\boldsymbol{x})\right|^{\frac{1}{2}}\,c^2 \tag{3.16}$$

where c^2 is given by (3.15). These measures correspond to a prediction interval and length of that prediction interval in single response problems.

3.3 The Interactive Optimization Approach

Even though Taguchi's RPD considers a single response, it actually corresponds to a multi objective optimization problem where mean and variance of the response are considered as the objectives to satisfy. From this point of view, we can say that for an RPD problem involving M responses there are *at least* $2M$ objectives to be considered in the multi objective optimization problem. With the addition of objectives such as that on the area of the prediction region this number increases.

For two responses, the RPD problem can be expressed as the following MRSO problem:

$$
\begin{aligned}
(P_1) \quad & Min\ |\hat{\mu}_1(\boldsymbol{x}) - t_1| \\
& Min\ |\hat{\mu}_2(\boldsymbol{x}) - t_2| \\
& Min\, \hat{\sigma}_1^2(\boldsymbol{x}) \\
& Min\, \hat{\sigma}_2^2(\boldsymbol{x}) \\
& Min\, A(\boldsymbol{x}) \\
& s.t. \\
& \boldsymbol{x} \in \boldsymbol{S}
\end{aligned}
\tag{3.17}
$$

where $\hat{\mu}_i(\boldsymbol{x})$ and $\hat{\sigma}_i^2(\boldsymbol{x})$ denote response surface models for mean and variance of the i^{th} response variable, respectively, $\boldsymbol{x}$ is the vector of controllable input variable values to be determined and t_i is the target value for response i.

For this specific problem we briefly define several concepts from multiobjective decision making area. Let $\boldsymbol{x}, \boldsymbol{x}' \in \boldsymbol{S}$ be two points in the objective space and $\boldsymbol{z}(\boldsymbol{x}) = (z_1(\boldsymbol{x}), \cdots, z_5(\boldsymbol{x}))$ and $\boldsymbol{z}(\boldsymbol{x}') = (z_1(\boldsymbol{x}'), \cdots, z_5(\boldsymbol{x}'))$. $\boldsymbol{z}(\boldsymbol{x}')$ is set to dominate $\boldsymbol{z}(\boldsymbol{x})$ if and only if $z_i(\boldsymbol{x}') \leqslant z_i(\boldsymbol{x})\ \forall i \in \{1, \cdots, 5\}$ and $z_i(\boldsymbol{x}') < z_i(\boldsymbol{x})$ for at least one i. If there exists such an $\boldsymbol{x}' \in \boldsymbol{S}$, then $\boldsymbol{z}(\boldsymbol{x})$ is set to be dominated. If there does not exist such an $\boldsymbol{x}' \in \boldsymbol{S}$, then $\boldsymbol{z}(\boldsymbol{x})$ is set to be non dominated. Naturally, we are interested in non dominated points only.

3.3.1 The Interactive Procedure

In order to solve problem (P_1) given by (3.17), we suggest an interactive procedure which is a modification of the STEM algorithm. At this stage, we change our notation slightly to ensure a better understanding of the solution procedure. The optimization model of interest (P_1), given by (3.17), is converted into the model (P_1') provided as:

$$\begin{array}{lrcll} (P_1) & Min\ |\hat{\mu}_1(\boldsymbol{x}) - t_1| & \rightarrow & Min\, z_1(\boldsymbol{x}) & (P_1') \\ & Min\ |\hat{\mu}_2(\boldsymbol{x}) - t_2| & \rightarrow & Min\, z_2(\boldsymbol{x}) & \\ & Min\, \hat{\sigma}_1^2(\boldsymbol{x}) & \rightarrow & Min\, z_3(\boldsymbol{x}) & \\ & Min\, \hat{\sigma}_2^2(\boldsymbol{x}) & \rightarrow & Min\, z_4(\boldsymbol{x}) & \\ & Min\, A(\boldsymbol{x}) & \rightarrow & Min\, z_5(\boldsymbol{x}) & \\ & & s.t. & & \\ & & \boldsymbol{x} \in \boldsymbol{S} & & \end{array} \tag{3.18}$$

As briefly mentioned in Chapter 2, the STEM algorithm suggests that, before a decisive interaction is established certain alterations on (P_1') model are to be done. Accordingly, ideal objective vector $(\boldsymbol{z}^*)$, nadir objective vector $(\boldsymbol{z}^{nad})$ and weight coefficients $(\boldsymbol{w})$ are to be calculated. The components of the ideal objective vector are obtained by minimizing each of the objective functions individually subject to the constraints as:

$$\begin{array}{l} Min\, z_j(\boldsymbol{x}) + \zeta \sum_{j=1}^{5} z_j(\boldsymbol{x}) \\ s.t. \\ \boldsymbol{x} \in \boldsymbol{S} \end{array} \tag{3.19}$$

where $j \in \{1, 2, \cdots, 5\}$, ζ is a very small constant and the second term in the objective function is a standard augmentation term to avoid dominated points [87]. Resulting solutions are written in corresponding rows of the payoff matrix given as:

$$\boldsymbol{P} = \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{15} \\ z_{21} & z_{22} & \cdots & z_{25} \\ \vdots & \vdots & \ddots & \vdots \\ z_{51} & z_{52} & \cdots & z_{55} \end{bmatrix} \tag{3.20}$$

where z_{jk} denotes the value of objective k found by solving Equation (3.19) for j^{th} objective subject to $\boldsymbol{x} \in \boldsymbol{S}$. In other words, the solutions of minimizing each response form the corresponding row of payoff matrix. Diagonal elements of the payoff matrix are the ideal objective values, z_j^*. By using the maximum of each column, nadir point of each objective, z_j^{nad} [59] is approximated. In other words, we find the payoff nadir vector. Then by using z_j^* and z_j^{nad} values, weights of the objectives ($\boldsymbol{w}$) are found by using the equations (2.9)-(2.11).

Using the above mentioned values, (P_1') is converted into the weighted Tchebycheff problem for the initialization phase of the STEM, (P_1''), as:

$$\begin{aligned} (P_1'') \quad & Min \max_{j \in \{1,2,\cdots,5\}} \left[w_j \left| z_j(\boldsymbol{x}) - z_j^* \right| \right] \\ & s.t. \\ & \boldsymbol{x} \in \boldsymbol{S} \end{aligned} \tag{3.21}$$

where $\boldsymbol{x}$ is the vector of controllable input parameters and $j \in \{1, 2, \cdots, 5\}$. The aim is to minimize the maximum distance between the solution and the ideal objective values. We convert (P_1'') into (P_1''') to manipulate the min max objective function.

$$\begin{aligned} (P_1''') \quad & Min \ a \\ & s.t. \\ & a \geqslant w_j \left(z_j(\boldsymbol{x}) - z_j^* \right) \\ & \boldsymbol{x} \in \boldsymbol{S} \end{aligned} \tag{3.22}$$

where $a \in \boldsymbol{R}$ and $j \in \{1, 2, \cdots, 5\}$. After solving (P_1'''), we represent the solutions to the DM and interaction with the DM starts. The following part explains the interaction with DM at a given iteration for one and two response design parameter optimization problems.

3.3.1.1 Interaction with the DM

In order to communicate with the DM better, the solutions found at each iteration of the interactive procedure are represented to the DM by using the visual aids displayed in Figure 3.2.

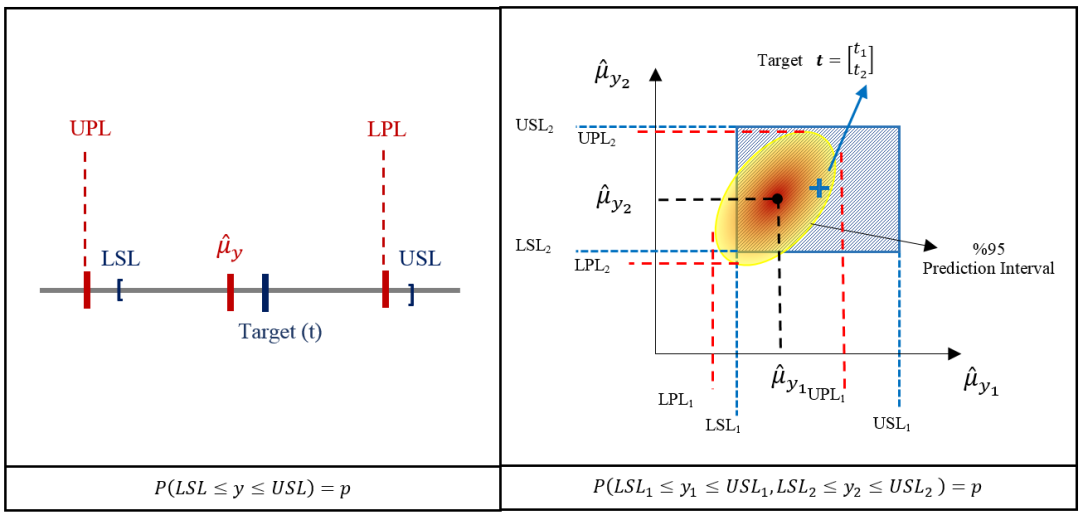

Figure 3.2: Visualization of a solution for single response problem (on the left) and binary response problem (on the right) at an iteration

As illustrated in Figure 3.2 (on the right), prediction region and simultaneous prediction intervals for each response, area of the prediction region, specification region and the probability of conformance to specifications for an unknown future value at a design solution are presented to the DM at each iteration. The aim of this visual support is to help the DM in determining the values that s/he can sacrifice from acceptable objective values and to inform the DM about the quality level that can be obtained at the presented solution. We expect that the DM learns the relationship between the objective values and the visualization of the solutions; that is s/he can understand the structure of the problem through the iterations and start to make more appropriate inferences about the objective functions' values. In addition, s/he can define the value to be sacrificed as a percentage of the current value.

We consider the single response problem as a special case of the two response problem in our study. In Figure 3.2 (on the left), for single response problems, the performance measures represented to the DM at a given iteration are illustrated. In this case, to be illustrated in Chapter 4, prediction region and area become prediction interval and distance between upper and lower limits of the prediction interval, respectively.

Suppose that at the h^{th} iteration, the DM finds value of the i^{th} objective, $z_i(\boldsymbol{x}^h)$,

acceptable, but decides to sacrifice as much as Δ_i^h from this objective to improve the others. Then, the corresponding weight of the objective, w_i, is taken as zero to drop $z_i(\boldsymbol{x}^h)$ from the objective set and a new constraint is added to the mathematical model to ensure that $z_i(\boldsymbol{x}^{h+1})$ is not worse than $\left(z_i(\boldsymbol{x}^h) + \Delta_i^h\right)$ at the next iteration $h+1$. Thus, (P_1''') assumes the following form:

$$
\begin{aligned}
(P_1'''') \quad & Min \;\; a \\
& s.t. \\
& a \geqslant w_j \left(z_j(\boldsymbol{x}) - z_j^*\right) \qquad \forall j \neq i \\
& z_i(\boldsymbol{x}^{h+1}) \leqslant z_i(\boldsymbol{x}^h) + \Delta_i^h \\
& z_j(\boldsymbol{x}^{h+1}) \leqslant z_j(\boldsymbol{x}^h) \qquad \forall j \neq i \\
& \boldsymbol{x} \in \boldsymbol{S}
\end{aligned}
\tag{3.23}
$$

The iterations continue until the DM finds all objective function values as satisfactory or acceptable, and desires to stop the optimization process.

3.3.2 Convergence of the Interactive Procedure

As we have previously stated it is not possible to comment on convergence of STEM according to a value function since it does not assume an underlying value function. The convergence of the solution procedure highly depends on how much the DM sacrifices from the objective function values at each iteration. To assume an underlying value function does not help to estimate the values to be sacrificed at an iteration. Thus, a satisfactory solution may be reached either in a short or long span of time. In some cases, a satisfactory solution may not exist due to the nature of the process influenced by factors such as technology, methods and materials used in the process. Then, the iterations proposed by the optimization procedure can help the DM to discover the difficulty of obtaining satisfactory robust design solutions and justify a tolerance design study.

In our approach, the DM is allowed to search the solution space back and forth. This provides flexibility to explore and learn the structure of the solution space. Thus, we believe that the DM learns structure of the problem through the iterations and searches the solution space better in time so that the time to reach

a satisfactory solution is not expected to be long. However, in some cases the DM may be tired of answering questions and willing to stop before a potential satisfactory solution is reached.

3.3.3 Nonlinearity of the Mathematical Models

In MRSO problems, the linear regression models fit to the performance measures may be nonlinear in term of the controllable input variables (i.e., second order models). Therefore, the objective functions $z_1(\boldsymbol{x})$ - $z_5(\boldsymbol{x})$ are typically nonlinear. We give specifics for an example problem in Chapter 4. Thus, a nonlinear multi objective optimization problem is solved at each iteration of the interactive solution procedure explained previously. In order to solve those problems, we use BARON [82,91] under MATLAB. BARON guarantees to find the global optimal solution under mild assumptions. In our study, BARON terminated with the proved-global optimal solution in most of the cases. In one exception for the two response problem illustrated in Chapter 4, BARON did not guarantee global optimality. In order to reach global optimum, the area of the prediction region function is partitioned into regions and the optimization is performed for each region. Then the global optimum is obtained by picking the optimum of the regional optima. That is a heuristic approach to handle the case specific to the provided example. Further investigations on how the structure of the function affects the solution are required to provide better solution approaches which guarantee the global optimality.

CHAPTER 4

ILLUSTRATIVE EXAMPLES

In this chapter, we illustrate the solution procedure on two examples. First, we consider a two response product and process design problem studied in the literature. Then, we illustrate our procedure on a single response problem which we generated. Latter example clarifies the data transformation when the response does not satisfy the assumptions of OLS regression. In each illustration, we exemplify the interactive procedure by acting as the DM.

4.1 Two Response Product and Process Design Optimization Problem

We illustrate the solution procedure on the polymer example presented by Myers and Montgomery [64] and used in many studies such as Vining [92], Ko et. al. [42] and Köksalan and Plante [43]. The aim of the experiment is to determine the settings of the parameters; reaction time (x_1), reaction temperature (x_2) and amount of catalyst (x_3), to maximize the conversion (y_1) of a polymer and achieve a target value of 57.5 for the thermal activity (y_2). The values within $(80, 100)$ and $(55, 60)$ are acceptable for y_1 and y_2, respectively.

In the original experiment each run involves one observation as given in Table 4.1. However, to construct the prediction region and to find its area we need to estimate the variance-covariance matrix.

Table4.1: Polymer Experiment Data

x_1	x_2	x_3	y_1(conversion)	y_2(thermal activity)
-1	-1	-1	74	53.2
1	-1	-1	51	62.9
-1	1	-1	88	53.4
1	1	-1	70	62.6
-1	-1	1	71	57.3
1	-1	1	90	67.9
-1	1	1	66	59.8
1	1	1	97	67.8
-1.68	0	0	76	59.1
1.68	-1.68	0	79	65.9
0	-1.68	0	85	60.0
0	1.68	0	97	60.7
0	0	-1.68	55	57.4
0	0	1.68	81	63.2
0	0	0	81	59.2
0	0	0	75	60.4
0	0	0	76	59.1
0	0	0	83	60.6
0	0	0	80	60.8
0	0	0	91	58.9

For this purpose, we generate a specified number of replications for each run by assuming an underlying model for variances of responses and covariance depending on the controllable input variables. In the literature, replicating experimental runs five times is a common application. Fewer number of replications might be insufficient to make reliable statistical inferences. Yet, increasing the number of replications brings additional experimental costs, that might not be practical. Thus, in this study, we generate five replications for each run. The following models, introduced by Ko et al. [42], are used:

$$\begin{bmatrix} y_{1i}(\boldsymbol{x}) \\ y_{2i}(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} y_1(\boldsymbol{x}) \\ y_2(\boldsymbol{x}) \end{bmatrix} + \boldsymbol{\epsilon}_i\,, \quad i = 1, 2, \cdots, 5 \tag{4.1}$$

where the original experiment data shown in Table 4.1 is represented by $y_1(\boldsymbol{x})$

and $y_2(\boldsymbol{x})$, and

$$\boldsymbol{\epsilon}_i \sim N\left(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}\sigma_{11}(\boldsymbol{x}) & \sigma_{12}(\boldsymbol{x})\\ \sigma_{21}(\boldsymbol{x}) & \sigma_{22}(\boldsymbol{x})\end{bmatrix}\right) \tag{4.2}$$

where $\sigma_{11}(\boldsymbol{x}) = exp(3 - x_1^2 - 3\,x_3^2)$, $\sigma_{22}(\boldsymbol{x}) = exp(2 - 2\,x_1^2 - x_3^2)$ and $\sigma_{12}(\boldsymbol{x}) = \sigma_{21}(\boldsymbol{x}) = 0.03\,\sigma_{11}(\boldsymbol{x})\,\sigma_{22}(\boldsymbol{x})$. The variance takes largest value at $x_1 = x_3 = 0$ by this setting.

Using the generated data presented in Tables 4.2-4.4, we estimate the responses, their variances and the correlation coefficient as follows:

$$\begin{aligned}
\hat{\mu}_1(\boldsymbol{x}) &= 81.1 + 1.03\,x_1 + 3.81\,x_2 + 6.17\,x_3 \\
&\quad - 2.02\,x_1^2 + 3.14\,x_2^2 - 5.21\,x_3^2 + 1.97\,x_1x_2 + 11.7\,x_1\,x_3 - 4\,x_2\,x_3 \\
\hat{\mu}_2(\boldsymbol{x}) &= 60.2 + 3.51\,x_1 + 2.26\,x_3 \\
\log\sigma_1^2(\boldsymbol{x}) &= 1.04 + 0.02\,x_1 + 0.001\,x_3 - 0.371\,x_1^2 - 1.31\,x_3^2 - 0.019\,x_1\,x_3 \\
\log\sigma_2^2(\boldsymbol{x}) &= 0.73 - 0.084\,x_1 + 0.078\,x_3 - 0.88\,x_1^2 - 0.411\,x_3^2 + 0.019\,x_1\,x_3 \\
tanh^{-1}\hat{\rho}_{12} &= 0.139 - 0.0595\,x_1 + 0.0364\,x_3 \\
&\quad - 0.0161\,x_1^2 - 0.0335\,x_3^2 + 0.12\,x_1\,x_3
\end{aligned} \tag{4.3}$$

Table4.2: The replications generated for the first response, y_1, for polymer example and the measures calculated from the data

x_1	x_2	x_3	y_{11}	y_{12}	y_{13}	y_{14}	y_{15}	$\bar{y}_1$	s_1^2	$\log s_1^2$
-1	-1	-1	74.06	73.10	74.58	73.74	74.10	73.92	0.30	-0.52
1	-1	-1	50.86	52.23	50.69	50.61	51.08	51.10	0.43	-0.36
-1	1	-1	88.47	88.39	88.64	89.52	88.70	88.74	0.20	-0.69
1	1	-1	69.22	69.54	70.34	69.46	69.90	69.69	0.19	-0.72
-1	-1	1	70.42	71.05	70.87	70.29	71.19	70.76	0.15	-0.81
1	-1	1	90.31	91.16	90.64	89.90	90.34	90.47	0.22	-0.66
-1	1	1	65.07	65.14	65.75	65.17	66.27	65.48	0.27	-0.57
1	1	1	97.62	97.25	97.21	97.20	96.46	97.15	0.18	-0.75
-1.68	0	0	77.13	75.81	75.68	74.81	74.89	75.66	0.88	-0.06
1.68	0	0	78.64	78.38	77.28	77.54	79.93	78.35	1.10	0.04
0	-1.68	0	81.86	91.54	85.54	90.37	82.89	86.44	18.96	1.28
0	1.68	0	90.79	98.89	97.43	101.85	94.45	96.68	17.95	1.25
0	0	-1.68	55.01	54.92	54.98	54.95	55.01	54.97	0.00	-2.82
0	0	1.68	81.08	81.07	80.94	81.03	81.05	81.03	0.00	-2.51
0	0	0	84.75	74.62	77.51	87.30	85.17	81.87	30.07	1.48
0	0	0	77.96	77.43	74.09	76.72	76.82	76.60	2.23	0.35
0	0	0	73.31	79.83	75.07	73.07	75.68	75.39	7.38	0.87
0	0	0	83.72	81.16	83.28	81.21	78.91	81.66	3.71	0.57
0	0	0	76.71	84.37	81.25	79.64	74.34	79.26	15.23	1.18
0	0	0	86.57	97.20	93.01	86.43	93.81	91.40	22.55	1.35

Table4.3: The replications generated for the second response, y_2, for polymer example and the measures calculated from the data

x_1	x_2	x_3	y_{21}	y_{22}	y_{23}	y_{24}	y_{25}	$\bar{y}_2$	s_2^2	$\log s_2^2$
-1	-1	-1	52.97	53.16	54.26	52.21	53.43	53.21	0.55	-0.26
1	-1	-1	62.20	61.48	62.10	63.09	62.47	62.27	0.34	-0.47
-1	1	-1	53.78	53.15	53.81	54.06	53.44	53.65	0.13	-0.89
1	1	-1	62.37	62.25	62.27	62.35	62.85	62.42	0.06	-1.22
-1	-1	1	57.49	58.10	57.22	56.45	57.15	57.28	0.36	-0.45
1	-1	1	67.36	67.99	67.77	68.32	67.22	67.73	0.20	-0.70
-1	1	1	59.12	59.83	59.57	60.26	59.75	59.71	0.17	-0.77
1	1	1	67.28	68.01	67.36	67.49	67.06	67.44	0.13	-0.90
-1.68	0	0	58.96	58.90	58.58	58.87	59.06	58.88	0.03	-1.48
1.68	0	0	66.21	65.86	65.82	65.90	65.97	65.95	0.02	-1.62
0	-1.68	0	55.18	66.64	57.62	59.69	61.78	60.18	19.02	1.28
0	1.68	0	54.37	62.13	62.05	64.23	62.18	60.99	14.54	1.16
0	0	-1.68	57.07	57.83	57.43	56.37	57.36	57.21	0.29	-0.53
0	0	1.68	63.73	62.70	62.36	65.05	62.69	63.31	1.22	0.08
0	0	0	57.18	59.60	59.23	61.61	56.06	58.74	4.71	0.67
0	0	0	66.47	57.04	58.93	61.82	59.88	60.83	12.91	1.11
0	0	0	57.01	55.26	59.58	59.66	56.66	57.63	3.72	0.57
0	0	0	60.08	58.39	55.99	58.83	61.35	58.93	4.03	0.60
0	0	0	61.44	61.37	62.69	62.09	62.36	61.99	0.33	-0.48
0	0	0	53.29	60.12	58.43	50.11	58.80	56.15	18.15	1.26

Table4.4: The correlation coefficient values, ρ, calculated from the generated data for each run and corresponding transformed values

x_1	x_2	x_3	ρ	$\frac{1}{2}\log\frac{1+\rho}{1-\rho}$
-1	-1	-1	0.57	0.28
1	-1	-1	-0.78	-0.46
-1	1	-1	0.70	0.38
1	1	-1	0.14	0.06
-1	-1	1	0.53	0.26
1	-1	1	-0.03	-0.01
-1	1	1	0.03	0.01
1	1	1	0.40	0.18
-1.68	0	0	-0.01	-0.01
1.68	0	0	0.42	0.20
0	-1.68	0	0.67	0.35
0	1.68	0	0.87	0.58
0	0	-1.68	-0.11	-0.05
0	0	1.68	0.31	0.14
0	0	0	-0.13	-0.06
0	0	0	0.43	0.20
0	0	0	-0.71	-0.38
0	0	0	-0.56	-0.28
0	0	0	-0.24	-0.10
0	0	0	0.95	0.80

Now, we need to convert these estimated models into the performance measures (or objectives) defined in Section 3.2.1 of Chapter 3, that are distances to corresponding targets, response variances and area of prediction region to move on to the optimization stage. Throughout this section, the objectives are denoted as $z_j(\boldsymbol{x})$.

1. *Distance to corresponding targets*

$$\begin{aligned} z_1(\boldsymbol{x}) &= |\hat{\mu}_1(\boldsymbol{x}) - t_1| \\ &= |81.1 + 1.03\,x_1 + 3.81\,x_2 + 6.17\,x_3 \\ &\quad - 2.02\,x_1^2 + 3.14\,x_2^2 - 5.21\,x_3^2 \\ &\quad + 1.97\,x_1\,x_2 + 11.7\,x_1\,x_3 - 4\,x_2\,x_3 - 100| \\ z_2(\boldsymbol{x}) &= |\hat{\mu}_2(\boldsymbol{x}) - t_2| = |60.2 + 3.51\,x_1 + 2.26\,x_3 - 57.5| \end{aligned} \tag{4.4}$$

2. *Response variances*

   In the optimization stage, we use estimated models for log-transformed response variances as objectives. It is equivalent to minimize response

variances in the original scale or in the log scale since the log is a monotonic transformation.

$$\begin{aligned} z_3(\boldsymbol{x}) = \log \hat{\sigma}_1^2(\boldsymbol{x}) &= 1.04 + 0.02\, x_1 + 0.001\, x_3 \\ &\quad - 0.371\, x_1^2 - 1.31\, x_3^2 - 0.019\, x_1\, x_3 \\ z_4(\boldsymbol{x}) = \log \hat{\sigma}_2^2(\boldsymbol{x}) &= 0.73 - 0.084\, x_1 + 0.078\, x_3 \\ &\quad - 0.88\, x_1^2 - 0.411\, x_3^2 + 0.019\, x_1\, x_3 \end{aligned} \tag{4.5}$$

3. *Area of the prediction region*

In order to form the area of the prediction region as a function of controllable input variables, ρ and $\boldsymbol{\Sigma}$ are required to be estimated.

The empirical model for $tanh^{-1}\hat{\rho}$ is given as:

$$\begin{aligned} tanh^{-1}\hat{\rho} &= 0.139 - 0.0595\, x_1 + 0.0364\, x_3 \\ &\quad - 0.0161\, x_1^2 - 0.0335\, x_3^2 + 0.12\, x_1\, x_3 \end{aligned} \tag{4.6}$$

If we follow the back transformation procedure explained in Chapter 3, we obtain ρ in the original scale as:

$$\hat{\rho} = \frac{\mathrm{e}^{\left(\boldsymbol{x}^T \hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}} + \dfrac{m\, RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}{2\, m\, (n-p+1+3\, n\, v_0) + 3\, RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}\right)} - 1}{\mathrm{e}^{\left(\boldsymbol{x}^T \hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}} + \dfrac{m\, RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}{2\, m\, (n-p+1+3\, n\, v_0) + 3\, RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}}}\right)} + 1} \tag{4.7}$$

where $n = 20$ (the number of observations), $p = 5$ (the number of regressors), $m = 14$ and

$$\boldsymbol{x} = \begin{bmatrix} 1 \\ x_1 \\ x_3 \\ x_1^2 \\ x_3^2 \\ x_1\, x_3 \end{bmatrix}, \quad \hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}} = \begin{bmatrix} 0.1390 \\ -0.0595 \\ 0.0364 \\ -0.0161 \\ -0.0335 \\ 0.1200 \end{bmatrix}, \tag{4.8}$$

$$RSS_{\hat{\boldsymbol{\beta}}_{tanh^{-1}\hat{\rho}}} = 1.5514\,, \quad v_0 = \boldsymbol{x}^T \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{x}\,,$$

where $\boldsymbol{X}$ is the design matrix specifying levels of the regressors at each

observation as:

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_{11} & x_{13} & x_{11}^2 & x_{13}^2 & x_{11}\,x_{13} \\ 1 & x_{21} & x_{23} & x_{21}^2 & x_{23}^2 & x_{21}\,x_{23} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n3} & x_{n1}^2 & x_{n3}^2 & x_{n1}\,x_{n3} \end{bmatrix}, \quad n = 20. \tag{4.9}$$

In Equation (4.9), an entity x_{ij} is the level of the decision variable j at observation i. Hence, the entities are obtained according to Table 4.1.

Thus, by using response variances and $\hat{\rho}$, we form $\hat{\boldsymbol{\Sigma}}$ in the original scale according to (3.10) by using:

$$\begin{aligned} \hat{\sigma}_1^2(\boldsymbol{x}) &= \mathrm{e}^{\left(\boldsymbol{x}^T \hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_1^2(\boldsymbol{x})} + \dfrac{14\, RSS_{\hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_1^2(\boldsymbol{x})}}}{28\,(16 + 60\, v_0) + 3\, RSS_{\hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_1^2(\boldsymbol{x})}}}\right)} \\ \hat{\sigma}_2^2(\boldsymbol{x}) &= \mathrm{e}^{\left(\boldsymbol{x}^T \hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_2^2(\boldsymbol{x})} + \dfrac{14\, RSS_{\hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_2^2(\boldsymbol{x})}}}{28\,(16 + 60\, v_0) + 3\, RSS_{\hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_2^2(\boldsymbol{x})}}}\right)} \end{aligned} \tag{4.10}$$

where $\boldsymbol{x}$ and v_0 are given by (4.8) and

$$\hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_1^2(\boldsymbol{x})} = \begin{bmatrix} 1.0400 \\ 0.0200 \\ 0.0010 \\ -0.3710 \\ -1.3100 \\ -0.9190 \end{bmatrix}, \quad \hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_2^2(\boldsymbol{x})} = \begin{bmatrix} 0.7300 \\ -0.0840 \\ 0.0780 \\ -0.8800 \\ -0.4110 \\ 0.0190 \end{bmatrix}, \tag{4.11}$$

$$RSS_{\hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_1^2(\boldsymbol{x})}} = 1.3307\,, \qquad RSS_{\hat{\boldsymbol{\beta}}_{\log \hat{\sigma}_2^2(\boldsymbol{x})}} = 3.4416$$

We present natural tolerance limits (or $3\,\sigma$ limits) to DM which include 99.73% of the variable for a normal distribution. In other words, we present 99.73% prediction region at each iteration. Since we use the formulation of MVR regression in order to show the prediction region, we need to use the same set of regressors in empirical models of the response means. However, we fit separate models for the means of the responses by using OLS regression, that is, we may have different set of regressors. For illustrative purposes, as a common set of regressors we choose the union of the regressors included in each mean model then assign 0 value to the coefficients

of the regressors which are not used in corresponding model. In this case, we have nine regressors which are included in the estimated model of first response mean. Thus, the area of 99.73% prediction region is obtained according to Equation (3.16) by setting $(n, r, M) = (20, 9, 2)$. Hence, the last performance measure, $z_5(\boldsymbol{x})$ becomes:

$$z_5(\boldsymbol{x}) = \left|2\,\hat{\boldsymbol{\Sigma}}(\boldsymbol{x})\right|^{\frac{1}{2}}\, c^2 \tag{4.12}$$

where c^2 is given by (3.15).

4.1.1 The Interactive Procedure

Before starting the interactive procedure, we need to find the payoff matrix, $\boldsymbol{P}$, ideal and nadir objective vectors, $\boldsymbol{z}^*$ and $\boldsymbol{z}^{nad}$, and weighting coefficients, $\boldsymbol{w}$, as we explain previously. Using the formulations given by equations (3.19) and (3.20), the payoff matrix, $\boldsymbol{P}$ is obtained as:

$$\boldsymbol{P} = \begin{bmatrix} 0.0001 & 11.0057 & -3.2831 & -1.8180 & 2.2250 \\ 23.4915 & 0.0000 & 0.3790 & 0.4218 & 15.3341 \\ 21.6478 & 6.9936 & -3.7934 & -2.8500 & 2.5736 \\ 14.2822 & 12.3936 & -3.7228 & -2.8702 & 2.4601 \\ 5.8121 & 12.3936 & -3.7228 & -2.8702 & 1.2030 \end{bmatrix} \tag{4.13}$$

and using $\boldsymbol{P}$, $\boldsymbol{z}^*$ and $\boldsymbol{z}^{nad}$ are obtained as explained in Section 3.3.1 and depicted in Figure 2.2:

$$\boldsymbol{z}^* = \begin{bmatrix} 0.0001 \\ 0.0000 \\ -3.7934 \\ -2.8702 \\ 1.2030 \end{bmatrix}, \quad \boldsymbol{z}^{nad} = \begin{bmatrix} 23.4915 \\ 12.3936 \\ 0.3790 \\ 0.4218 \\ 15.3341 \end{bmatrix} \tag{4.14}$$

and finally $\boldsymbol{w}$ is determined by the equations (2.9)-(2.11) as:

$$\boldsymbol{w} = \begin{bmatrix} 0.1935 \\ 0.1935 \\ 0.2128 \\ 0.2219 \\ 0.1783 \end{bmatrix} . \tag{4.15}$$

Once the necessary calculations are available, the interactive procedure is ready to be performed. In the illustration of the procedure, no real decision maker is collaborated with and no underlying utility function is preassumed. We exemplify the steps of the interactive process by considering the cases on behalf of the DM. That is to say, the procedure is carried on by considering example responses from the DM such as what the DM would like to have or would say in a particular situation.

First, we set iteration counter to zero ($h = 0$) and in order to present the initial solution to the DM, we solve the problem given by equation (3.22) using the values obtained in equations (4.14) and (4.15). That is, we solve

$$\begin{aligned} (P^0) \quad & Min \;\; a \\ & s.t. \\ & a \geqslant w_1 \; (z_1(\boldsymbol{x}) - 0.0001) \\ & a \geqslant w_2 \; (z_2(\boldsymbol{x}) - 0) \\ & a \geqslant w_3 \; (z_3(\boldsymbol{x}) + 3.7934) \\ & a \geqslant w_4 \; (z_4(\boldsymbol{x}) + 2.8702) \\ & a \geqslant w_5 \; (z_5(\boldsymbol{x}) - 1.2030) \\ & 1.68 \geqslant x_1 \geqslant -1.68 \\ & 1.68 \geqslant x_2 \geqslant -1.68 \\ & 1.68 \geqslant x_3 \geqslant -1.68 \end{aligned} \tag{4.16}$$

where $z_1(\boldsymbol{x})$-$z_5(\boldsymbol{x})$ are given by equations (4.4), (4.5) and (4.12). The format of the presentation may require care in order to obtain correct preference information and not to overload the DM with information. However, we do not address these issues here. Mainly, some or all of the information in Table 4.5 can be provided to the DM.

Table4.5: Initial solution, corresponding values of the objectives and additional information, p, which is the probability of being within specification limits

h	x_1	x_2	x_3	$\hat{\mu}_1(\boldsymbol{x})$	$\hat{\mu}_2(\boldsymbol{x})$	$\hat{\sigma}_1^2(\boldsymbol{x})$	$\hat{\sigma}_2^2(\boldsymbol{x})$	$A(\boldsymbol{x})$	$\hat{\rho}$	p
0	-1.1	1.58	-1.68	95.05	52.55	0.01	0.23	6.57	0.13	$1.6\,10^{-7}$

Probability of conforming specifications is very low as seen in the results given in Table 4.5. In addition, in Figure 4.1, it is shown that $\hat{\boldsymbol{\mu}}_2(\boldsymbol{x})$ is not within the corresponding specifications. Thus, the DM may sacrifice from area, $A(\boldsymbol{x})$, of the prediction region in order to improve the mean values of the responses. Suppose that area of the prediction region up to 10 is acceptable for the DM thus s/he sacrifices 3.4433 units from $A(\boldsymbol{x})$ given by Equation (3.16).

After taking the DM's preferences, we set $h = 1$ and another mathematical model (P^1) is to be formed. We remove $A(\boldsymbol{x})$ from the objective set and restrict its value by 10 (equivalently $6.5567 + 3.4433$). As a result of this relaxation, we expect that the area will increase.

$$
\begin{aligned}
(P^1) \quad & Min \;\; a \\
& s.t. \\
& a \geqslant w_1 \; (z_1(\boldsymbol{x}) - 0.0001) \\
& a \geqslant w_2 \; (z_2(\boldsymbol{x}) - 0) \\
& a \geqslant w_3 \; (z_3(\boldsymbol{x}) + 3.7934) \\
& a \geqslant w_4 \; (z_4(\boldsymbol{x}) + 2.8702) \\
& 10 \geqslant z_5(\boldsymbol{x}) \\
& 1.68 \geqslant x_1 \geqslant -1.68 \\
& 1.68 \geqslant x_2 \geqslant -1.68 \\
& 1.68 \geqslant x_3 \geqslant -1.68
\end{aligned}
\tag{4.17}
$$

where $z_1(\boldsymbol{x})$-$z_5(\boldsymbol{x})$ are given by equations (4.4), (4.5) and (4.12). We solved (P^1) and present the solutions and corresponding objective values to the DM as given in Table 4.6 and Figure 4.2.

As shown in Table 4.6 and Figure 4.2 mean values of the responses are improved

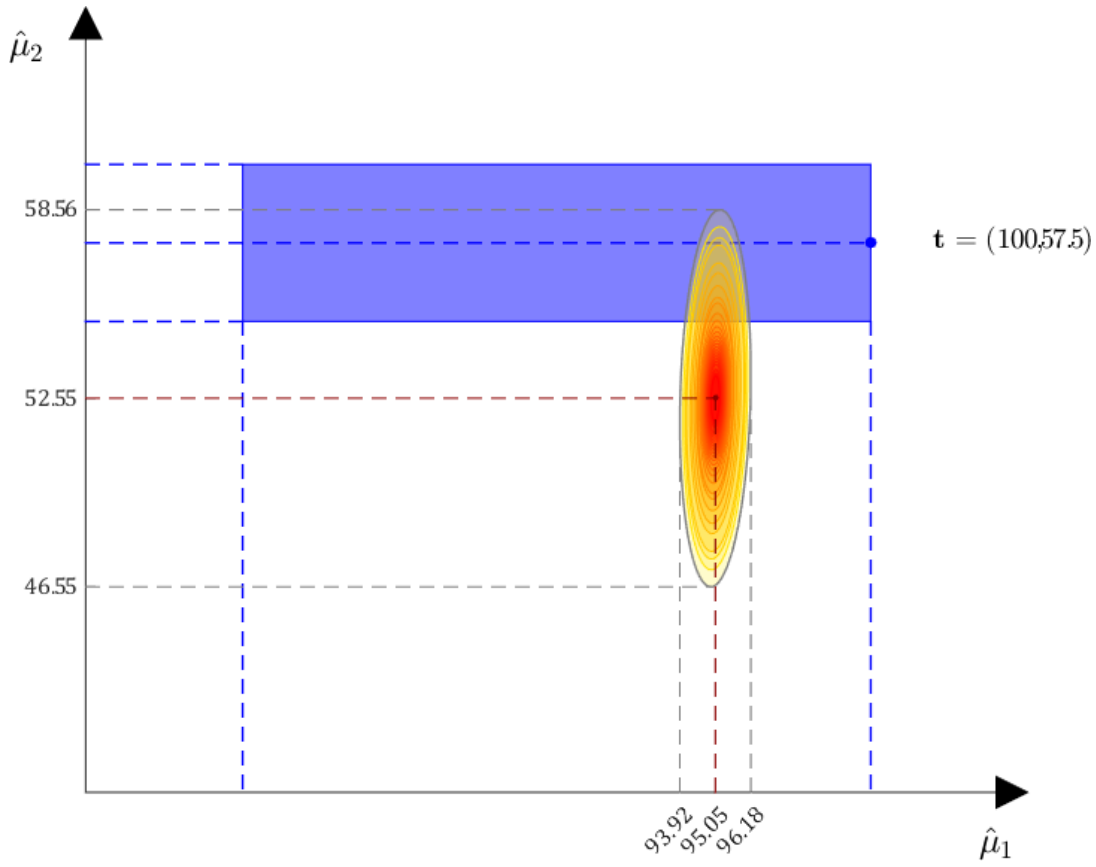

Figure 4.1: Visualization of the solution ($h = 0$) for the two response problem

Table4.6: First iteration results and corresponding objective values and additional information, p, which is the probability of being within specification limits

h	x_1	x_2	x_3	$\hat{\mu}_1(\boldsymbol{x})$	$\hat{\mu}_2(\boldsymbol{x})$	$\hat{\sigma}_1^2(\boldsymbol{x})$	$\hat{\sigma}_2^2(\boldsymbol{x})$	$A(\boldsymbol{x})$	$\hat{\rho}$	p
1	-0.96	1.68	-1.62	95.67	53.19	0.02	0.31	10	0.11	$5.32\,10^{-4}$

and the area of the prediction region is at its limit. This shows that there is a tradeoff between those objectives. In addition, probability of conforming specifications is slightly increased. Since $\hat{\boldsymbol{\mu}}_2(\boldsymbol{x})$ is still far from its specifications, the DM does not find this acceptable. S/he may sacrifice more from the area of the prediction region to improve $\hat{\boldsymbol{\mu}}_2(\boldsymbol{x})$. S/he may think that approximately 3.5 unit increase in the area of the prediction region improves $\hat{\boldsymbol{\mu}}_2(\boldsymbol{x})$ by approximately 0.5 unit. Then, the DM may sacrifice 20 more units from area to obtain value of $\hat{\boldsymbol{\mu}}_2(\boldsymbol{x})$ within its specifications.

After taking the DM's preferences, we set $h = 2$ and form the corresponding mathematical model (P^2). $A(\boldsymbol{x})$ has been already removed from the objective

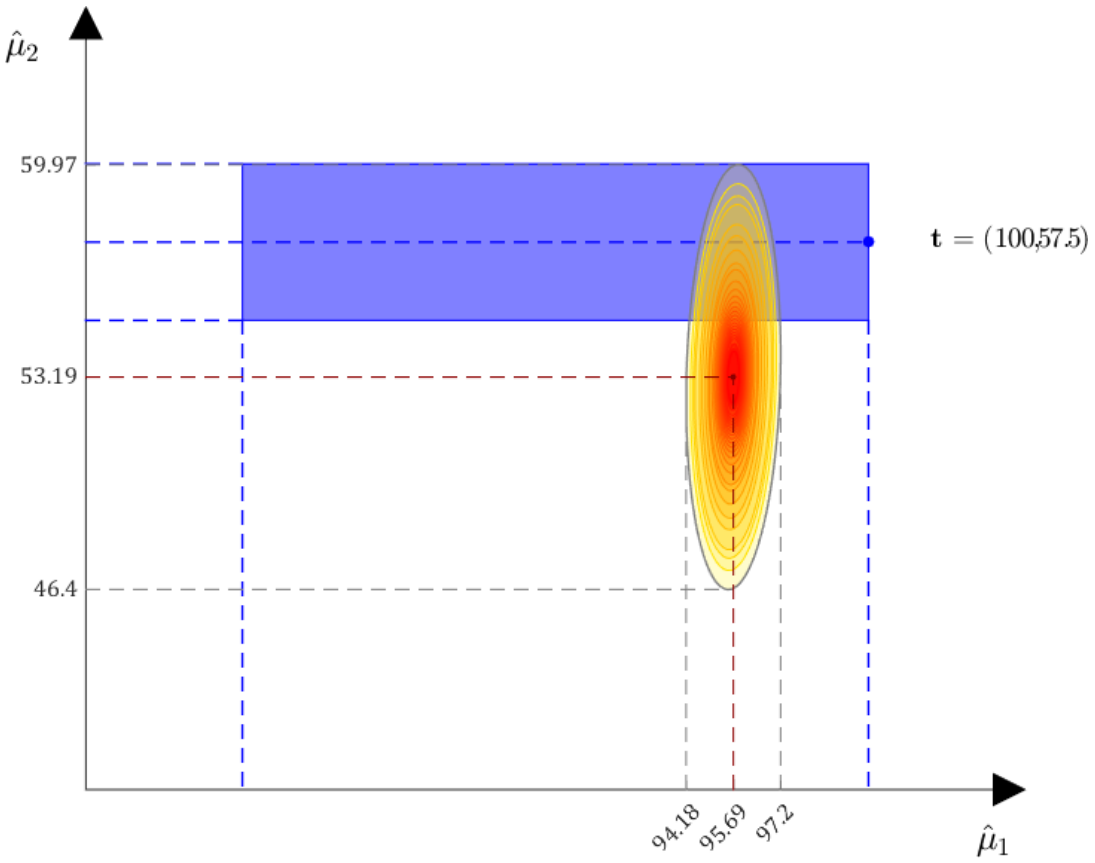

Figure 4.2: Visualization of the solution ($h = 1$) for the two response problem

set. We only change its allowable limit by 30.

$$
\begin{aligned}
(P^2) \quad & Min \;\; a \\
& s.t. \\
& a \geqslant w_1 \;(z_1(\boldsymbol{x}) - 0.0001) \\
& a \geqslant w_2 \;(z_2(\boldsymbol{x}) - 0) \\
& a \geqslant w_3 \;(z_3(\boldsymbol{x}) + 3.7934) \\
& a \geqslant w_4 \;(z_4(\boldsymbol{x}) + 2.8702) \\
& 30 \geqslant z_5(\boldsymbol{x}) \\
& 1.68 \geqslant x_1 \geqslant -1.68 \\
& 1.68 \geqslant x_2 \geqslant -1.68 \\
& 1.68 \geqslant x_3 \geqslant -1.68
\end{aligned}
\tag{4.18}
$$

where $z_1(\boldsymbol{x})$-$z_5(\boldsymbol{x})$ are given by equations (4.4), (4.5) and (4.12). (P^2) is solved and the solutions and corresponding objective values are presented to the DM

as given in Table 4.7 and Figure 4.3.

Table4.7: Second iteration results and corresponding objective values and additional information, p, which is the probability of being within specification limits

h	x_1	x_2	x_3	$\hat{\mu}_1(\boldsymbol{x})$	$\hat{\mu}_2(\boldsymbol{x})$	$\hat{\sigma}_1^2(\boldsymbol{x})$	$\hat{\sigma}_2^2(\boldsymbol{x})$	$A(\boldsymbol{x})$	$\hat{\rho}$	p
2	-0.94	1.68	-1.12	96.89	54.39	0.15	0.59	26.56	0.11	0.21

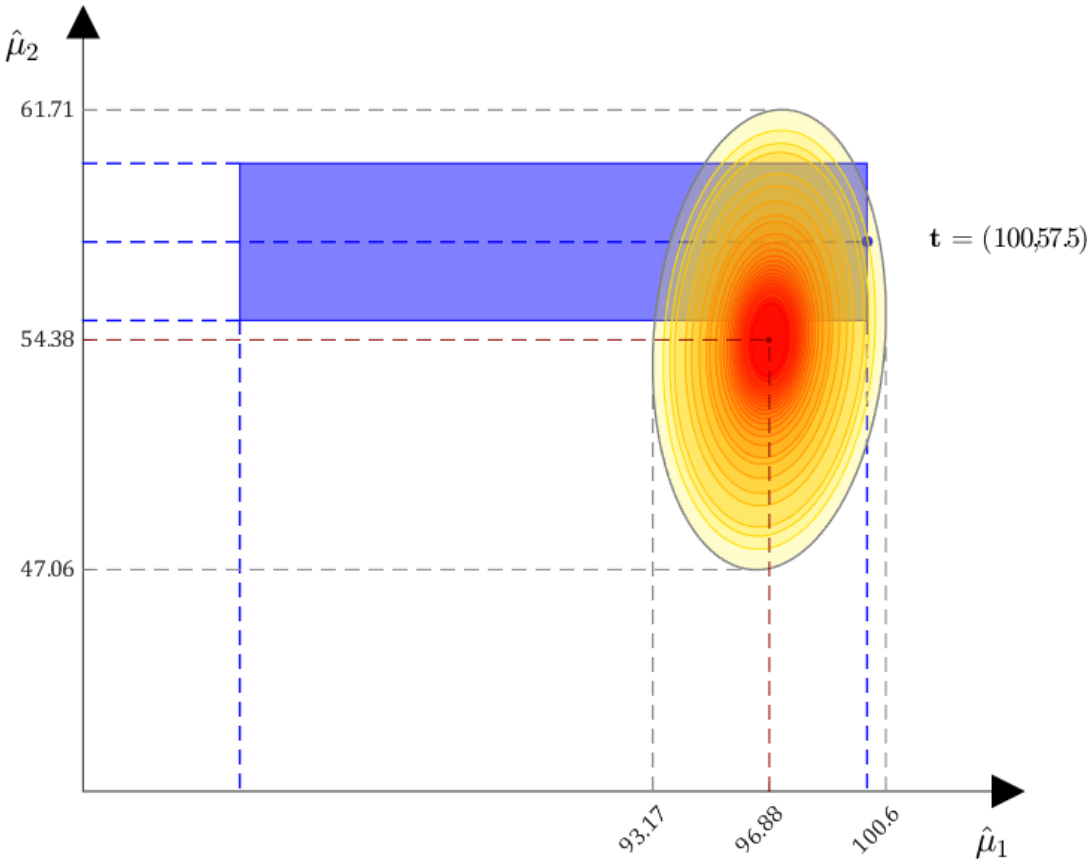

Figure 4.3: Visualization of the solution ($h = 2$) for the two response problem

Table 4.7 and Figure 4.3 show that the mean of the second response is still out of its specifications. In addition, the area of the prediction region is not on the limit determined by the DM. This shows that increasing the area will no longer be helpful to improve $\hat{\boldsymbol{\mu}}_2(\boldsymbol{x})$. Now, the DM may find the value of $\hat{\boldsymbol{\mu}}_1(\boldsymbol{x})$ as acceptable and sacrifice from the corresponding objective value by 6.8846 which means that the distance between $\hat{\boldsymbol{\mu}}_1(\boldsymbol{x})$ and its target is allowed to take values up to 10. Thus, we remove $\hat{\boldsymbol{\mu}}_1(\boldsymbol{x})$ from the objective set and keep the constraint

on $A(\boldsymbol{x})$ unchanged. We restrict the distance between $\hat{\boldsymbol{\mu}}_1(\boldsymbol{x})$ and corresponding target value by 10. Hence, the next problem (P^3) becomes:

$$
\begin{aligned}
(P^3) \quad & Min \ a \\
& s.t. \\
& 10 \geqslant z_1(\boldsymbol{x}) \\
& a \geqslant w_2 \ (z_2(\boldsymbol{x}) - 0) \\
& a \geqslant w_3 \ (z_3(\boldsymbol{x}) + 3.7934) \\
& a \geqslant w_4 \ (z_4(\boldsymbol{x}) + 2.8702) \\
& 30 \geqslant z_5(\boldsymbol{x}) \\
& 1.68 \geqslant x_1 \geqslant -1.68 \\
& 1.68 \geqslant x_2 \geqslant -1.68 \\
& 1.68 \geqslant x_3 \geqslant -1.68
\end{aligned}
\tag{4.19}
$$

where $z_1(\boldsymbol{x})$-$z_5(\boldsymbol{x})$ are given by equations (4.4), (4.5) and (4.12). (P^3) is solved and the solutions and corresponding objective values are presented to the DM as given in Table 4.8 and Figure 4.4.

Table4.8: Third iteration results and corresponding objective values and additional information, p, which is the probability of being within specification limits

h	x_1	x_2	x_3	$\hat{\mu}_1(\boldsymbol{x})$	$\hat{\mu}_2(\boldsymbol{x})$	$\hat{\sigma}_1^2(\boldsymbol{x})$	$\hat{\sigma}_2^2(\boldsymbol{x})$	$A(\boldsymbol{x})$	$\hat{\rho}$	p
3	-0.47	1.68	-1.62	90	54.91	0.04	0.54	17.81	0.05	0.45

It can be observed from the solutions provided by Table 4.8 and Figure 4.4, the constraint on the area becomes redundant, since it does not reach its limit specified by the DM. That means that even though the DM sacrifices from area of the prediction region it may not get worse as long as the variances are in the objective set. Thus, the DM needs to sacrifice some units from the variances to improve the second objective. Since it is not easy to understand variances as values, we allow the DM to state his/her preferences on variances by percentages. In this step, the DM may understand that it is not possible to obtain a solution that minimizes the area of the prediction region and the distance between the mean values of the responses to their targets. Then, s/he may decide that the

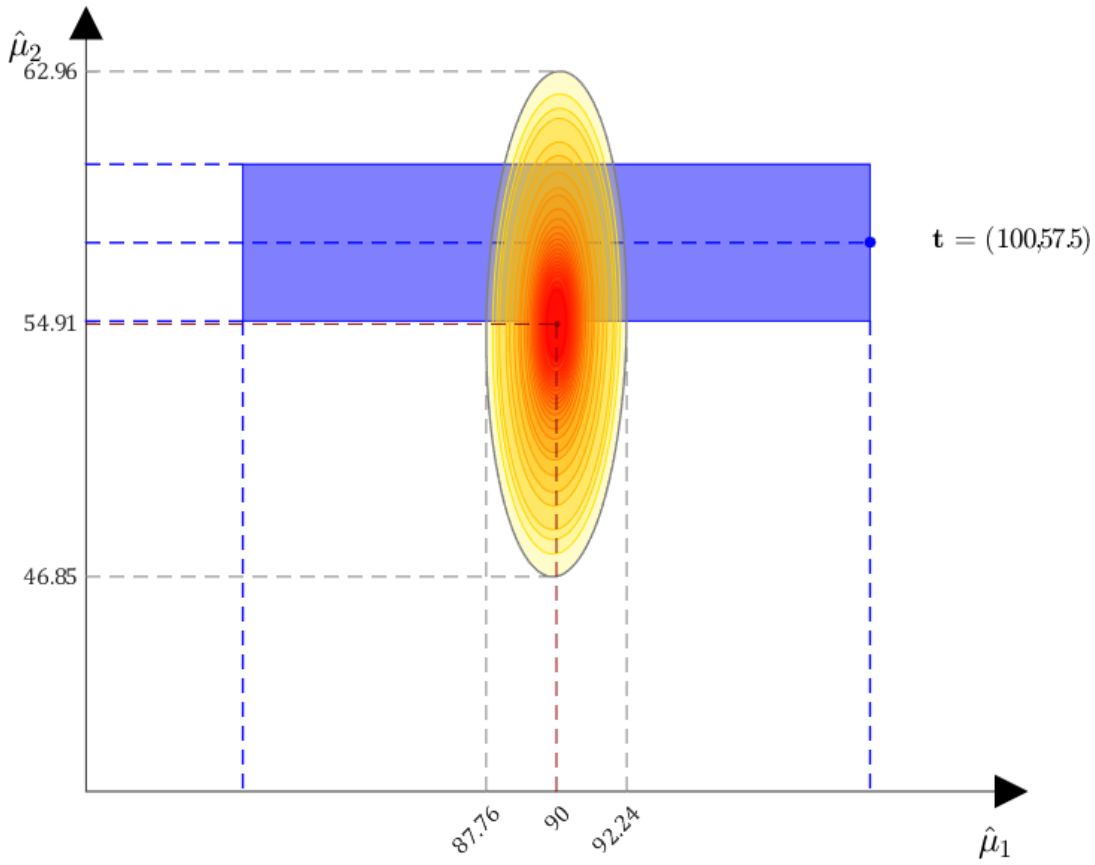

Figure 4.4: Visualization of the solution ($h = 3$) for the two response problem

area of the prediction region is more important than the individual values of variances. As the area is limited by 30, s/he may no longer need to limit the variances and decide to set them free to see how the other objectives are affected. Thus, we remove variances from the objective set and keep the constraint on $A(\boldsymbol{x})$ the same. We maintain restricting the distance between $\hat{\boldsymbol{\mu}}_1(\boldsymbol{x})$ and its corresponding target value by 10. To proceed, the problem is reformulated as

(P^4):

$$
\begin{aligned}
(P^4) \quad & Min \ a \\
& s.t. \\
& 10 \geqslant z_1(\boldsymbol{x}) \\
& a \geqslant w_2 \ (z_2(\boldsymbol{x}) - 0) \\
& 30 \geqslant z_5(\boldsymbol{x}) \\
& 1.68 \geqslant x_1 \geqslant -1.68 \\
& 1.68 \geqslant x_2 \geqslant -1.68 \\
& 1.68 \geqslant x_3 \geqslant -1.68
\end{aligned}
\tag{4.20}
$$

where $z_1(\boldsymbol{x})$, $z_2(\boldsymbol{x})$ and $z_5(\boldsymbol{x})$ are given by equations (4.4), (4.5) and (4.12). (P^4) is solved and the solutions and corresponding objective values are presented to the DM as given in Table 4.9 and Figure 4.5.

Table4.9: Fourth iteration results and corresponding objective values and additional information, p, which is the probability of being within specification limits

h	x_1	x_2	x_3	$\hat{\mu}_1(\boldsymbol{x})$	$\hat{\mu}_2(\boldsymbol{x})$	$\hat{\sigma}_1^2(\boldsymbol{x})$	$\hat{\sigma}_2^2(\boldsymbol{x})$	$A(\boldsymbol{x})$	$\hat{\rho}$	p
4	-0.55	1.31	-0.77	90	56.56	0.79	1.25	30	0.08	0.92

The area of the prediction region and the distance between $\hat{\boldsymbol{\mu}}_1(\boldsymbol{x})$ and its target are on their limits. We observe the best value of the second objective so far. That directly affects the probability of conformance which is increased to 0.92.

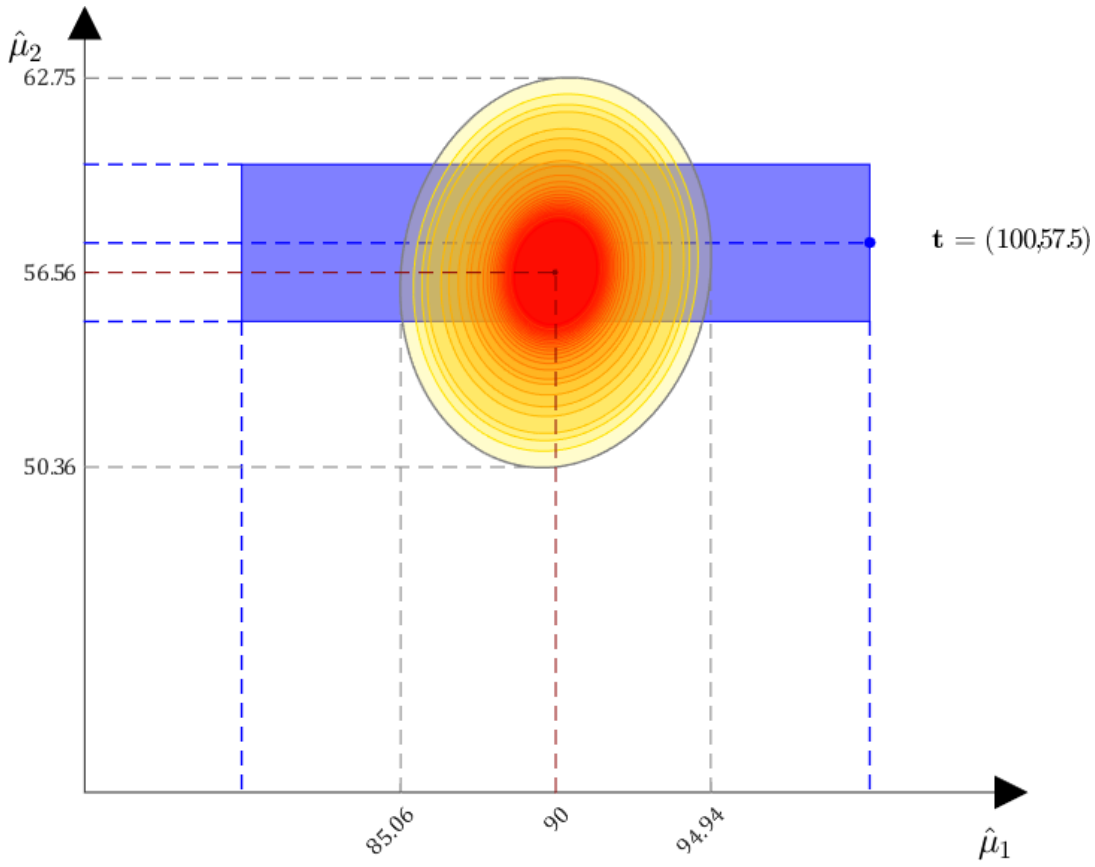

Figure 4.5: Visualization of the solution ($h = 4$) for the two response problem

We expect that the DM learns about his/her problem and his/her preferences through the iterations. It is obvious that there is no solution minimizing the area of the prediction region while bringing the means of the responses to their targets with current limitations of the system. In order to improve the objectives, the DM needs to improve the current technology or equipment or so on. Thus, we assume that this solution is acceptable for the DM and s/he is willing to stop the procedure in this step.

4.2 Single Response Product and Process Design Optimization Problem

In order to present how our method may be applied on a single response problem whose response is a non-normally distributed random variable, we assume an experimental layout shown in Table 4.10.

Table4.10: The generated data for the single response problem, corresponding sample variances, s^2, and transformed values

x	z_1	z_2	z_3	z_4	z_5	s^2	$\log s^2$	y_1	y_2	y_3	y_4	y_5
1	7.72	3.30	13.96	13.94	11.53	20.92	3.04	2.04	1.19	2.64	2.64	2.44
3	27.11	75.13	56.67	140.6	73.55	$17.34\,10^2$	7.46	3.30	4.32	4.04	4.95	4.30
5	735.58	367.82	352.41	773.27	175.38	$6.83\,10^4$	11.13	6.60	5.91	5.86	6.65	5.17
7	$1.43\,10^3$	$1.55\,10^3$	$2.4\,10^3$	$5.78\,10^3$	$5.47\,10^3$	$4.56\,10^6$	15.33	7.27	7.35	7.78	8.66	8.61

In order to illustrate the solution procedure, arbitrarily picked four different settings ($x_1 = 1$, $x_2 = 3$, $x_3 = 5$ and $x_4 = 7$) of one controllable variable, x, are studied. For each setting, we generate log-normally distributed response values replicated five times according to an underlying model. For a given setting i, each observation j on the response variable, y, is generated as follows:

$$y_{ij} = \mathrm{e}^{z_{ij}}\,, \quad i \in \{1, \cdots, 4\},\ j \in \{1, \cdots, 5\} \tag{4.21}$$

where

$$z_{ij} = \mu_i + \epsilon_{ij}\,, \quad \epsilon_{ij} \sim N(0, 2)\ and\ \mu_i = x_i\,. \tag{4.22}$$

In order to satisfy the assumptions of OLS regression, logarithmic transformation is applied to the response values and z_{ij} values are obtained, which are already known in our case, since we generate the data by those. Then, we fit a model for means of z_i's ($\mu_{\log y_i}$ values). Moreover, we calculate sample variances of z_i's for each setting and we transform those values into the log scale and fit a model for $\log \sigma_y^2(x)$. In addition, we calculate sample variances for each setting by using original data, i.e. $Var(y_i)$, and after transforming those values into the log scale, we fit a model for $\log \sigma^2_{\log y}(x)$.

$$\begin{aligned} \hat{\mu}_{\log y}(x) &= 1.27 + 0.95\,x \\ \log \hat{\sigma}^2_{\log y}(x) &= -0.93 - 0.08\,x + 0.01\,x^2 \\ \log \hat{\sigma}^2_{y}(x) &= 0.98 + 2.135\,x \end{aligned} \tag{4.23}$$

Now, we can calculate the performance measures explained in Section 3.2.1 of Chapter 3 which are distance to target, response variance and area of the prediction region. In a single response problem, variance-covariance matrix, prediction region and the area of the prediction region become variance, prediction interval and the length of the prediction interval, respectively.

1. *Distance to target*

$$z_1(x) = |\hat{\mu}_{\log y}(x) - \log t| = |1.27 + 0.95\,x - \log 200| \tag{4.24}$$

where t is the target value which is 200 in this example.

2. *Response variance*

In the optimization stage, we use estimated model for log-transformed response variance as objective. It is equivalent to minimization response variance in the original scale or in the log scale, since the log is a monotonic transformation.

$$z_2(x) = \log \sigma_y^2(x) = 0.98 + 2.135\,x \tag{4.25}$$

3. *Length of the prediction interval*

It is easy to show that in a single response problem, prediction regions corresponds to prediction interval. OLS regression formulation of $100\,(1-\alpha)\%$ prediction interval is

$$\hat{\mu}_{\log y} \pm t_{n-r-1}\left(\frac{\alpha}{2}\right)\sqrt{\hat{\sigma}^2_{\log y}\left(1 + \boldsymbol{x}_0^T\left(\boldsymbol{X}^T\boldsymbol{X}\right)\boldsymbol{x}_0\right)} \tag{4.26}$$

where

$$\boldsymbol{x}_0 = \begin{bmatrix} 1 \\ x \end{bmatrix}\,,\quad \boldsymbol{X} = \begin{bmatrix} 1 & 1 \\ 1 & 3 \\ 1 & 5 \\ 1 & 7 \end{bmatrix}\,, \tag{4.27}$$

$$n = 4\,,\ \ r = 1\,,\ \ \alpha = 0.0027 \textit{ and } t_2(0.00135) = 27.189.$$

$\hat{\sigma}^2_{\log y}$ is the estimated variance of z_i's in the original scale, that are obtained by using (3.4) - (3.6).

Length of 99.73% prediction interval, $L(\boldsymbol{x})$, is defined as

$$z_3(\boldsymbol{x}) = L(\boldsymbol{x}) = 2\left(t_{n-r-1}\left(\frac{\alpha}{2}\right)\sqrt{\hat{\sigma}^2_{\log y}\left(1 + \boldsymbol{x}_0^T\left(\boldsymbol{X}^T\boldsymbol{X}\right)\boldsymbol{x}_0\right)}\right) \tag{4.28}$$

4.2.1 The Interactive Procedure

As an initial phase of STEP method we calculate payoff matrix, $\boldsymbol{P}$, ideal and nadir objective vectors, $\boldsymbol{z}^*$ and $\boldsymbol{z}^{nad}$, and weighting coefficients, $\boldsymbol{w}$. Using the

formulations given by equations (3.19) and (3.20) the payoff matrix, $\boldsymbol{P}$ is obtained as:

$$\boldsymbol{P} = \begin{bmatrix} 0.00 & 9.99 & 35.30 \\ 3.07 & 3.12 & 43.00 \\ 0.21 & 9.52 & 35.25 \end{bmatrix} \tag{4.29}$$

and using $\boldsymbol{P}$, $\boldsymbol{z}^*$ and $\boldsymbol{z}^{nad}$ are obtained as explained in Section 3.3.1 and depicted in Figure 2.2:

$$\boldsymbol{z}^* = \begin{bmatrix} 0.00 \\ 3.1150 \\ 35.25 \end{bmatrix}, \quad \boldsymbol{z}^{nad} = \begin{bmatrix} 3.07 \\ 9.99 \\ 43.00 \end{bmatrix} \tag{4.30}$$

and finally $\boldsymbol{w}$ is determined by the equations (2.9)-(2.11) as:

$$\boldsymbol{w} = \begin{bmatrix} 0.54 \\ 0.37 \\ 0.10 \end{bmatrix}. \tag{4.31}$$

Once $\boldsymbol{P}$, $\boldsymbol{z}^*$, $\boldsymbol{z}^{nad}$ and $\boldsymbol{w}$ are available, the interactive procedure is ready to be performed. Similar to the previous example presented in Section 4.1, no real decision maker is collaborated with and we exemplify the steps of the interactive process by considering the cases on behalf of the DM.

For the very first iteration ($h = 0$) and the initial solution to the DM is to be presented. For this purpose, the problem given by equation (3.22) is solved for the single response by using the values obtained in equations (4.30) and (4.31). That is, we solve

$$\begin{aligned} (P^0) \quad & Min \ \ a \\ & s.t. \\ & a \geqslant w_1 \ (z_1(x) - 0.00) \\ & a \geqslant w_2 \ (z_2(x) - 3.12) \\ & a \geqslant w_3 \ (z_3(x) - 35.25) \\ & 7 \geqslant x \geqslant 1 \end{aligned} \tag{4.32}$$

where $z_1(x)$, $z_2(x)$ and $z_3(x)$ are given by equations (4.24), (4.25) and (4.28). Some or all of the information that corresponds to the solution of (P^0) can be represented to the DM as given in Figure 4.6.

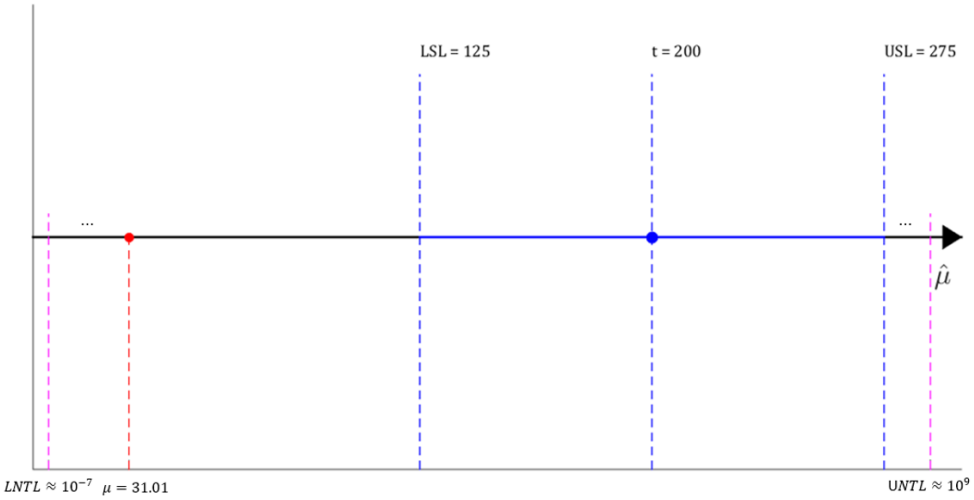

Figure 4.6: Visualization of the solution ($h = 0$) for the single response problem in the original scale

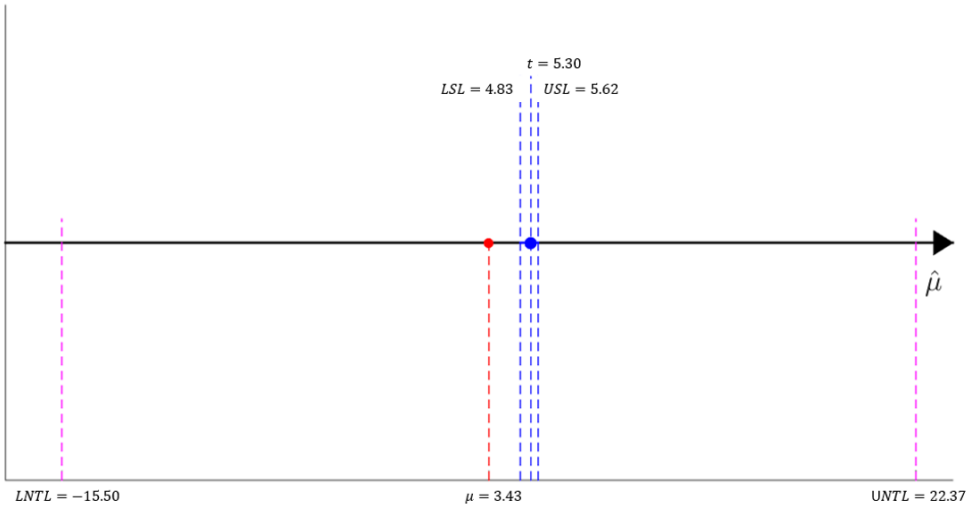

Figure 4.7: Visualization of the solution ($h = 0$) for the single response problem in the log scale

As we stated in (4.26), we find prediction intervals for z_i's. Then, we directly back transform them, due to the fact that the percentage of data remaining in the tails is preserved, since logarithmic transformation is a monotonic transformation. As we show in Figure 4.6, 99.73% prediction intervals which correspond to natural tolerance limits (NTLs) are too wide. This may partially indicate that estimation of prediction intervals in the original scale is not appropriate. Thus, for this specific case of single response problems where the response follows a

non normal distribution we prefer to represent solutions to the DM in the log scale.

Now, the DM is required to state his/her preferences according to Figure 4.7, since the prediction interval is wider than specification limits, we assume that the DM decides to sacrifice approximately 2.5 units from the mean value in order to decrease the length of the prediction interval. According to the DM's preference, we are to start another iteration $h = 1$ and another mathematical model (P^1) is formed by restricting the first objective by 6.

$$\begin{aligned} (P^1) \quad & Min \ \ a \\ & s.t. \\ & 6 \geqslant z_1(x) \\ & a \geqslant w_2 \ (z_2(x) - 3.12) \\ & a \geqslant w_3 \ (z_3(x) - 35.25) \end{aligned} \tag{4.33}$$

where $z_1(x)$, $z_2(x)$ and $z_3(x)$ are given by equations (4.24), (4.25) and (4.28).

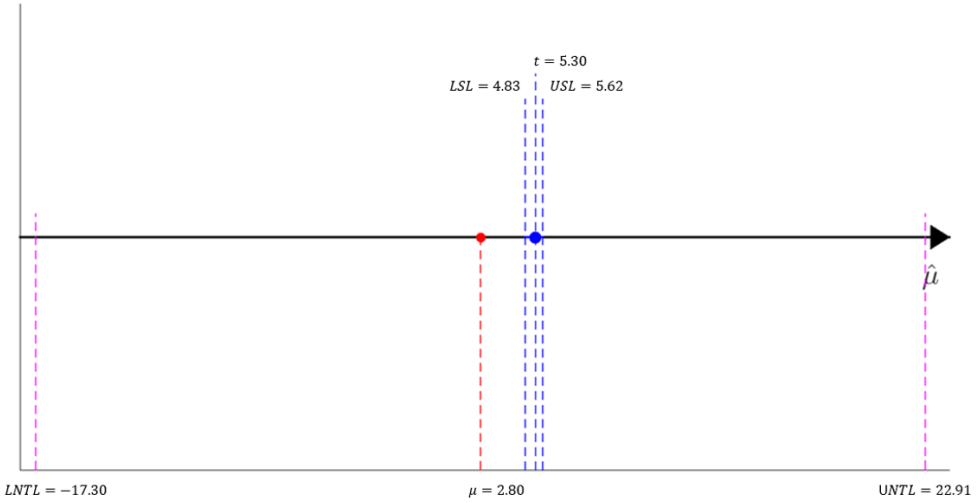

Figure 4.8: Visualization of the solution ($h = 1$) for the single response problem in the log scale

P^1 is solved and the solutions and corresponding objective values are presented to the DM as given in Figure 4.8. As observed from 4.8, sacrificing from mean value does not improve length of the prediction interval. Thus, the DM learns that it is not possible to decrease the length of the prediction interval with

current limitations and s/he is willing to stop sacrificing from the mean value of the response. Thus, s/he may decide to sacrifice from the length of the prediction interval in order to bring the mean value within the specification limits. We assume that s/he specifies the allowable limit of the length of the interval as 60. Now, the length of the prediction interval is expected to increase owing to this relaxation. The next problem to be solved for the second iteration, $h = 2$, becomes:

$$
\begin{aligned}
(P^2) \quad & Min \;\; a \\
& s.t. \\
& a \geqslant w_1 \;\; (z_1(x) - 0.00) \\
& a \geqslant w_2 \;\; (z_2(x) - 3.12) \\
& 60 \geqslant z_3(x)
\end{aligned}
\tag{4.34}
$$

where $z_1(x)$, $z_2(x)$ and $z_3(x)$ are given by equations (4.24), (4.25) and (4.28).

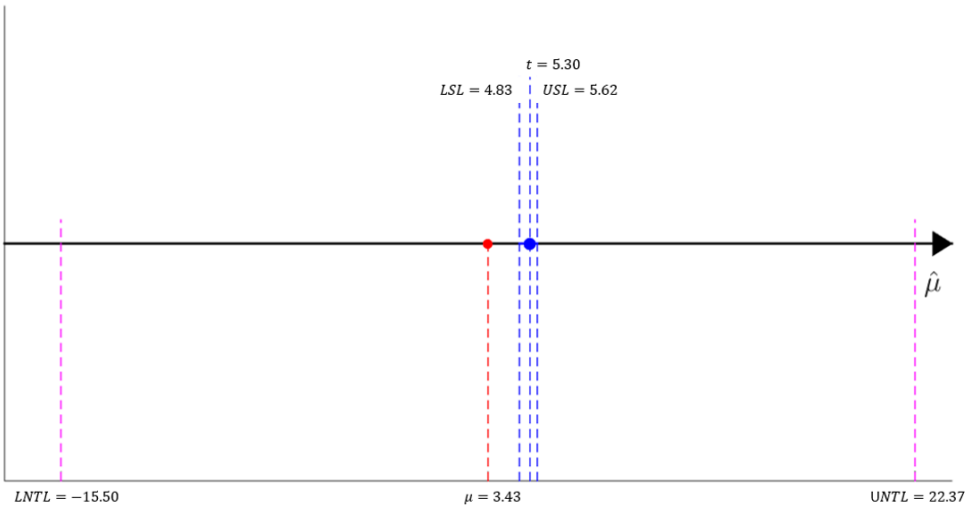

Figure 4.9: Visualization of the solution ($h = 2$) for the single response problem in the log scale

After presenting the results of (P^2) with Figure 4.9, the DM observes that the length of the prediction interval is not on its limit and there is no significant improvement on mean value. Since limiting the length of the prediction interval limits the variance of the response, the DM may want to remove the variance

from the objective set to improve the mean value. After taking into account this preference, the next problem for the third iteration, $h = 3$, becomes:

$$\begin{aligned} (P^3) \quad & Min \ \ a \\ & s.t. \\ & a \geqslant w_1 \ (z_1(x) - 0.00) \\ & 60 \geqslant z_3(x) \end{aligned} \tag{4.35}$$

where $z_1(x)$ and $z_3(x)$ are given by equations (4.24) and (4.28).

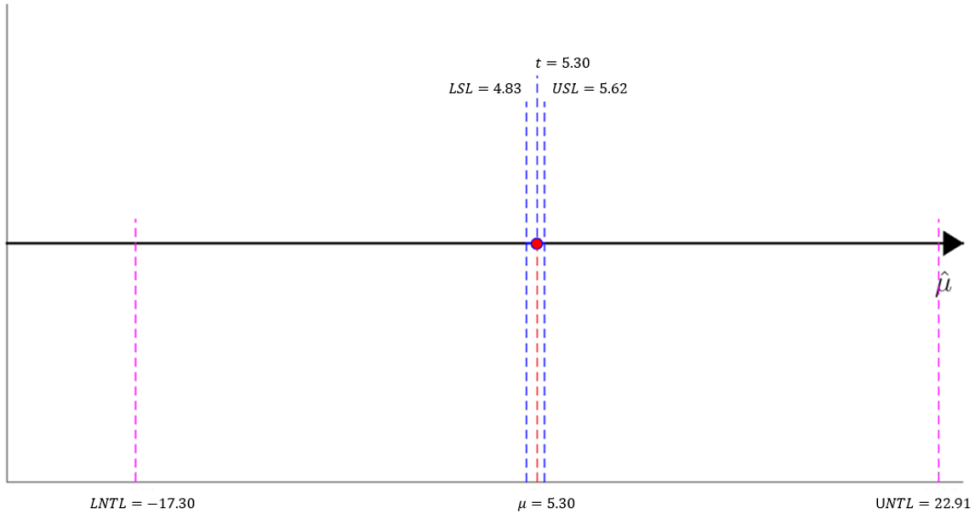

Figure 4.10: Visualization of the solution ($h = 3$) for the single response problem in the log scale

As observed from Figure 4.10, the mean value of the response is improved. It is almost at the target value. Thus, we assume that this is a desirable solution for the DM and the DM is willing to stop at this step.

CHAPTER 5

CONCLUSION

Within the scope of this thesis study, we address model building and optimization stages of the multi response surface optimization for two response product and process design problem. In this regard, we consider the general case where the responses may be correlated and variances of responses are not constant at the different settings of the controllable design parameters.

We mainly focus on optimization stage. We develop an interactive approach to two response product and process design problems and address the single response problem as a special case. This approach involves some concepts of STEM Method [5]. We define a set of performance measures (objectives) that represent the objectives of the problem and facilitate the communication with the DM at each iteration. The studied performance measures are distances between means of the responses and the corresponding targets, response variances and area of the prediction region. In addition, we use visual aids to ease the decision making at each iteration.

Furthermore, we study the model building stage. We are required to build the empirical models for means and variances of the responses and the correlation coefficient in order to formulate the performance measures to be used in the optimization stage. For this purpose, we utilize OLS regression which is a commonly studied approach in the literature [23]. Moreover, we consider data transformations due to the limiting assumptions of OLS regression. Owing to wide observation of log-normality, we restrict our focus on logarithmic transformation. The main difficulty of using data transformation is to back transform the data to the

original scale for the DM to have a better understanding on the performance measures. Therefore, to obtain the estimates of the performance measures in the original scale, we follow the estimation approach presented in [84] instead of performing direct back transformation.

To illustrate the steps of the interactive procedure, the developed method is applied on two examples. The first example is for two response problems. In that example, we show how the defined performance measures and their reflections on the visual aids help the interaction with the DM. Similarly, in the second example, application of the method on a single response problem is illustrated.

Compared to the literature, we explicitly consider the preferences of the DM on the objectives through the interactive procedure, yet most of the approaches such as desirability function based and loss function approaches aggregate multiple objectives into a single objective function. Aggregation implicitly enforces a global preference on the objectives of the problem, however the preferences can change among the DMs. Thus, such aggregations may fail to represent the preferences of DMs satisfactorily. For instance, the loss function approach cannot consider the cases where the solutions closer to the lower specification limit can be preferred, since it is defined as a symmetric function. Moreover, some of the studies in the literature such as desirability function based approaches cannot consider the possible correlations between the responses. In our approach, the performance measures (i.e., area of the prediction region) we use to show joint behaviour of the responses provides better insight to the DM on the problem. Besides, the most of the interactive approaches in the literature use point estimation of the response means and determine the optimal setting of the controllable input variables with respect to these estimations. In addition, most of them do not consider the correlations between responses and heterogeneity of the error variances. Those may lead to unrealistic solutions in practice. In our method, we consider the possible estimation errors by presenting prediction regions to the DM at each iteration. To improve the perception, the density along the prediction region is depicted by colouring the contour lines. Contrary to some of the studies, we take into account the heterogeneity of the variance by formulating the variance-covariance structure as a function of controllable input

variables.

In order to achieve the aforementioned improvements, we encounter several difficulties related to modelling and estimation throughout this study. Since we consider a general case where the variances are heterogeneous and possible correlations exist among the responses, none of the parametric regression approaches discussed in Chapter 3 dominates the others when their disadvantages are considered besides advantages. Thus, we prefer to use OLS regression in order to exploit its well-known properties for fitting separate models to means and variances of the responses and correlation coefficient. Then, we use those models to predict variance-covariance matrix to be used in the MVR regression formulation of the prediction region. That is a rough estimate of the prediction region which requires further improvements in order to achieve realistic solutions. In that manner, the idea of combining some of the regression methods might be considered. Apart from those, multivariate normality is required to perform those estimations in our study. However, this may not be the case in real problems and non-normality of the responses may be encountered as we illustrate for a single response problem. To extend our approach to those cases where multivariate normality might not be present, non parametric methods can be utilized to be able to make inferences on joint behaviour of the responses.

In some robust product and process design problems, responses are categorical. Our method can be extended to cover these cases by considering the use of empirical modelling approaches such as logistic regression and Poisson regression. However, development of more appropriate performance measures for interaction with the DM is an area that needs to be studied further.

Finally, we developed our method for up to two responses. In order to extend our approach for the cases where three or more responses are of interest, we mainly need to consider how the solutions and corresponding performance measures are represented to the DM. For three response problems, we may still use current framework by representing prediction ellipsoid and using volume of the ellipsoid. For more responses we may think of showing binary combinations of the responses to obtain prediction regions or defining additional performance

measures such as multivariate capability indices to facilitate the communication with the DM.

REFERENCES

[1] A. E. Ames, N. Mattucci, S. MacDonald, G. Szonyi, and D. M. Hawkins. Quality loss functions for optimization across multiple response surfaces. *Journal of Quality Technology*, 29(3):339, 1997.

[2] M. K. Ardakani and S. S. Wulff. An overview of optimization formulations for multiresponse surface problems. *Quality and Reliability Engineering International*, 29(1):3–16, 2013.

[3] M. I. Awad and J. V. Kovach. Multiresponse optimization using multivariate process capability index. *Quality and Reliability Engineering International*, 27(4):465–477, 2011.

[4] M. S. Bartlett and D. Kendall. The statistical analysis of variance-heterogeneity and the logarithmic transformation. *Supplement to the Journal of the Royal Statistical Society*, pages 128–138, 1946.

[5] R. Benayoun, J. De Montgolfier, J. Tergny, and O. Laritchev. Linear programming with multiple objective functions: Step method (stem). *Mathematical Programming*, 1(1):366–375, 1971.

[6] S. Bera and I. Mukherjee. An integrated approach based on principal component and multivariate process capability for simultaneous optimization of location and dispersion for correlated multiple response problems. *Quality Engineering*, 25(3):266–281, 2013.

[7] J. M. Bland and D. G. Altman. Statistics notes: measurement error proportional to the mean. *British Medical Journal*, 313(7049):106, 1996.

[8] G. Box. Signal-to-noise ratios, performance criteria, and transformations. *Technometrics*, 30(1):1–17, 1988.

[9] G. E. Box and N. R. Draper. The bayesian estimation of common parameters from several responses. *Biometrika*, 52(3-4):355–365, 1965.

[10] G. E. Box and N. R. Draper. *Empirical model-building and response surfaces*, volume 424. Wiley New York, 1987.

[11] G. E. Box and R. D. Meyer. Dispersion effects from fractional designs. *Technometrics*, 28(1):19–27, 1986.

[12] G. E. Box and K. Wilson. On the experimental attainment of optimum conditions. *Journal of the Royal Statistical Society. Series B (Methodological)*, 13(1):1–45, 1951.

[13] C.-H. Chiao and M. Hamada. Analyzing experiments with correlated multiple responses. *Journal of Quality Technology*, 33(4):451, 2001.

[14] N. R. Costa, J. Lourenço, and Z. L. Pereira. Desirability function approach: a review and performance evaluation in adverse conditions. *Chemometrics and Intelligent Laboratory Systems*, 107(2):234–244, 2011.

[15] N. R. Costa and Z. L. Pereira. Multiple response optimization: a global criterion-based method. *Journal of Chemometrics*, 24(6):333–342, 2010.

[16] K. Dehnad. *Quality control, robust design, and the Taguchi method.* Springer Science & Business Media, 1989.

[17] E. Del Castillo and D. Montgomery. A nonlinear programming solution to the dual response problem. *Journal of Quality Technology*, 25(3):199–204, 1993.

[18] E. Del Castillo, D. C. Montgomery, and D. R. McCarville. Modified desirability functions for multiple response optimization. *Journal of Quality Technology*, 28:337–345, 1996.

[19] G. C. Derringer. Simultaneous optimization of several response variables. *Journal of Quality Technology*, 12:214–219, 1980.

[20] G. C. Derringer. A balancing act-optimizing a products properties. *Quality Progress*, 27(6):51–58, 1994.

[21] R. Ding, D. K. Lin, and D. Wei. Dual-response surface optimization: a weighted mse approach. *Quality Engineering*, 16(3):377–385, 2004.

[22] J. Figueira, S. Greco, and M. Ehrgott. *Multiple criteria decision analysis: state of the art surveys*, volume 78. Springer Science & Business Media, 2005.

[23] F. S. Fogliatto and S. L. Albin. Variance of predicted response as an optimization criterion in multiresponse experiments. *Quality Engineering*, 12(4):523–533, 2000.

[24] A. M. Geoffrion, J. S. Dyer, and A. Feinberg. An interactive approach for multi-criterion optimization, with an application to the operation of an academic department. *Management science*, 19(4-part-1):357–368, 1972.

[25] A. M. Geoffrion, J. S. Dyer, and A. Feinberg. An interactive approach for multi-criterion optimization, with an application to the operation of an academic department. *Management science*, 19(4-part-1):357–368, 1972.

[26] E. Harrington. The desirability function. *Industrial quality control*, 21(10):494–498, 1965.

[27] A. Hedayat, N. Sloane, and J. Stufken. Orthogonal arrays: theory and applications, 1999.

[28] W. J. Hill and W. G. Hunter. A review of response surface methodology: a literature survey. *Technometrics*, 8(4):571–590, 1966.

[29] C.-L. Hwang and A. S. M. Masud. *Multiple Objective Decision Making — Methods and Applications*. Springer-Verlag Berlin Heidelberg, 1979.

[30] I.-J. Jeong and K.-J. Kim. D-stem: a modified step method with desirability function concept. *Computers & Operations Research*, 32(12):3175–3190, 2005.

[31] I.-J. Jeong and K.-J. Kim. An interactive desirability function method to multiresponse optimization. *European Journal of Operational Research*, 195(2):412–426, 2009.

[32] I.-J. Jeong, K.-J. Kim, and S. Y. Chang. Optimal weighting of bias and variance in dual response surface optimization. *Journal of Quality Technology*, 37(3):236–247, 2005.

[33] S. K. Karna and R. Sahai. An overview on taguchi method. *International Journal of Engineering and Mathematical Sciences*, 1(January-June):11–18, 2012.

[34] R. B. Kazemzadeh, M. Bashiri, A. C. Atkinson, and R. Noorossana. A general framework for multiresponse optimization problems based on goal programming. *European Journal of Operational Research*, 189(2):421–429, 2008.

[35] A. Khuri and M. Conlon. Simultaneous optimization of multiple responses represented by polynomial regression functions. *Technometrics*, 23(4):363–375, 1981.

[36] A. I. Khuri. 12 multiresponse surface methodology. *Handbook of Statistics*, 13:377–406, 1996.

[37] A. I. Khuri and J. A. Cornell. *Response surfaces: designs and analyses*, volume 152. CRC Press, 1996.

[38] A. I. Khuri and S. Mukhopadhyay. Response surface methodology. *Wiley Interdisciplinary Reviews: Computational Statistics*, 2(2):128–149, 2010.

[39] K.-J. Kim and D. K. Lin. Dual response surface optimization: a fuzzy modeling approach. *Journal of Quality Technology*, 30(1):1–10, 1998.

[40] K.-J. Kim and D. K. Lin. Simultaneous optimization of mechanical properties of steel by maximizing exponential desirability functions. *Applied Statistics*, pages 311–325, 2000.

[41] K.-J. Kim and D. K. Lin. Optimization of multiple responses considering both location and dispersion effects. *European Journal of Operational Research*, 169(1):133–145, 2006.

[42] Y.-H. Ko, K.-J. Kim, and C.-H. Jun. A new loss function-based method for multiresponse optimization. *Journal of Quality Technology*, 37(1):50–59, 2005.

[43] M. Koksalan and R. Plante. Interactive multi-criteria optimization for multiple response product and process design. *Manufacturing and Service Operations Management*, 5(4):334–347, 2003.

[44] P. Korhonen, H. Moskowitz, and J. Wallenius. Multiple criteria decision support-a review. *European Journal of Operational Research*, 63(3):361–375, 1992.

[45] P. J. Korhonen and J. Laakso. A visual interactive method for solving the multiple criteria problem. *European Journal of Operational Research*, 24(2):277–287, 1986.

[46] S. Kushwaha, S. Sikdar, I. Mukherjee, and P. K. Ray. A modified desirability function approach for mean-variance optimization of multiple responses. *International Journal of Software Science and Computational Intelligence (IJSSCI)*, 5(3):7–21, 2013.

[47] M. H. Kutner, C. J. Nachtsheim, J. Neter, and W. Li. Applied linear statistical models. 2005. McGraw-Hill Irwin New York.

[48] C. E. Land. Confidence interval estimation for means after data transformations to normality. *Journal of the American statistical Association*, 69(347):795–802, 1974.

[49] D.-H. Lee, I.-J. Jeong, and K.-J. Kim. A posterior preference articulation approach to dual-response-surface optimization. *IIE Transactions*, 42(2):161–171, 2009.

[50] D.-H. Lee, K.-J. Kim, and M. Köksalan. A posterior preference articulation approach to multiresponse surface optimization. *European Journal of Operational Research*, 210(2):301–309, 2011.

[51] D.-H. Lee, K.-J. Kim, and M. Köksalan. An interactive method to multiresponse surface optimization based on pairwise comparisons. *IIE Transactions*, 44(1):13–26, 2012.

[52] K.-H. Lee, I.-S. Eom, G.-J. Park, and W.-I. Lee. Robust design for unconstrained optimization problems using the taguchi method. *The American Institute of Aeronautics and Astronautics Journal*, 34(5):1059–1063, 1996.

[53] M.-S. Lee and K.-J. Kim. Expected desirability function: consideration of both location and dispersion effects in desirability function approach. *Quality Technology & Quantitative Management*, 4(3):365–377, 2007.

[54] P.-H. Lee and B.-J. Yum. Multi-characteristics parameter design: A desirability function approach based on process capability indices. *International Journal of Reliability, Quality and Safety Engineering*, 10(04):445–461, 2003.

[55] D. K. Lin and W. Tu. Dual response surface optimization. *Journal of Quality Technology*, 27(1):34–39, 1995.

[56] Y. Ma and T. Tian. Optimal weighted approach in dual-response surface optimization. In *Management and Service Science, 2009. MASS'09. International Conference on*, pages 1–4. IEEE, 2009.

[57] D. M. Mandy and C. Martins-Filho. Seemingly unrelated regressions under additive heteroscedasticity: theory and share equation applications. *Journal of Econometrics*, 58(3):315–346, 1993.

[58] W. Mendenhall, T. Sincich, and N. S. Boudreau. *A second course in statistics: regression analysis*, volume 5. Prentice Hall Upper Saddle River^ eNew Jersey New Jersey, 1996.

[59] K. Miettinen. *Nonlinear multiobjective optimization*, volume 12. Kluwer Academic Publishers, Dordrecht, 1999.

[60] K. Miettinen, F. Ruiz, and A. P. Wierzbicki. Introduction to multiobjective optimization: interactive approaches. In *Multiobjective Optimization*, pages 27–57. Springer, 2008.

[61] M. Mollaghasemi and G. W. Evans. Multicriteria design of manufacturing systems through simulation optimization. *Systems, Man and Cybernetics, IEEE Transactions on*, 24(9):1407–1411, 1994.

[62] D. C. Montgomery, V. M. Bettencourt, et al. Multiple response surface methods in computer simulation. *Simulation*, 29(4):113–121, 1977.

[63] D. C. Montgomery, E. A. Peck, and G. G. Vining. *Introduction to linear regression analysis*, volume 821. John Wiley & Sons, 2012.

[64] R. Myer and D. C. Montgomery. Response surface methodology: process and product optimization using designed experiment. *John Wiley and Sons, New York*, pages 343–350, 2002.

[65] R. H. Myers and W. H. Carter. Response surface techniques for dual response systems. *Technometrics*, 15(2):301–317, 1973.

[66] R. H. Myers, A. I. Khuri, and W. H. Carter. Response surface methodology: 1966–l988. *Technometrics*, 31(2):137–157, 1989.

[67] R. H. Myers, A. I. Khuri, and G. Vining. Response surface alternatives to the taguchi robust parameter design approach. *The American Statistician*, 46(2):131–139, 1992.

[68] V. N. Nair, B. Abraham, J. MacKay, G. Box, R. N. Kacker, T. J. Lorenzen, J. M. Lucas, R. H. Myers, G. G. Vining, J. A. Nelder, et al. Taguchi's parameter design: a panel discussion. *Technometrics*, 34(2):127–161, 1992.

[69] U. Olsson. Confidence intervals for the mean of a log-normal distribution. *Journal of Statistics Education*, 13(1):n1, 2005.

[70] G.-J. Park, T.-H. Lee, K. H. Lee, and K.-H. Hwang. Robust design: an overview. *AIAA journal*, 44(1):181–191, 2006.

[71] K. S. Park and K.-J. Kim. Optimizing multi-response surface problems: how to use multi-objective optimization techniques. *IIE Transactions*, 37(6):523–532, 2005.

[72] M. S. Phadke. *Quality engineering using robust design*. Prentice Hall PTR, 1989.

[73] J. J. Pignatiello Jr. Strategies for robust multiresponse quality engineering. *IIE Transactions*, 25(3):5–15, 1993.

[74] R. D. Plante. Multicriteria models for the allocation of design parameter targets. *European Journal of Operational Research*, 115(1):98–112, 1999.

[75] M. Ramezani, M. Bashiri, and A. C. Atkinson. A goal programming-topsis approach to multiple response optimization using the concepts of non-dominated solutions and prediction intervals. *Expert Systems with Applications*, 38(8):9557–9563, 2011.

[76] C. R. Rao. *Linear statistical inference and its applications*. John Wiley & Sons, 1973.

[77] L. P. Rees, E. R. Clayton, and B. W. Taylor. Solving multiple response simulation models using modified response surface methodology within a lexicographic goal programming framework. *IIE Transactions*, 17(1):47–57, 1985.

[78] J. L. D. Ribeiro, F. S. Fogliatto, and C. S. ten Caten. Minimizing manufacturing and quality costs in multiresponse optimization. *Quality Engineering*, 13(2):191–201, 2000.

[79] A. J. Richard and W. W. Dean. Applied multivariate statistical analysis. *Prenticee Hall, London*, 265, 2002.

[80] T. J. Robinson, C. M. Borror, and R. H. Myers. Robust parameter design: a review. *Quality and Reliability Engineering International*, 20(1):81–101, 2004.

[81] P. J. Ross. Taguchi techniques for quality engineering, 1996. *Mcgraw-Hill International Editions*.

[82] N. V. Sahinidis. *BARON 14.3.1: Global Optimization of Mixed-Integer Nonlinear Programs,* User's Manual, 2014.

[83] H. K. Shah, D. C. Montgomery, and W. M. Carlyle. Response surface modeling and optimization in multiresponse experiments using seemingly unrelated regressions. *Quality Engineering*, 16(3):387–397, 2004.

[84] H. Shen and Z. Zhu. Efficient mean estimation in log-normal linear models. *Journal of Statistical Planning and Inference*, 138(3):552–567, 2008.

[85] W. S. Shin and A. Ravindran. Interactive multiple objective optimization: Survey i—continuous case. *Computers & Operations Research*, 18(1):97–114, 1991.

[86] V. K. Srivastava and D. E. Giles. *Seemingly unrelated regression equations models: estimation and inference*, volume 80. CRC Press, 1987.

[87] R. E. Steuer. *Multiple criteria optimization: theory, computation, and applications*. Wiley, 1986.

[88] G. Taguchi. *Introduction to quality engineering: designing quality into products and processes*. Asian Productivity Organization, 1990.

[89] G. Taguchi, S. Chowdhury, and Y. Wu. *Taguchi's Quality Engineering Handbook*. Wiley, 2005.

[90] L. Tang and K. Xu. A unified approach for dual response surface optimization. *Journal of Quality Technology*, 34(4):437, 2002.

[91] M. Tawarmalani and N. V. Sahinidis. A polyhedral branch-and-cut approach to global optimization. *Mathematical Programming*, 103:225–249, 2005.

[92] G. Vining. A compromise approach to multiresponse optimization. *Journal of Quality Technology*, 30:309–313, 1998.

[93] G. G. Vining and R. H. Myers. Combining taguchi and response surface philosophies: a dual response approach. *Journal of Quality Technology*, 22(1), 1990.

[94] W. J. Welch, T.-K. Yu, S. M. Kang, and J. Sacks. Computer experiments for quality control by parameter design. *Journal of Quality Technology*, 22(1):15–22, 1990.

[95] F.-C. Wu. Optimization of correlated multiple quality characteristics using desirability function. *Quality Engineering*, 17(1):119–126, 2004.

[96] K. Xu, D. K. Lin, L.-C. Tang, and M. Xie. Multiresponse systems optimization using a goal attainment approach. *IIE Transactions*, 36(5):433–445, 2004.

[97] O. P. Yadav, G. Thambidorai, B. Nepal, and L. Monplaisir. A robust framework for multi-response surface optimization methodology. *Quality and Reliability Engineering International*, 30(2):301–311, 2014.

[98] A. Zellner. An efficient method of estimating seemingly unrelated regressions and tests for aggregation bias. *Journal of the American statistical Association*, 57(298):348–368, 1962.

[99] S. Zionts and J. Wallenius. An interactive programming method for solving the multiple criteria problem. *Management science*, 22(6):652–663, 1976.