

INTERACTIVE TWO RESPONSE PRODUCT AND PROCESS DESIGN
OPTIMIZATION UNDER MODEL PARAMETER UNCERTAINTY

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UNCERTAINTY**

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ABSTRACT

INTERACTIVE TWO RESPONSE PRODUCT AND PROCESS DESIGN OPTIMIZATION UNDER MODEL PARAMETER UNCERTAINTY

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In this study, we address two response product and process design optimization problems. Finding meaningful solutions to these problems requires simultaneous consideration of the responses represented as empirical functions of relevant design parameters. Many of the existing approaches assume that the preferences of the decision maker (DM) are known prior to the solution procedure. This is a strong assumption that is hard to justify in practice. Other approaches incorporate DM's preferences into the solution process in an interactive manner. Of these, only two approaches consider model parameter uncertainty in the empirical functions. We demonstrate the deficiencies of these two interactive approaches that consider model parameter uncertainty in detail with examples. To overcome the issues with the existing approaches, we develop two interactive optimization approaches considering DM's preferences under model parameter uncertainty. We empower the DM to consider the area of the joint prediction region and the distances of the response means from their target values as performance measures. To facilitate the interaction with the DM, we produce

visual aids on joint confidence and prediction regions of the responses at solutions under consideration. The main differences between our two approaches arise from the differences in the empirical model building. The first is for the case when a closed-form function for the joint prediction region is available, and the second is when it is not available. The latter complicates the process of navigating towards desirable solutions. We illustrate the developed approaches on a two response problem widely used in the literature.

Keywords: Multi-response problems, robust product and process design optimization, multi-response surface optimization, interactive multi-objective optimization approaches, model parameter uncertainty

ÖZ

MODEL PARAMETRE BELİRSİZLİĞİ ALTINDA ETKİLEŞİMLİ İKİ YANITLI ÜRÜN VE SÜREÇ TASARIM OPTİMİZASYONU

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Bu çalışmada, iki yanıtlı ürün ve süreç tasarım optimizasyonu problemlerini ele aldık. Bu problemlere anlamlı çözümler bulunması, ilgili tasarım parametrelerinin ampirik fonksiyonları olarak temsil edilen yanıtların birlikte gözetilmesini gerektirmektedir. Mevcut yaklaşımların çoğu, karar vericinin (KV) tercihlerinin çözüm sürecinden önce bilindiğini varsayar. Bu, pratikte doğrulanması zor olan güçlü bir varsayımdır. Diğer çalışmalar, KV'nin tercihlerini etkileşimli bir şekilde çözüm sürecine dahil etmektedir. Bu yaklaşımların sadece ikisi ampirik fonksiyonlardaki model parametre belirsizliğini dikkate almaktadır. Model parametre belirsizliğini dikkate alan bu iki etkileşimli yaklaşımın eksikliklerini örneklerle detaylı bir şekilde gösterdik. Mevcut yaklaşımlarla ilgili eksiklikleri gidermek için, model parametre belirsizliği altında KV'nin tercihlerini göz önünde bulunduran iki etkileşimli optimizasyon yaklaşımı geliştirdik. Yaklaşımlarımız, KV'nin, ortak tahmin bölgesinin alanını ve yanıt ortalamalarının hedef değerlerinden uzaklıklarını, performans ölçüleri olarak dikkate alması sağlamaktadır. KV ile etkileşimi

kolaylařtırmak iin, deęerlendirilen zmlerde yanıtların ortak gven ve tahmin blgeleri iin yardımcı grseller retiyoruz. İki yaklařımımız arasında ampirik model oluřtırmada kullanılan yntemlerden kaynaklanan farklılıklar bulunmaktadır. İlki, ortak tahmin blgesi iin kapalı formda bir fonksiyonun mevcut olduęunda, ikincisi ise byle bir fonksiyon mevcut olmadıęında kullanılabilir. İkinici durum, istenen zmlere doęru ynelme srecini karmařıklařtırmaktadır. Geliřtirdięimiz yaklařımları literatrde yaygın olarak kullanılan iki yanıtlı bir problem zerinde rneklendirdik.

Anahtar Kelimeler: ok yanıtlı problemler, robust rn ve sre tasarım optimizasyonu, ok yanıtlı yzey optimizasyonu, etkileřimli ok amalı optimizasyon yaklařımları, model parametre belirsizlięi



To my family...

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LIST OF ABBREVIATIONS

ALS	Adaptive Least Squares
ANOVA	Analysis of Variance
CCD	Central Composite Design
CI	Confidence Interval
DA	Design Analyst
DM	Decision Maker
DOE	Design of Experiments
DRO	Dual-Response Surface Optimization
GDF	Geoffrion-Dyer-Feinberg
GLM	General Linear Model
GLS	Generalized Least Squares
HC	Heteroskedasticity Consistent
LAL	Lower Acceptable Limit
LTB	Larger-The-Better
MCDM	Multi-Criteria Decision Making
MOO	Multi-Objective Optimization
MRO	Multi-Response surface Optimization
NTB	Nominal-The-Best
MINLP	Mixed Integer Nonlinear Program
ML	Maximum Likelihood
MRS	Marginal Rate Substitution
MSE	Mean Square Error
MVR	Multivariate Regression

OLS	Ordinary Least Squares
PCA	Principal Component Analysis
PI	Prediction Interval
RIDFA	Robust Interactive Desirability Function Approach
RPD	Robust Parameter Design
RSM	Response Surface Methodology
R&R	Repeatability and Reproducibility
SLPL	Simultaneous Lower Prediction Limit
SPI	Simultaneous Prediction Interval
SUPL	Simultaneous Upper Prediction Limit
SUR	Seemingly Unrelated Regression
SPV	Scaled Prediction Variance
STB	Smaller-The-Better
STEM	STEP Method
S/N	Signal-To-Noise
UAL	Upper Acceptable Limit
WLS	Weighted Least Squares



CHAPTER 1

INTRODUCTION

Development of high quality industrial products and processes through design involves a common problem of selecting "optimal" settings of design parameters. Typically, the quality of a product or process is multidimensional where optimal design parameter settings for one quality characteristic (or response) is not necessarily optimal for others due to their conflicting nature. Such problems are referred to as *multi-response problems* (Khuri, 1996; Jeong, 2011). Finding meaningful solutions to these problems requires simultaneous consideration of multiple responses affected by several factors (*i.e.*, design parameters and uncontrollable factors), mostly, in an unknown manner, which leads designers to investigate those affects experimentally.

Several approaches have been developed to address multiresponse problems since the early works of Lind et al. (1960, as cited in Khuri, 1996) and Harrington (1965, as cited in Derringer and Suich, 1980). The common folklore is to solve these problems through three main stages: data collection, empirical model building, and optimization. Using the data collected through designed experiments, responses are represented as response surface models (*i.e.*, empirical functions of relevant design parameters) and then treated as objectives or constraints together with additional performance measures in finding the optimal design parameter settings. Such methods are known as *Multi-Response surface Optimization (MRO)* approaches (Park and Kim, 2005).

Key Aspects. The aforementioned three-stage methodology is subject to uncertainty from various sources of errors, namely, measurement errors (*i.e.*, inaccuracies in measurements due to measurement system), random errors in

response observations due to noise factors (*i.e.*, unknown factors or known but uncontrollable factors), and model uncertainty (*i.e.*, errors in estimating model structure and its parameters). Even when measurement errors are minimized and the true model structure is selected, there still exists uncertainty associated with model parameters due to random errors (*i.e.*, intrinsic variation in the response observations when the same design parameter setting is repeated) and sampling variability (*i.e.*, a different set of experimental data may yield different model parameters). Disregarding these issues may result in selecting design parameter settings where responses perform worse than anticipated (Apley and Kim, 2011; Chapman et al., 2014; Ouyang et al., 2017). Moreover, variances of random errors (or variances of responses) often differ by design parameter settings, which brings the concept of *robustness* in the context of product and process design, formally established by Taguchi (1986, as cited in Robinson et al., 2004), into the forefront. Taguchi’s *robust parameter design (RPD)* aims to select the settings of design parameters in a way that the product or process is robust (or minimally sensitive) to the variation in response observations transmitted from noise factors. Despite all the criticisms on Taguchi’s RPD methodology (*e.g.*, experimental procedures and data analysis methods), there is great consensus that quality philosophy must incorporate the concept of robustness since more stable settings may be of interest even if the distances of estimated response values to their respective targets are somewhat larger. Furthermore, conventional response surface modeling approaches such as ordinary least squares (OLS) regression assume constant error variance over experimental region (*i.e.*, homoskedasticity or equal robustness), which may result in invalid response surface models under unequal robustness (or heteroskedasticity).

Besides, the data obtained at the first stage of MRO may be multivariate in nature. That is to say, cross-correlations (hereafter called as correlations ¹) may exist among the responses. Ignoring possible correlations among the responses at empirical model building and optimization stages may lead to unrealistic decisions which cannot be confirmed in practice.

¹ Serial correlation (*i.e.*, autocorrelation of the random errors across experimental runs) is not usually expected in multiresponse problems since the experimental run sequence is typically randomized.

MRO can be viewed from a *Multi-objective Optimization (MOO)* perspective in the sense that multiple conflicting performance measures as functions of relevant design parameters are considered at the optimization stage and there is no unique way of determining the optimal settings of design parameters. To find a satisfactory compromise, preference information of the decision maker (DM) (*i.e.*, the person (or a group of people's consensus) who is in charge of evaluating quality performance of the product or process of interest), on the trade-offs among performance measures should be incorporated into the solution procedure.

Limitations of the Existing MRO Approaches. MRO approaches can be grouped under three categories of MOO literature according to the timing that preferences of the DM are taken into account as prior, interactive (or progressive) and posterior preference articulation methods (Park and Kim, 2005).

The majority of the existing MRO approaches are prior approaches in which preferences of the DM are assumed to be known exactly at the outset. This is a strong assumption that is hard to justify in practice. Such approaches typically combine multiple performance measures into a single function and optimize the resulting function, such as the so-called desirability function (Harrington, 1965; Derringer and Suich, 1980) or loss function (Khuri and Conlon, 1981; Pignatiello, 1993) approaches. They assume that all DMs evaluate with the same function type, whereas the preference structure depends on the particular DM and the problem context. The parameters of these functions could be determined according to the DM's preferences, process economics and statistics (Dolgun et al., 2020), yet; finding them is typically difficult (Keeney and Raiffa, 1976), (Hwang et al., 1979, pp. 30-34), (Steuer, 1986, pp. 3-4) even if the general structure of the function captures the true structure of DM's utility function. Although many of such studies consider at least one of model parameter uncertainty, unequal robustness of responses or possible correlations among responses, they cannot overcome the major drawback of difficulty in adequate representation of the DM's preferences by a single function.

Interactive approaches, on the other hand, extract the DM's preference information progressively during the solution procedure rather than requiring all complete

preference information in advance. In this way, the DM learns about the possible solutions throughout the solution procedure and better understands her/his preferences. Several MRO approaches utilize interactive MOO approaches. As early as 1977, Montgomery and Bettencourt made an application of interactive MOO to the MRO problem. Then, it was not until Köksalan and Plante (2003) that researchers started using more sophisticated interactive MOO approaches to address MRO problems. Further interactive approaches for the MRO problems were developed, such as Park and Kim (2005); Lee et al. (2012); Jeong and Lee (2020); He et al. (2021). Of these, only Park and Kim (2005); He et al. (2021) consider model parameter uncertainty in the response surface models while others use point estimates in their optimization procedures. Those two approaches, on the other hand, neglect the unequal robustness of responses and possible correlations among responses. Özateş (2015), in her interactive approach to two-response product and process design optimization problems, is the first to consider unequal robustness and possible correlations among responses under model parameter uncertainty. However, she uses rough estimates in constructing performance measures, which may lead to unrealistic solutions in practice. Specifically, unequal robustness is ignored in empirical model building although an RPD scenario is assumed.

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 efficient solutions are identified. There are a few MRO approaches considered as posterior preference articulation methods. These approaches first find representative set of solutions, then they either use an additional performance measure in selecting the final solution without incorporating DM's preferences (Moslemi et al., 2018; Bashiri et al., 2020) or progressively take the preferences of the DM to facilitate DM's final solution selection process (Lee et al., 2011, 2018). Thus, we consider those approaches either as prior or interactive approaches, respectively.

Thesis Contributions. In this thesis, we address product and process design problems with two responses. To overcome the issues with the existing approaches, we develop two interactive optimization approaches considering DM's preferences

under model parameter uncertainty. We empower the DM to consider the area of the joint prediction region, which represents uncertainty due to model parameters and random errors, and the distances of estimated response values from their target values as performance measures. To facilitate the interaction with the DM, we produce visual aids on performance measures such as joint confidence and prediction regions of the responses at design parameter settings under consideration. At each interaction iteration, the design analyst (DA) supports the DM in converting her/his verbal preferences into mathematical expressions and searching the solution space. The procedure continues until the DM is satisfied with a solution.

We consider four parametric linear regression methods for empirical model building and estimate the model parameters using the method of least squares, a widely used approach in MRO literature. However, due to their limiting assumptions, none of those regression methods can efficiently model the general case where possible correlations exist among the responses and variances of random errors are not constant over the experimental region. Consequently, along with the DM's preferences and model parameter uncertainty, our approaches can consider either *(i)* possible correlations among the responses assuming equal robustness or *(ii)* unequal robustness assuming no correlations among responses.

The main differences between our two approaches arise from the differences in the empirical model building. The first is for the case when the area of the joint prediction region is available as a closed-form function of design parameters, and the second is for the case when it can only be numerically estimated at given design parameter settings. The latter complicates the process of navigating toward desirable solutions.

We illustrate the developed approaches on a two-response problem widely used in MRO literature for the aforementioned two cases, *(i)* and *(ii)*.

Furthermore, upon a comprehensive literature review on interactive MRO approaches, we select the two most relevant studies taking model parameter uncertainty into account in their solution procedures and demonstrate their deficiencies in detail with examples.

Our contributions can be summarized as follows.

- We demonstrate the deficiencies of existing interactive approaches considering model parameter uncertainty.
- We develop the first interactive MRO approach properly considering possible correlations among responses under model parameter uncertainty.
- We develop the first interactive MRO approach properly considering the unequal robustness of responses under model parameter uncertainty.
- We incorporate methods from econometrics literature into MRO literature (*e.g.*, recent developments on WLS (Romano and Wolf, 2017)).
- We develop a bootstrapping procedure to consider uncertainty associated with SUR predictions for illustrative purposes.

The Organization of the Thesis. The thesis is organized as follows. In Chapter 2, we provide a brief background on response surface methodology (RSM) and Taguchi's RPD and we broadly review existing MRO approaches. We review the most relevant MRO approaches to this thesis and demonstrate their deficiencies in Chapter 3. We devote Chapter 4 to providing common methodological background on our approaches. In Chapter 5, we develop our first approach. Then, we illustrate the first approach for two cases where MVR and WLS regression are used in empirical model building. Similarly, in Chapter 6, after explaining our second approach, we provide an illustrative example demonstrating empirical modeling with SUR regression. Finally, in Chapter 7, we discuss the strengths and the limitations of our approaches compared to the existing methods, as well as addressing further issues to set the ground for future research directions.

CHAPTER 2

LITERATURE REVIEW

Built on the foundations of response surface methodology (RSM), several multiresponse surface optimization (MRO) approaches have been developed since the early works of Lind et al. (1960, as cited in Khuri, 1996) and Harrington (1965, as cited in Derringer and Suich, 1980). In mid 1980s, a significant step was taken in quality improvement by Taguchi's robust parameter design (RPD). Although the methodology of RPD had been the matter of much debate, its philosophy has been incorporated into RSM resulting in the development of RSM approaches as alternatives to Taguchi's RPD. This integration has also influenced the evolution of MRO literature, in terms of considering robustness. Consequently, we view RSM and Taguchi's RPD as the key foundations within the MRO literature.

In this chapter, we briefly review RSM and RPD in Section 2.1. We devote Section 2.2 to discussing the existing MRO approaches categorized regarding their optimization stages.

2.1 Response Surface Methodology and Robust Parameter Design

In this section, we briefly review classical RSM, RPD, and RSM approaches to RPD problems.

Response Surface Methodology (RSM). RSM is a comprehensive framework that employs statistical and mathematical techniques for the design and improvement of industrial processes and products. It finds wide application in situations where multiple input variables (*i.e.*, design parameters) influence the performance measure or quality characteristic, known as the response, which is

typically measured on a continuous scale (Myers et al., 2009, p. 1). RSM combines modeling strategies with sequential experimentation to gain insights into the system under study. It aims to establish a functional relationship between the response of interest and the input factors, which allows for determining the optimal conditions for the design parameter settings.

While earlier studies can be traced back to the 1930s, Box and Wilson (1951) are widely acknowledged as the pioneers of RSM (Myers et al., 1989). Their groundbreaking work focuses on determining the optimal conditions in the chemical industry to achieve maximum yield based on a sequential experimental investigation. It has played a significant role in inspiring further exploration in the field, leading to extensive applications in various sectors, including chemical processing, food, and textiles (Myers et al., 1992).

Conventional RSM focuses on optimizing the mean of a single response, assuming constant response variance (Khuri, 1996). A low-order polynomial is typically used within a small design parameter space, with the choice of first-order or second-order models, based on the stage of sequential experimentation. The parameters of the response surface models are estimated using ordinary least squares (OLS) method. Once the small region around the optimum, where the true response surface typically displays curvature, is identified, a second-order model is used to determine the optimal conditions. Practical experience shows that second-order models are effective in real response surface problems (Myers et al., 2009, p. 5). In Chapter 4, we briefly discuss the experimentation stages and commonly used response surface models to establish the methodological background for this thesis study.

For a deeper understanding of RSM, we refer to notable review papers, including those by Hill and Hunter (1966); Myers et al. (1989, 2004); Khuri and Mukhopadhyay (2010), which cover different time periods in the field. Additionally, we refer to the dedicated books on RSM that provide comprehensive coverage such as Box and Draper (1987); Khuri and Cornell (1996); Myers et al. (2009).

Robust Parameter Design (RPD). RPD is a methodology within the field of quality engineering introduced by Genichi Taguchi in the 1950s in Japan and later in the 1980s in the United States. It aims to improve the quality of a system (*i.e.*, a product or a process) by determining the optimal configuration of design parameters that minimize the system's sensitivity to uncontrollable variations.

The main premise of RPD is that not all input factors can be controlled in a designed experiment. There are additional factors known as *noise factors* that are difficult, costly, or impossible to control. In this context, the goal is to select the settings of design parameters (also referred to as *controllable factors*) in a manner that the system remains *robust* or minimally sensitive to the variations transmitted by the noise factors.

To achieve this goal, Taguchi proposed a set of techniques, including experimental design and analysis. Taguchi used orthogonal arrays where an orthogonal array of design parameters (inner array) is crossed with an orthogonal array of noise factors (outer array). In this way, each row of the inner array is repeatedly conducted by systematically varying noise factors using the outer array. This arrangement, known as *crossed arrays*, allows for the evaluation of noise factor effects. Furthermore, Taguchi introduced performance criteria referred to as signal-to-noise (S/N) ratios. These ratios are formulated based on the specific objective of the experiment, which may fall into categories such as smaller-the-better (STB), larger-the-better (LTB), or target-is-best. Depending on the desired goal, the S/N ratios are derived from the average quadratic loss, combining the mean and variance of the response into a single value at each row of the inner array. Once the response values are observed, they are treated as replicates for the development of S/N ratios. Analysis of variance (ANOVA) is used to identify significant design parameters, and the optimum setting of these parameters is determined by selecting the levels with the highest mean S/N ratio on the main effect plots. The specified setting is recommended to be tested through confirmation experiments to verify whether the predicted performance is realized or not.

For further details on RPD, we refer to Phadke (1989) and Taguchi et al. (2005).

We also recommend exploring overview studies such as Robinson et al. (2004); Myers et al. (2004); Park et al. (2006); Khuri and Mukhopadhyay (2010), and their bibliographies for additional references.

Taguchi's techniques provide a user-friendly framework that can be readily adopted and applied, even by practitioners with limited statistical knowledge. Consequently, they have gained high popularity among practitioners and statisticians, resulting in their widespread application across various fields (Park et al., 2006; Karna and Sahai, 2012). However, despite being a significant advancement in quality improvement, the Taguchi method has faced criticisms such as Box (1988); Welch et al. (1990); Nair (1992). It has been demonstrated that this method struggles to estimate interactions between design parameters and requires a large number of experimental runs. Additionally, S/N ratios employed by the method are unable to differentiate factors that affect the mean from those that affect the variance. To overcome those drawbacks, RSM approaches have been developed.

RSM Approaches to Taguchi's RPD. Two main RSM approaches were introduced to the RPD: *i*) dual response surface optimization (DRO) approaches, and *ii*) single model approaches. The former, introduced by Vining and Myers (1990), is the initial effort to combine RSM with RPD philosophy as an alternative to Taguchi's method. Inspired by Myers and Carter (1973), Vining and Myers (1990) proposed that sample mean and variance of the response can be modeled as functions of the relevant design parameters the coefficients of which are estimated by the method of least squares. Then, the estimated variance function is minimized subject to the equality constraint that sets the response mean function equal to the response target value. Then, Myers et al. (1992) proposed a single model approach using a combined array introduced by Welch et al. (1990). As the name suggests, a single model containing both the design parameters and noise factors as independent variables is fit for the response of interest. Although the combined arrays were proposed as better alternatives addressing the issues with the crossed arrays, Kunert et al. (2007) ran an experiment in which the crossed array found an effect on the variance that cannot be seen from the combined array. Thus, the crossed arrays seem to have their own advantages.

In our study, we assume crossed array layout for data collection, assumptions of which are detailed in Sec. 4.1. Hence, in this section, we discuss the advances in DRO since such methods are special cases of MRO problems when an RPD scenario is assumed.

Del Castillo and Montgomery (1993) proposed the use of nonlinear programming to optimize the problem formulated by Vining and Myers (1990) with inequality constraints. Demonstrating that small sacrifices from bias performance may lead to a greater return in variance performance, Lin and Tu (1995) proposed a different formulation minimizing mean square error (MSE). Copeland and Nelson (1996) extended the formulation of Lin and Tu (1995) by restricting the distance between the response mean and its target, and by using nonlinear programming in solving the resulting problem. Ding et al. (2004) extended Lin and Tu (1995)'s work to a weighted MSE. The authors proposed a data-driven approach to determine the weights without incorporating the DM's preferences. To address this issue, Jeong et al. (2005) proposed pairwise comparisons that incorporate the DM's trade-off on bias and variance for the determination of the weights in the weighted MSE. Then, they minimize the resulting weighted MSE. Shin and Cho (2009) pointed out that the weighted MSE is not capable of representing any potentially optimal solutions (*i.e.*, *nondominated* solutions formally defined in Section 3.1). To overcome this deficiency, they suggested the using lexicographic weighted Tchebbychef approach. Some further extensions include the use of fuzzy membership functions (Kim and Lin, 1998), the formulation based on goal programming (Tang and Xu, 2002), and maximizing process capability index, C_{pk} , (Bendersky et al., 2022).

The DM's preferences are either taken prior to the solution procedure or completely neglected in the aforementioned approaches. Köksoy and Doganaksoy (2003) is the first to address DRO in an interactive manner utilizing the NIMBUS method (Miettinen and Mäkelä, 2000) where the mean and variance functions are considered as objectives. Extending the work of Jeong et al. (2005), Lee and Kim (2012) proposed an interactive approach that extracts the preferences of the DM where weighted MSE is considered as the DM's utility function weights of which are updated progressively throughout the solution process.

On the other hand, some DRO approaches are posterior approaches. Lee et al. (2010) utilize *e-constraint method* (Haimes et al., 1971) in finding a representative set of nondominated solutions without taking the preferences of the DM, then the DM selects the final solution from the generated solution set. Jeong and Lee (2019) proposes another posterior approach that generates a set of nondominated solutions revising the *e-constraint method* formulation of Lee et al. (2010) to represent the nondominated solution space by an evenly distributed points on the objective space.

DRO approaches focus on addressing single-response problems, which can be viewed as special cases of MRO problems. In many DRO approaches, the DM's preferences are either taken prior to the solution procedure or completely neglected. Only two studies (Köksoy and Doganaksoy, 2003; Lee and Kim, 2012) consider the preferences of the DM in an interactive manner. Furthermore, the majority of these approaches do not take into account the uncertainty associated with the coefficients of the response surface models as well as the heterogeneity of variances that naturally occur in RPD problems. Easily adaptable for single-response problems, our approaches to two-response problems overcome the limitations of the DRO approaches.

For further understanding of the RSM alternatives to the RPD, we refer to some review papers by Robinson et al. (2004); Khuri and Mukhopadhyay (2010); Le and Shin (2018) that cover both DRO and single model approaches, and some useful books (Myers et al., 2009; Montgomery, 2020).

Before moving forward, it is worth mentioning that the term *dual response* was originally used in Myers and Carter (1973) to refer to the response surface models for the means of two quality characteristics. Vining and Myers (1990) continued using the same term in their work addressing single response problems to refer to the two separate response surface models for the mean and variance of a single quality characteristic. In this study, we solely use the term *response* to denote the quality characteristic itself and use the term *performance measure* in referring to an additional response surface model such as for the variance of a quality characteristic.

2.2 Multi-Response Surface Optimization

The development of Taguchi's RPD highlighted the importance of reducing variance in designing quality products and processes. In response to this, RSM approaches have been extended to consider response variance. Although, it is common for multiple responses to be of interest in the context of product or process development (Jeong, 2011), conventional RSM approaches, including alternatives to Taguchi's RPD, primarily focus on a single response. Over time, RSM has evolved into a richer set of techniques to consider multiple responses and their variances in addition to their means, leading to today's definition of the Multi-Response surface Optimization (MRO) problem.

There are different viewpoints on the classification of existing MRO approaches, such as Ramezani et al. (2011) and Yadav et al. (2014). Similar to Park and Kim (2005), we consider MRO as a form of multi-objective optimization (MOO). Hwang et al. (1979); Steuer (1986); Miettinen (1999); Figuera et al. (2005) are useful references for MOO approaches.

MOO aims to address the presence of multiple conflicting and/or incommensurate objectives, naturally leading to a set of potentially optimal solutions (*i.e.*, *nondominated* solutions formally defined in Section 3.1). Similarly, in the optimization stage of MRO, multiple conflicting performance measures, such as means and variances of responses, are taken into account as functions of relevant design parameters, where the optimal setting for one performance measure may not be optimal for others. MRO approaches typically seek to identify a final solution. In addition to generating potentially optimal solutions, MOO research also addresses the task of reaching a final solution. Since there is no unique way to achieve that, it incorporates the preference information of the DM on the trade-offs among the performance criteria to obtain a satisfactory compromise. Hwang et al. (1979, pp. 7-11) classify MOO approaches into prior, interactive (or progressive), and posterior preference articulation methods according to the timing that the preferences of the DM are taken into account. We categorize MRO approaches similarly.

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. There are a few MRO approaches considered as posterior preference articulation methods. These approaches first find representative set of solutions, then they either use an additional performance measure in selecting the final solution without incorporating DM's preferences (Moslemi et al., 2018; Bashiri et al., 2020) or progressively take the preferences of the DM to facilitate DM's final solution selection process (Lee et al., 2011, 2018). Thus, we consider those approaches either as prior or interactive approaches, respectively.

We present a critical review of some of the existing prior and interactive MRO approaches in Sections 2.2.1 and 2.2.2. Our review focuses on key aspects such as the methodology used for building response surface models, the performance criteria employed for evaluating solutions, and the method of searching for solutions (excluding the employed mathematical optimization algorithms).

2.2.1 Prior Approaches

Prior preference articulation approaches require all the necessary information about the preferences of the DM prior to the solution procedure. The majority of the approaches in MRO literature including well-known conventional approaches such as desirability function and loss function approaches are categorized into prior preference articulation methods. These approaches typically aggregate the objectives into a single function to optimize them simultaneously, which is a very similar approach to assuming a utility function to be optimized. It is worth mentioning that, in addition to the prior approaches, this section also includes the MRO approaches that completely ignore the preferences of the DM (*i.e.*, no preference approaches).

The desirability function approach is the most popular approach for MRO problems due to its simplicity and availability in many software packages resulting in its wide application in practice. Introduced by Harrington (1965 as cited in Derringer and Suich, 1980), desirability functions convert an estimated response

$\hat{y}_i(\mathbf{x})$ into a value, so-called *desirability*, ranged in $[0, 1]$. The transformation is performed in a way that the desirability value, d_i , increases as $\hat{y}_i(\mathbf{x})$ becomes more desirable. The individual desirability functions are combined in an overall desirability function, D , that is also ranged in $[0, 1]$. The desirability function approaches vary by their individual and overall desirability function formulations. The most widely used individual desirability function formulations were introduced by Derringer and Suich (1980). Their approach use a geometric mean of the individual desirability values as the overall desirability, which is later extended by Derringer (1994) to consider the relative importance of the responses through the use of a weighted geometric mean. There have been many extensions of the desirability function approaches including those of Del Castillo et al. (1996) and Kim and Lin (2000). Costa et al. (2011) provide a detailed review of the further extensions. Later, He et al. (2012, 2017); Akteke-Öztürk et al. (2017); Li et al. (2022) addressed the uncertainty in response surface models in constructing the desirability functions. He et al. (2017); Li et al. (2022) also addressed unequal robustness of the response variances in the optimization. However, they ignore this issue in building empirical models. The major drawback of the desirability functions is that they typically ignore possible correlations among the responses.

The second most widely used MRO approach is the loss function approach. Pignatiello (1993) was the first to extend Taguchi's single-response quadratic loss function to a multi response loss by considering the variance-covariance structure of the responses. Then, Vining (1998) suggested a new function to consider the variance-covariance structure of the predicted responses. The generalized distance approach introduced by Khuri and Conlon (1981) is a special case of Vining (1998) when the preference parameters are ignored. Combining the strengths of the works of Pignatiello (1993) and Vining (1998), Ko et al. (2005) introduced a new loss function which includes three main components to consider the deviation of predicted responses from their targets, unequal robustness, and model parameter uncertainty. Built upon Ko et al. (2005), Ouyang et al. (2016) addressed model parameter uncertainty via prediction regions, and Ouyang et al. (2017) considered implementation errors in their loss function. Wang et al. (2016) and Wang et al. (2020) proposed Bayesian approaches extending Ko et al.

(2005). The loss function approach, in general, takes into account the unequal robustness of responses, model parameter uncertainty, and potential correlations among the responses. However, these approaches tend to formulate the loss function as a summation of all the corresponding performance measures, among which trade-offs are not allowed. The preference parameters are used only in considering trade-offs among response means and process economics. Dolgun et al. (2020) focused on how to extract and incorporate these trade-offs effectively. Moreover, although loss functions develop performance measures to consider unequal robustness, they often assume constant variance in building empirical models.

Another common prior MRO approach is to maximize a multivariate process capability index as an overall performance measure, taking into account both estimated response means and response variances. Some examples of such approaches include the works of Plante (2001); Awad and Kovach (2011); Bera and Mukherjee (2013). The key idea behind the use of a process capability index is to consider unequal robustness in the optimization process. However, it is worth noting that these approaches often use OLS to determine the coefficients of the empirical models for the response means, which contradicts their main premise.

Some other studies include maximizing the probability of meeting specifications for all responses simultaneously (Chiao and Hamada, 2001), utilization of goal programming (Kazemzadeh et al., 2008; Ramezani et al., 2011) and goal attainment (Xu et al., 2004).

Recently, Moslemi et al. (2018); Bashiri et al. (2020) proposed posterior preference approaches. These approaches first generate a set of nondominated solutions and then select the final solution among them based on a statistical distance measure. Notably, these methods do not consider the DM's preferences at any stage of their solution processes. Hence, we consider them as no preference methods which assume the same preference structure for every DM.

The prior MRO approach literature offers a more extensive consideration of statistical aspects, such as correlations among responses, model parameter uncertainty,

and unequal robustness, compared to the interactive MRO approaches discussed in the next section. However, similar to the interactive MRO approaches, these methods tend to ignore the inherent heterogeneity in response variances in an RPD scenario. More importantly, in these approaches, the proper determination of the preference parameter values based on the DM's preference structure is critical. Albeit seemingly easy to apply, the prior MRO approaches may suffer from the difficulty of specifying all the required preference information of the DM in advance. It is widely acknowledged that it is not likely for a DM to know about her/his complete preference structure in advance. The DM typically better understands and develops her/his preferences regarding the possible solutions throughout the decision-making process.

2.2.2 Interactive Approaches

Interactive approaches extract the preferences of the DM progressively during the solution procedure. Typically, the approach and software generate a solution for the DM to evaluate and the DM either directly adjusts the preference parameter values or provides feedback to the analyst for adjustments. The optimization problem is then solved using the updated preference parameters. The procedure continues until a satisfactory solution is reached. Employing such an iterative procedure helps the DM to better understand and develop her/his preferences as s/he learns more about the problem (Park and Kim, 2005; Steuer, 1986, pp. 35-56). Some early examples of interactive procedures are STEM (Benayoun et al., 1971), GDF (Geoffrion et al., 1972), Z-W method (Zionts and Wallenius, 1976), and visual interactive approach (Korhonen and Laakso, 1986). We refer to Shin and Ravindran (1991); Miettinen et al. (2008), particularly for a review of interactive approaches.

Although most of the existing interactive MRO approaches follow the aforementioned general progressive scheme, they differ in terms of the information presented to the DM, the information obtained from the DM, and consequently, how the problem transformed into a single objective optimization problem.

Montgomery and Bettencourt (1977) and Park and Kim (2005) applied the GDF

algorithm (Geoffrion et al., 1972) to MRO problems with some modifications. In these methods, the DM is expected to specify values of marginal rates of substitution between the responses of the solution under consideration. Providing such values accurately enough may not be easy for the DM. Salmasnia et al. (2013) proposed an approach utilizing the GDF method to overcome one of the drawbacks of Park and Kim (2005) by incorporating correlations among responses using principal component analysis (PCA). However, they utilize the principal components of the response means when interacting with the DM, and it may be difficult for the DM to relate the principal components to the original responses.

Köksalan and Plante (2003) developed an interactive approach by using univariate process capability indices by modifying the parametric multi-criteria optimization proposed by Korhonen and Laakso (1986). In this approach, 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 at each iteration. C_{pk} values may not be sufficient to represent the preferences of the DM satisfactorily since C_{pk} is a measure combining the mean and variance of a response into a single function preventing the DM to make trade-offs among means and variances.

By employing the MSE criterion, Köksoy (2006) extended the DRO approach introduced by Lin and Tu (1995) to address multi-response problems. MSE functions are constructed for each response based on experimental data collected through a combined array, which are then treated as objective functions. The NIMBUS method (Miettinen and Mäkelä, 2000) is employed to solve the MOO problem. However, Köksoy (2006) may not effectively capture the preferences of the DM since the MOO problem is structured in a way that it allows the DM to make trade-offs among MSE functions, but not trade-offs among means and variances of responses.

Jeong and Kim (2003, 2005, 2009) developed interactive desirability function approaches. In these approaches, the DM is allowed to adjust the parameters of the desirability functions. Jeong and Kim (2003), and Jeong and Kim (2005) limit the DM to adjust the shape and bounds of the desirability functions, respectively.

Jeong and Kim (2009) extended those approaches by allowing the DM to adjust all the preference parameters, namely, shape, bound, and target. However, the DM may have difficulties in adjusting the preference parameter values directly since it is not straightforward to relate the parameters to the objectives that are relevant to the DM. Recently, He et al. (2021) extended the approach proposed by Jeong and Kim (2009) in a way to consider the uncertainty associated with the model parameters in solving optimization models.

Lee et al. (2012) assumed a general monotone utility function that encompasses various preference structures. The preferences of the DM are extracted through a series of pairwise comparisons. Estimated utility functions, such as weighted desirability functions, are constructed and updated based on the DM's preference information. Building upon this research, Jeong and Lee (2020) extended the approach by modifying the estimated utility functions into an overall capability index constructed as a weighted sum of individual capability index functions noting that the aggregation can be achieved in other ways. This modification allows for considering robustness in a limited manner, where the DM is not permitted to make trade-offs between means and variances of the responses.

Lee et al. (2011); Lee and Lee (2016); Lee and Jeong (2017); Lee et al. (2018) proposed posterior preference articulation approaches supported by interactive solution selection procedures. They all utilize e -constraint method (Haimes et al., 1971) in finding a representative set of nondominated solutions without taking the preferences of DM. To facilitate the DM's solution selection from a large set of solutions, Lee et al. (2011) use the interactive solution selection method by Köksalan and Sagala (1995) based on pairwise comparisons. Lee and Lee (2016) modify Lee et al. (2011)'s approach with the aim of decreasing the number of pairwise comparisons. Instead of Köksalan and Sagala (1995)'s interactive selection method, they utilize K-means clustering and present the centroids of the clusters to the DM for pairwise comparisons. Lee and Jeong (2017), on the other hand, extends Lee et al. (2011) by proposing a hybrid approach exploring e space progressively based on the DM's preferences and generating small sets of representative solutions for pairwise comparisons. Lee et al. (2018) extend P-DRO (Lee et al., 2010) for multi-response problems, incorporating

multiple response means and variances into separate overall desirability functions, parameters of which are determined by the DM prior to the solution procedure. In the solution selection process, the overall mean and variance desirability values of the responses are presented to the DM. However, it may be hard for the DM to comprehend the effect of the overall desirability function values on the solutions. Moreover, the DM is not allowed to make interactive trade-offs among response means, focusing only on the trade-off between overall mean desirability and overall variance desirability.

Although we classify posterior approaches with an interactive selection procedure as part of the interactive approaches category, they have certain drawbacks compared to fully interactive approaches. One disadvantage is that, utilizing *e*-constraint method may produce some infeasible solutions. Furthermore, these approaches are not efficient as they require substantial effort to obtain a non-dominated solution set including regions that may not be desirable for the DM. For instance, Lee and Jeong (2017)'s method is motivated by preventing the generation of a large set of representative solutions at once including solutions not of interest to the DM, it still has inefficiencies due to producing infeasible and/or redundant solutions. Additionally, the representative solution set typically involves a large number of points, which increases the cognitive effort for the DM, despite the attempts of these methods to alleviate this through interactive selection procedure. As an example, Lee et al. (2012) demonstrate that their approach achieves a satisfactory solution with fewer comparisons than that of Lee et al. (2011).

We summarize our evaluation of interactive MRO approaches based on the key MRO aspects in Table 2.1. While these approaches have the advantage compared to prior approaches in that they consider the DM's preferences progressively rather than considering all preference information prior to solution process, none of them simultaneously address model parameter uncertainty and robustness. Table 2.1 shows that the most commonly considered aspect is robustness of solutions in addition to their mean performance. However, except for Jeong and Lee (2020), all approaches considering robustness ignore the heterogeneity of response variances in building response surface models, which is against the

nature of RPD where response variance is inherently a variable of interest as demonstrated in Luner (1994). Possible correlations among the responses are only considered by Salmasnia et al. (2013), but as mentioned earlier, their interactive procedure involves the use of principal components that the DM may not fully comprehend. Furthermore, model parameter uncertainty is only addressed by Park and Kim (2005); He et al. (2021), which is a major drawback of interactive approaches. Even when measurement errors are minimized and the true model structure is selected, uncertainty associated with model parameters remains due to random errors and sampling variability. Neglecting this issue may lead to the selection of design parameter settings where the system performs worse than anticipated. The next chapter evaluates the two interactive MRO approaches (Park and Kim, 2005; He et al., 2021) that consider this issue and demonstrates the deficiencies in their solution procedures.

Özates (2015) develops the first interactive approach to two-response product and process design optimization problems considering unequal robustness and possible correlations among responses under model parameter uncertainty. Still, this study uses rough estimates in constructing performance measures, which may lead to unrealistic solutions in practice. Specifically, unequal robustness is ignored in empirical model building although an RPD scenario is assumed.

Table 2.1: Evaluation of interactive MRO approaches based on key MRO aspects

Existing Studies	Search	Model Parameter Uncertainty	Heteroskedasticity	Robustness	Correlation
He et al. (2021)	Interactive	✓		✓	
Jeong and Lee (2020)	Interactive			✓	
Lee et al. (2018)	Posterior with interactive selection			✓	
Salmasnia et al. (2017)	Interactive			✓	
Lee and Jeong (2017)	Posterior with interactive selection				
Lee and Lee (2016)	Posterior with interactive selection				
Salmasnia et al. (2013)	Interactive			✓	✓
Lee et al. (2012)	Interactive				
Lee et al. (2011)	Posterior with interactive selection				
Jeong and Kim (2009)	Interactive				
Köksoy (2006)	Interactive			✓	
Park and Kim (2005)	Interactive	✓			
Jeong and Kim (2005)	Interactive				
Köksalan and Plante (2003)	Interactive			✓	
Jeong and Kim (2003)	Interactive				
Montgomery and Bettencourt (1977)	Interactive				

CHAPTER 3

EVALUATION OF RELEVANT MRO APPROACHES THAT CONSIDER MODEL PARAMETER UNCERTAINTY

The three-stage MRO methodology is influenced by uncertainties arising from various error sources during the data collection and empirical model building stages. Those uncertainties propagate to the optimization stage and affect the precision of the expected outcomes of the decisions. Therefore, it is critical to consider those uncertainties to obtain realistic solutions that are confirmed in practice. Even if we assume that the measurement errors are minimized and the true model structure is selected, there still exists uncertainty associated with model parameters due to random errors and sampling variability. Neglecting this issue may result in the selection of design parameter settings at which the system performs worse than predicted. Besides, to be able to make informed decisions, the DM should be informed about the fact that the response values presented to her/him are the expected values and subject to variation. Without explicit consideration of model parameter uncertainty, the outcomes of the selected design parameter settings may not be desirable for the DM. As we discuss in Section 2.2.1, only two of the existing interactive MRO approaches consider such uncertainties. The rest use point estimates in searching the desirable design parameter settings, which is the major drawback of the existing interactive approaches.

Measuring model parameter uncertainty may be a challenging task depending on the method utilized in building empirical models. Typically, the variance of predicted responses denoted as $\text{Var}(\hat{y}(\mathbf{x}))$ where $\hat{y}(\mathbf{x})$ represents a response surface model, is used as a measure in this context. This measure can also

be expressed as a confidence interval. Some existing MRO approaches utilize Bayesian posterior probabilities in considering model uncertainty. However, it is not the aim of the chapter to discuss how model parameter uncertainty should be measured. Our aim is rather to evaluate the two interactive MRO approaches that explicitly consider model parameter uncertainty (Park and Kim, 2005; He et al., 2021) from a MOO perspective. Treating their model parameter uncertainty measures as part of the objective set, our goal is to point out their limitations in addressing model parameter uncertainty effectively in their interactive search procedures. To this end, we first present initial insights into some concepts from the MOO area in Section 3.1. Then, we review the approaches by Park and Kim (2005) and He et al. (2021), and demonstrate the issues with their solution procedures in Sections 3.2 and 3.3. In our demonstrations, we use the data of the polymer experiment the details of which are given in Appendix A.

3.1 Multi Objective Optimization Preliminaries

We formulate the MRO problem as a multi objective optimization (MOO) problem where objective functions are performance measures (*i.e.*, functions of relevant design parameters).

$$\begin{aligned}
& \text{"Min"} \quad \{z_1(\mathbf{x}), z_2(\mathbf{x}), \dots, z_m(\mathbf{x})\} \\
& \text{subject to} \\
& \mathbf{x} \in \Omega
\end{aligned} \tag{3.1}$$

Let $\Omega \in \mathbb{R}$ be the compact feasible region denoting the experimental region. z_j denotes the j^{th} performance measure bounded over Ω where $j \in \{1, 2, \dots, m\}$ and $\mathbf{x}$ is the vector of K design parameters. We use quotation marks since minimizing a vector of objectives is not a well defined mathematical operation when there is no point in Ω at which all objectives are simultaneously minimized.

Let $\mathbf{z}(\mathbf{x}) = (z_1(\mathbf{x}), \dots, z_m(\mathbf{x}))$ and $\mathbf{z}(\mathbf{x}') = (z_1(\mathbf{x}'), \dots, z_m(\mathbf{x}'))$ denote two points in the objective space where $\mathbf{x}$ and $\mathbf{x}'$ are elements of Ω .

$\mathbf{z}(\mathbf{x}')$ is said to dominate $\mathbf{z}(\mathbf{x})$, if and only if $z_j(\mathbf{x}') \leq z_j(\mathbf{x}) \forall j = \{1, 2, \dots, m\}$ and $z_j(\mathbf{x}') < z_j(\mathbf{x})$ for at least one j . If there exists such an $\mathbf{x}' \in \Omega$, then $\mathbf{z}(\mathbf{x})$ is said to be *dominated* and $\mathbf{x}$ is *inefficient*. If there does not exist such an $\mathbf{x}' \in \Omega$, then $\mathbf{z}(\mathbf{x})$ is said to be *nondominated* and $\mathbf{x}$ is *efficient*.

If $\mathbf{z}(\mathbf{x})$ is dominated and there is no $\mathbf{x}' \in \Omega$ with $z_j(\mathbf{x}') < z_j(\mathbf{x}) \forall j = \{1, 2, \dots, m\}$, then $\mathbf{z}(\mathbf{x})$ is said to be *weakly nondominated* and $\mathbf{x}$ is *weakly efficient*.

If a nondominated point is dominated by some convex combination of other nondominated points, then it is said to be *unsupported* nondominated point. Such points do not occur in linear programs; however, they are likely to occur in integer and nonlinear programs (Steuer, 1986, pp. 419-450).

Naturally, we are interested in the set of nondominated points only.

3.2 Revised GDF Procedure

Park and Kim (2005) emphasize that MOO approaches can be successfully utilized in solving MRO problems in which a design solution preferred based on its performance with respect to only the response means may not be satisfactory due to the randomness involved in the predicted responses. As a first attempt to consider this issue in an interactive solution procedure, they revised the GDF method (Geoffrion et al., 1972), a well-known method in MOO literature, without considering the possible correlations among the responses. In measuring the uncertainty associated with the predicted responses, Park and Kim (2005) take the prediction variances of the responses into account during their solution procedure. They assume constant variance of the responses; hence, the term uncertainty refers to the randomness in the model parameters.

The prediction variance for response i at a design parameter setting, $\mathbf{x}_0$, is formulated as,

$$\text{Var}[\hat{y}_i(\mathbf{x}_0)] = \sigma_i^2 v_i(\mathbf{x}_0), \quad (3.2)$$

where $\hat{y}_i(\mathbf{x}_0)$ is the estimated value of response i , σ_i^2 is the unknown variance assumed to be constant, and $v_i(\mathbf{x}_0)$ measures the impact of a design solution on

the prediction variance which varies by the design parameter settings.

Park and Kim (2005) incorporate the idea that $\mathbf{x}_0$ is considered to be more reliable than another solution, $\mathbf{x}_1$, for response i when $v_i(\mathbf{x}_0)$ is smaller than $v_i(\mathbf{x}_1)$ into the GDF method. The steps of the revised GDF procedure are summarized as follows:

Step 0. Set $h = 1$ denoting the iteration count and find an initial feasible design parameter setting $\mathbf{x}^{(1)} \in \Omega$.

Step 1. Ask the DM to specify the trade-off weights $\mathbf{w}(\mathbf{x}^{(h)})$ between the desirability values at $\mathbf{x}^{(h)}$, $\mathbf{d}(\mathbf{x}^{(h)})$.

Step 2. Find the directional vector $\mathbf{r}^{(h)} = \mathbf{g}^{(h)} - \mathbf{x}^{(h)}$, by solving

$$\mathbf{g}^{(h)} = \arg \max_{\mathbf{g} \in \Omega} \mathbf{w}^T(\mathbf{x}^{(h)}) \nabla_{\mathbf{x}} \mathbf{d}^T(\mathbf{x}^{(h)}) \mathbf{g} \quad (3.3)$$

where $\nabla_{\mathbf{x}} \mathbf{d}(\mathbf{x}^{(h)})$ is the gradient matrix of the desirability vector $\mathbf{d}(\mathbf{x})$ evaluated at $\mathbf{x}^{(h)}$.

Step 3. Ask the DM to select the optimal step size $t^{(h)*}$, based on both information $\mathbf{d}(\mathbf{x}^{(h)} + t^{(h)} \mathbf{r})$ and $\mathbf{v}(\mathbf{x}^{(h)} + t^{(h)} \mathbf{r})$ detailed for several values of $t^{(h)} \in [0, 1]$. Let $\mathbf{x}^{(h+1)} = \mathbf{x}^{(h)} + t^{(h)*} \mathbf{r}$. If the new solution $\mathbf{x}^{(h+1)}$ is satisfactory, stop. Otherwise, set $h = h + 1$ and go to Step 1.

The desirability vector, $\mathbf{d}(\mathbf{x})$, is obtained prior to the solution procedure. The entity i of the vector is a function of $\hat{y}_i(\mathbf{x})$, which is simply a function of $\mathbf{x}$. Hence, it is denoted by $d_i(\mathbf{x})$. $\mathbf{w}(\mathbf{x}^{(h)})$ is the absolute value of the DM's marginal rate of substitution (*i.e.*, indifference tradeoff) between the desirability of response i and the reference desirability at the design parameter setting $\mathbf{x}^{(h)}$, and $\mathbf{v}(\mathbf{x})$ is the vector of individual prediction variances of responses, $v_i(\mathbf{x})$.

The vector of trade-off weights, $\mathbf{w}(\mathbf{x}^{(h)})$, and the gradient matrix, $\nabla_{\mathbf{x}} \mathbf{d}(\mathbf{x}^{(h)})$, represent the gradient of the DM's utility function and provide its local linear approximation to be maximized at $\mathbf{x}^{(h)}$ in Step 2. Each entity i is obtained by determining the DM's i^{th} marginal rate of substitution which matches a change in the i^{th} desirability by a compensatory change in the reference desirability

while all other desirability values remain at their current values. The reference desirability can either be selected arbitrarily or by asking the DM to ensure that marginal rates of substitution are sensible for the DM.

The revised GDF stops when either (i) the DM finds the current solution satisfactory or (ii) the DM prefers none of the solutions with $t^{(h)} > 0$ over the current solution.

Issues with the revised GDF procedure. The revised GDF procedure does not consider the prediction variances of the estimated response means in determining the tradeoff weights and consequently in finding the directional vector in Step 2. In this way, the resulting directions may increase the values of the prediction variances and may lead the search towards solutions that are not desirable for the DM. In some cases, these solutions may even be dominated with respect to the objective set that consists of both $\mathbf{d}(\mathbf{x})$ and $\mathbf{v}(\mathbf{x})$. When this is the case, the DM may not find a preferred solution at a $t^{(h)} > 0$ and the procedure may prematurely converge to a solution far from the most desirable solution for the DM. In fact, the authors mention that a vital deterioration may occur in some of the previous prediction variances after a revision of the tradeoff weights in Step 1. They state that the process may either terminate or force a reconsideration of the assessment before proceeding to further steps. However, they do not suggest a way to reconsider the assessment. In reconsideration, the DM may need to select a direction where both desirability values get worse to improve the prediction variances. Although this may intrinsically happen due to the nonlinearity of the objectives, the GDF method determines the directional vector in a way to lead the search towards regions where at least one of the considered objectives improves. Therefore, the revised GDF does not have any mechanism to search for solutions that improve the prediction variances while both of the desirabilities worsen simultaneously since it does not consider the prediction variances in determining the directional vector.

Furthermore, the process of selecting the step size may impose a high cognitive burden on the DM. Park and Kim (2005) present the values of the desirability functions and the prediction variances to the DM in tables where $t^{(h)}$ is first

incremented by 0.1, then further incremented by 0.01 within the interval chosen by the DM. However, by this approach, a total of 20 solutions are presented to the DM in a single iteration, which is more than a DM can handle. Additionally, when the DM's underlying utility function is concave in the design parameter space, satisfying the assumption of the GDF method, the utility value improves until some $t^{(h)} > 0$ in the selected direction and then deteriorates beyond that point. In this case, selecting a single interval to further search for a more desirable solution may not be effective. It may be better to consider two intervals in the neighborhood of the $t^{(h)} > 0$ where the best solution is observed for 0.1 increments. However, in such a scenario, displaying 30 solutions may greatly complicate the interaction with the DM. On the other hand, if the underlying utility function of the DM is not concave in the design parameter space, then the best solution in the selected direction may not be in the neighborhood of the $t^{(h)} > 0$ at which the best solution is observed for 0.1 increments. In addition to these issues, interpreting the values of the prediction variances may be difficult for the DM throughout this process.

Moreover, for the GDF method to work and converge, the underlying utility function should be differentiable and concave on the design parameter space, Ω . Differentiability may not be a critical issue since this is an interactive procedure; however, violation of the concavity assumption may affect the performance of the converged solutions. Because of the individual objective functions, the utility function may not be concave on Ω and it may not be an easy task to check this assumption.

Finally, GDF has its own downsides even when its assumptions are satisfied. The DM may have difficulty in providing marginal rates of substitution accurately enough as demonstrated by Wallenius (1975), which may affect the final solution performance. In addition, due to the nonlinearity of the objectives, some of the solutions obtained in the step size selection may dominate some of the others obtained during the same process for different $t^{(h)} > 0$ values.

Demonstrations. We demonstrate some of the aforementioned issues on the example problem, known as the polymer experiment, which is also used by Park

and Kim (2005) for illustrative purposes. The polymer experiment involves two responses, the desirability functions of which are given by,

$$d_1(\mathbf{x}) = \begin{cases} \frac{\hat{y}_1(\mathbf{x})-80}{100-80}, & 80 \leq \hat{y}_1(\mathbf{x}) \leq 100 \\ 0, & \text{otherwise,} \end{cases} \quad (3.4)$$

$$d_2(\mathbf{x}) = \begin{cases} \frac{\hat{y}_2(\mathbf{x})-55}{57.5-55}, & 55 \leq \hat{y}_2(\mathbf{x}) \leq 57.5 \\ \frac{60-\hat{y}_2(\mathbf{x})}{60-57.5}, & 57.5 \leq \hat{y}_2(\mathbf{x}) \leq 60 \\ 0, & \text{otherwise.} \end{cases} \quad (3.5)$$

To simulate the responses of the DM, we assume that the DM has an underlying overall utility function of the following form,

$$U(\mathbf{x}) = - \sum_{j=1}^4 \omega_j^p (z_j^* - z_j(\mathbf{x}))^p \quad (3.6)$$

where ω_j is the weight and z_j^* is the ideal value of the objective j . We differentiate the importance weights in the underlying utility function by using $\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3, \omega_4)$ and the marginal rates of substitution by using $\mathbf{w} = (w_1, w_2)$. The objectives are $z_1(\mathbf{x}) = \frac{(v_1^{\max} - v_1(\mathbf{x}))}{(v_1^{\max} - v_1^{\min})}$, $z_2(\mathbf{x}) = \frac{(v_2^{\max} - v_2(\mathbf{x}))}{(v_2^{\max} - v_2^{\min})}$, $z_3(\mathbf{x}) = d_1(\mathbf{x})$, and $z_4(\mathbf{x}) = d_2(\mathbf{x})$. To prevent scaling problems, we transform $v_i(\mathbf{x})$ values into $[0, 1]$ interval in formulating $z_1(\mathbf{x})$ and $z_2(\mathbf{x})$ in a similar manner to the formulations of the desirability functions. We select $v_i^{\min}$ and $v_i^{\max}$ values as the ideal and nadir values for $v_i(\mathbf{x}) \forall i \in \{1, 2\}$, respectively. Therefore, $z_1^* = z_2^* = 1$. We set $p = 4$, which puts more emphasis on the objectives that are farther from their respective ideal points.

We arbitrarily select $d_1(\mathbf{x})$ as the reference desirability, and we formulate i^{th} entity of $\mathbf{w}(\mathbf{x})$ at iteration h as,

$$w_1^{(h)} = 1 \quad \text{and} \quad w_2^{(h)} = \frac{\frac{\partial U(\mathbf{z}(\mathbf{x}^{(h)}))}{\partial z_4}}{\frac{\partial U(\mathbf{z}(\mathbf{x}^{(h)}))}{\partial z_3}}. \quad (3.7)$$

In selecting the optimal step size at an iteration h , we vary the value of $t^{(h)}$ within the range of $[0, 1]$ by increments of 0.01 to be able to find the best possible

solution that Park and Kim (2005) could reach by their step size selection approach. Then, we calculate the resulting utility values for each value of $t^{(h)}$ and select the step size that yields the maximum of the utility values as optimal.

We demonstrate that the revised GDF procedure may stop prematurely at an early iteration (*i.e.*, the first iteration) far from the DM's most desirable solution. Throughout the demonstrations, in finding the actual most desirable solution of the DM for a given ω , we solve the following mixed integer nonlinear program (MINLP),

$$\begin{aligned}
& \max - \sum_{j=1}^2 \omega_j^4 (1 - z_j(\mathbf{x}))^4 - \sum_{i=1}^2 \omega_{i+2}^4 (1 - d_i)^4 \\
& \text{subject to} \\
& d_1 \leq \frac{y_1(\mathbf{x}) - 80}{100 - 80} + M(1 - b_1) \\
& \frac{y_1(\mathbf{x}) - 80}{100 - 80} \leq 1 + M(1 - b_1) \\
& d_2 \leq \frac{y_2(\mathbf{x}) - 55}{57.5 - 55} + M(1 - b_2) \\
& d_2 \leq \frac{60 - y_2(\mathbf{x})}{60 - 57.5} + M(1 - b_2) \\
& d_i \leq M b_i \quad \forall i \in \{1, 2\} \\
& b_i \in \{0, 1\} \quad \forall i \in \{1, 2\} \\
& 0 \leq d_i \quad \forall i \in \{1, 2\} \\
& -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\},
\end{aligned} \tag{3.8}$$

where M is a sufficiently big number.

First, we assume that the prediction variances of the responses are of relatively less importance to the DM. We implement the revised GDF for $\omega = (0.15, 0.15, 0.35, 0.35)$, and $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$.

Table 3.1 shows the results of the first iteration where $t^{(1)*} = 0.24$ is selected by the DM based on the U values. We should note that Park and Kim (2005) present the DM with such tables in which $t^{(h)}$ is first incremented by 0.1, then further incremented by 0.01 within the interval chosen by the DM. Skipping these intermediate steps, we present the results in a single table for increments of

0.1 together with the optimal step size selected based on the increments of 0.01.

Table 3.1: Determination of the optimal step size, $t^{(1)*}$, for $\mathbf{w}(\mathbf{x}^{(1)}) = (1.00, 107.54)$

t	0.00	0.10	0.20	0.24	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	1.32	0.89	0.66	0.61	0.56	0.56	0.66	0.88	1.30	2.01	3.13	4.83
v_2	0.18	0.12	0.08	0.07	0.05	0.05	0.07	0.11	0.17	0.25	0.35	0.46
d_1	0.79	0.76	0.75	0.76	0.78	0.84	0.93	0.00	0.00	0.00	0.00	0.00
d_2	0.00	0.27	0.96	0.77	0.35	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.79	95.13	95.08	95.24	95.65	96.83	98.62	101.02	104.03	107.66	111.90	116.76
y_2	53.96	55.68	57.40	58.09	59.12	60.84	62.55	64.27	65.99	67.71	69.43	71.15
$U \times 10^2$	-19.40	-1.83	-0.06	-0.03	-0.28	-1.51	-1.53	-3.75	-14.00	-89.20	-455.37	-1839.83

Table 3.2 shows the results presented to the DM in the second iteration where none of the solutions for $t^{(2)} > 0$ gives better prediction variance values due to not considering them in determining the directional vector. Therefore, the revised GDF procedure stops in the second iteration.

Table 3.2: Determination of the optimal step size, $t^{(2)*}$, for $\mathbf{w}(\mathbf{x}^{(2)}) = (1.00, 0.96)$

t	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.61	0.69	0.82	0.99	1.22	1.53	1.92	2.43	3.07	3.86	4.83
v_2	0.07	0.08	0.10	0.13	0.16	0.20	0.24	0.29	0.34	0.40	0.46
d_1	0.76	0.76	0.77	0.78	0.81	0.84	0.88	0.93	0.98	0.00	0.00
d_2	0.77	0.88	0.53	0.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.24	95.23	95.38	95.69	96.16	96.79	97.57	98.51	99.61	100.87	102.28
y_2	58.09	57.21	56.33	55.46	54.58	53.70	52.82	51.95	51.07	50.19	49.31
$U \times 10^2$	-0.03	-0.09	-0.54	-2.89	-9.98	-28.60	-76.78	-188.90	-429.23	-914.14	-1839.83

We display the iterations of the revised GDF and the most desirable solutions for the true underlying weights $\boldsymbol{\omega} = (0.15, 0.15, 0.35, 0.35)$ and $\boldsymbol{\omega}' = (0.00, 0.00, 0.50, 0.50)$ in Figure 3.1 where the axes denote the predicted response values. We present the associated numerical results in Table 3.3 and Table 3.4. It is worth noting that even though Park and Kim (2005) do not consider the prediction variances in determining the directional vector, they take them into account in step size selection, which implies that the prediction variances are implicitly

assumed in the DM's objective set along with desirability values. Therefore, in our demonstrations, we assume that all four objectives are included in the DM's objective set, and consequently the DM's actual most desirable solution results from $\omega > \mathbf{0}$. We consider ω to simulate the responses of the DM in implementing the revised GDF procedure. In addition to the actual most desirable solution and the solution of the revised GDF, we display the most desirable solution for ω' which excludes the prediction variances of the responses from the DM's objective set and assigns equal importance to the desirability values to observe where the revised GDF stops in between these two points.

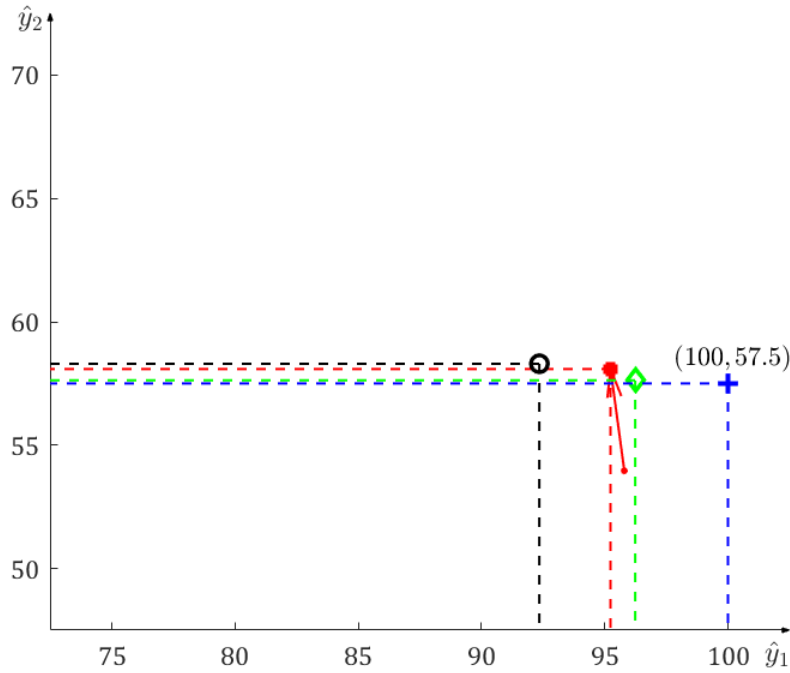


Figure 3.1: The most desirable solution for $\omega = (0.15, 0.15, 0.35, 0.35)$ (black circle), the solution of revised GDF for $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$ (red dot), the most desirable solution for $\omega' = (0.00, 0.00, 0.50, 0.50)$ (green diamond), and the target value (blue plus sign)

Table 3.3: The most desirable solutions displayed in Figure 3.1 for $\omega = (0.15, 0.15, 0.35, 0.35)$ and $\omega' = (0.00, 0.00, 0.50, 0.50)$

	v_1	v_2	d_1	d_2	y_1	y_2
ω	0.4019	0.0619	0.6174	0.6802	92.3475	58.2996
ω'	0.7418	0.0758	0.8117	0.9485	96.2346	57.6287

Table 3.4: The solution of the revised GDF for $\omega = (0.15, 0.15, 0.35, 0.35)$ and $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$

v_1	v_2	d_1	d_2	y_1	y_2
0.6089	0.0651	0.7618	0.7652	95.2363	58.0870

In Figure 3.1, the starting point of the red arrow represents the initial solution, while the endpoint represents the converged solution. The solution of the revised GDF dominates the actual most desirable solution with respect to the desirability values. This demonstrates a case where both of the desirability values need to deteriorate to direct the search towards the actual most desirable solution. Although this may intrinsically happen due to the nonlinearity of the objectives, the GDF method is designed to find the directional vector in a way to lead the search towards regions where at least one of the considered objectives improves. Therefore, the revised GDF may not lead the search to regions in which the desirability values simultaneously worsen without considering the prediction variances in determining the directional vector.

The outcome remains unchanged even when the step size selection problem (*i.e.*, $t^{(h)*} = \arg \max_{0 \leq t \leq 1} U(\mathbf{x}^{(h)} + t\mathbf{r}^{(h)})$) is solved to optimality without discretizing $t^{(h)}$. The procedure follows a similar pattern and terminates in the second iteration. We show the associated numerical results in Appendix B.1.

We additionally illustrate a case where the prediction variances of the responses are of relatively high importance to the DM. We implement the revised GDF procedure for $\omega = (0.35, 0.35, 0.15, 0.15)$ and the same initial solution. We

display the iterations of the revised GDF and the most desirable solutions for $\omega = (0.35, 0.35, 0.15, 0.15)$ and $\omega' = (0.00, 0.00, 0.50, 0.50)$ in Figure 3.2. We present the associated numerical results in Table 3.5 and Table 3.6.

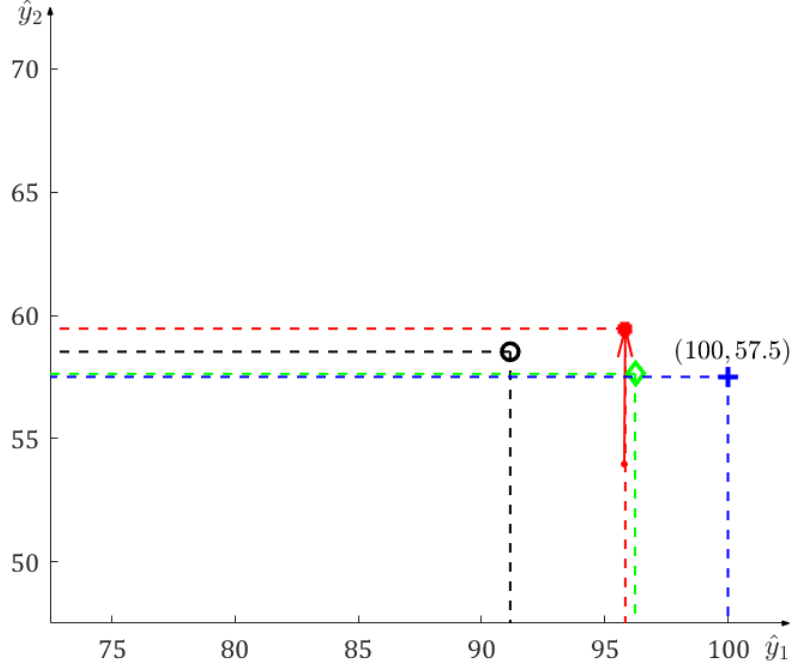


Figure 3.2: The actual most desirable solution for $\omega = (0.35, 0.35, 0.15, 0.15)$ (black circle), the solution of revised GDF for $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$ (red dot), the most desirable solution for $\omega' = (0.00, 0.00, 0.50, 0.50)$ (green diamond), the target value (blue plus sign)

Table 3.5: The most desirable solutions displayed in Figure 3.2 for $\omega = (0.35, 0.35, 0.15, 0.15)$ and $\omega' = (0.00, 0.00, 0.50, 0.50)$

	v_1	v_2	d_1	d_2	y_1	y_2
ω	0.3297	0.0593	0.5583	0.5916	91.1659	58.5210
ω'	0.7418	0.0758	0.8117	0.9485	96.2346	57.6287

Table 3.6: The solution of the revised GDF for $\omega = (0.35, 0.35, 0.15, 0.15)$ and $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$

v_1	v_2	d_1	d_2	y_1	y_2
0.5548	0.0519	0.7917	0.2154	95.8348	59.4616

Figure 3.2 demonstrate that the revised GDF is unable to deviate from the most desirable solution based on two objectives despite the objective weights for v_i 's being relatively higher than those for desirabilities. We provide the details of the iterations in Appendix B.2.

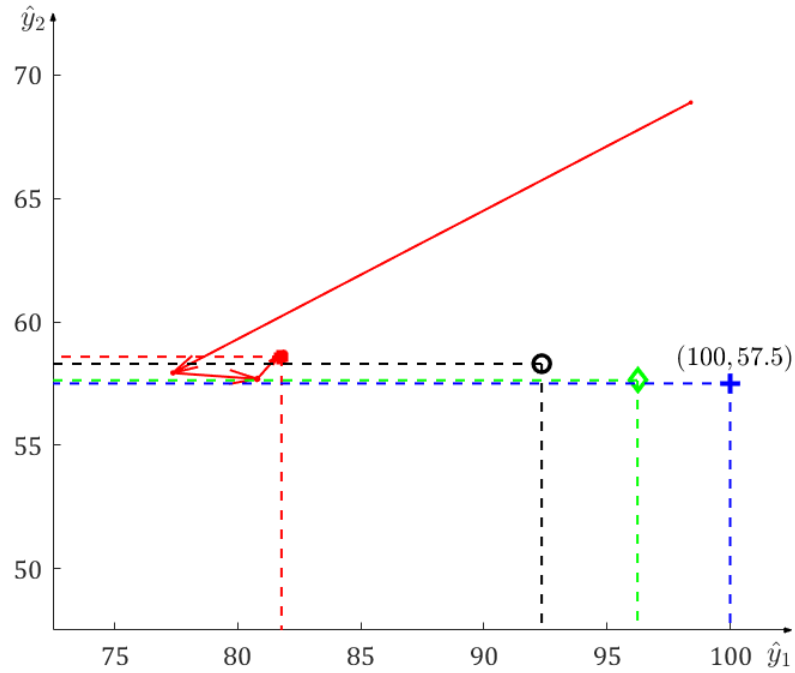


Figure 3.3: The actual most desirable solution for $\omega = (0.15, 0.15, 0.35, 0.35)$ (black circle), the solution of revised GDF for $\mathbf{x}^{(1)} = (1.3, -0.6, 1.4)$ (red dot), the most desirable solution for $\omega' = (0.00, 0.00, 0.50, 0.50)$ (green diamond), the target value (blue plus sign)

Table 3.7: The solution of the revised GDF (second row) for $\omega = (0.15, 0.15, 0.35, 0.35)$ and $\mathbf{x}^{(1)} = (1.3, -0.6, 1.4)$, and a dominating solution (third row)

v_1	v_2	d_1	d_2	y_1	y_2
0.4144	0.0764	0.0891	0.5660	81.7814	58.5851
0.3720	0.0743	0.5403	1.0000	90.8055	57.5000

We also implement the revised GDF procedure for the objective weights $\omega = (0.15, 0.15, 0.35, 0.35)$, and a different initial solution, $\mathbf{x}^{(1)} = (1.3, -0.6, 1.4)$. We observe that the location of the converged solutions may substantially change compared to the solution displayed in Figure 3.1, which implies that the revised GDF may demonstrate sensitivity to the initial solution although the authors state that the initial solution can be arbitrarily selected. Table 3.7 shows the solution of the revised GDF procedure in the second row. We provide further details of the iterations in Appendix B.3.

Differently from Table 3.4, Table 3.7 also includes a solution in the third row that dominates the solution obtained by the revised GDF procedure. To find the dominating solution, we solve the problem formulated in Eq. (B.1). This illustrates that the revised GDF has no mechanism to prevent the final solution from being dominated in terms of either four or two objectives. To investigate if the outcome changes to a nondominated solution when the step size selection problem is solved without discretizing $t^{(h)}$, we repeat the revised GDF procedure. Appendix B.3 includes the details of the iterations, which converge to a solution again dominated by the solution shown in the third row of Table 3.7. Hence, the issue is not related to the discretization of t values. The problem may arise from the failure to satisfy the assumptions of the GDF or from not considering prediction variances in determining the directional vector. Regardless of the specific reason, our findings indicate that the revised GDF may fail to converge to a nondominated solution.

Furthermore, we compare the revised GDF procedure to a random search. For

this evaluation, we assume a linear utility function and generate a large set of nondominated solutions by randomly changing the importance weights of the assumed linear utility function, given by Eq. (3.6) when $p = 1$. We use this function only to generate nondominated solutions. In simulating the DM's decisions, we still consider the DM's underlying utility in Eq. (3.6) for $p = 4$.

Table 3.8 shows the results for five different settings of the DM's objective weights. For each setting, we determine the worst (U_{worst}) and the best (U_{best}) values of the DM's utility observed in the generated nondominated solution set. Additionally, we calculate the utility value (U_{pk}) of the solution obtained from the revised GDF procedure for $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$. The normalized utility (U_{norm}) indicates the position of U_{pk} within the utility range of $[U_{\text{worst}}, U_{\text{best}}]$.

Table 3.8: Comparison with random selection of n nondominated solutions

ω	$U_{\text{worst}} \times 10^4$	$U_{\text{best}} \times 10^4$	$U_{\text{pk}} \times 10^4$	$U_{\text{norm}} \times 10^2$	$P_s \times 10^2$	$P_{f(3)} \times 10^2$	$P_{f(5)} \times 10^2$
(0.05, 0.05, 0.45, 0.45)	-820.22	-0.65	-1.22	99.93	94.01	16.93	26.59
(0.15, 0.15, 0.35, 0.35)	-308.19	-2.87	-2.92	99.98	99.95	0.15	0.25
(0.25, 0.25, 0.25, 0.25)	-140.35	-3.08	-11.97	93.52	82.22	44.43	62.43
(0.35, 0.35, 0.15, 0.15)	-283.88	-1.16	-32.05	89.07	45.49	90.59	98.05
(0.45, 0.45, 0.05, 0.05)	-775.72	-0.04	-78.66	89.86	46.05	90.24	97.93

P_s represents the ratio of the number of the nondominated solutions outperformed by the revised GDF's solution in terms of the overall utility value of the DM to the total number of generated nondominated solutions. This ratio helps us estimate the probability of success for the revised GDF. Using this success probability, we assess the performance of the revised GDF procedure against n randomly selected nondominated solutions. To measure the probability that at least one of the n randomly generated nondominated solutions has a utility value greater than the revised GDF's solution, we define $P_{f(n)} = 1 - P_s^n$.

Our findings in Table 3.8 indicate that there may be cases where $P_{f(n)}$ is considerably high even when $n = 3$ such as for $\omega \in \{(0.35, 0.35, 0.15, 0.15), (0.45, 0.45, 0.05, 0.05)\}$. In such cases, there is a high chance of finding a solution that the DM would prefer over the solution provided by the revised GDF by randomly selecting n nondominated solutions. On the other hand, for some ω

such as $(0.15, 0.15, 0.35, 0.35)$, we observe high P_s values. This illustrates that the performance of the revised GDF is sensitive to the DM's underlying importance weights and there may be situations where the benefits of the method are not substantial.

It is worth noting that we do not find it meaningful to discuss if there is any trend in the behavior of $P_{f(n)}$ with respect to the different ω selections based on such limited observations. The results vary by initial solutions. We provide two additional tables based on different initial solutions to illustrate how the results may change in Appendix B.5. For further insights, the analysis can be extended to include different examples, underlying utility functions, and initial solution selections.

Finally, we show that relatively dominated solutions may be observed for multiple $t^{(h)} > 0$ values presented to the DM for determining the optimal step size due to the nonlinearity of the objectives. To demonstrate this issue, we implement the original GDF procedure on a specific problem that we generated, ensuring that the assumptions of the procedure are satisfied.

We assume two objective functions, namely $f_1(x_1, x_2)$ and $f_2(x_1, x_2)$, both of which are concave over the decision space. Additionally, we consider an overall utility function $U(f_1, f_2)$, which is concave and increasing over the objective space. We provide the details of the assumed objective functions and the overall utility of the DM in Appendix B.6. We should note that in this demonstration, we show the deficiencies only attributed to the use of the GDF method and not the revisions by Park and Kim (2005).

We implement the GDF procedure for $\mathbf{x}^{(1)} = (-1, 1)$, an arbitrarily selected initial solution, and increment $t^{(1)}$ by 0.1. We obtain the results presented in Table 3.9 in the first iteration for $\mathbf{w}(\mathbf{x}^{(1)}) = (1.00, 2.50)$. We provide the details of the implementation steps such as finding trade-off weights in Appendix B.6.

Table 3.9: Determination of the optimal step size in the first iteration of the GDF method for $\mathbf{x}^{(1)} = (-1, 1)$ and $\mathbf{w}^{(1)} = (1.0, 2.5)$

t	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
$f_1(x_1, x_2)$	-2.00	-1.70	-1.60	-1.70	-2.00	-2.50	-3.20	-4.10	-5.20	-6.50	-8.00
$f_2(x_1, x_2)$	5.00	6.30	7.40	8.30	9.00	9.50	9.80	9.90	9.80	9.50	9.00
$U(f_1, f_2)$	-29.00	-16.58	-9.32	-5.78	-5	-6.50	-10.28	-16.82	-27.08	-42.50	-65.00

Table 3.9 shows that the solution at $t = 0.2$ dominates the solutions at $t = 0$ and $t = 0.1$. Similarly, the solution at $t = 0.7$ dominates the solution at $t = 1$. This way, the solutions at $t = 0.2$ and $t = 0.7$ become advantageous compared to other relatively nondominated solutions. There are examples from Behavioral Economics, which indicate that DMs tend to prefer alternatives that are presented alongside the options they dominate (Ariely, 2008, pp. 1-21). This potential bias in selecting the optimal step size may lead the search to regions that are not desirable for the DM.

3.3 Robust Interactive Desirability Function Approach (RIDFA)

He et al. (2021) proposed a robust interactive desirability function approach (RIDFA) incorporating model uncertainty into an interactive MRO procedure. The term "robustness" does not refer to the insensitivity to response variability, as in the context of RPD. Instead, He et al. (2021) consider the robustness against variability arising from the utilization of empirical models. According to their definition, a robust solution is a compromise solution at which the worst model forecasts in the confidence intervals of the responses are within the acceptable regions (*i.e.*, bounds on response values based on engineering requirements) for a given significance level (*i.e.*, type I error α) determined prior to the solution procedure.

For any design parameter setting, $\mathbf{x}$, the robust desirability functions for a

nominal-the-best (NTB) response is constructed as follows,

$$\hat{d}_R^{(h)} = \begin{cases} \min\left(\frac{\hat{\eta}(\mathbf{x}) - Y^{min}}{Y^T - Y^{min}}\right)s & \text{if } Y^{min} < \hat{y}^L(\mathbf{x}), \hat{y}^U(\mathbf{x}) < Y^T \\ \min\left(\frac{\hat{\eta}(\mathbf{x}) - Y^{min}}{Y^T - Y^{min}}\right)t & \text{if } Y^{min} < \hat{y}^L(\mathbf{x}) < Y^T < \hat{y}^U(\mathbf{x}) < Y^{max}, \hat{y}(\mathbf{x}) < Y^T \\ \min\left(\frac{Y^{max} - \hat{\eta}(\mathbf{x})}{Y^{max} - Y^T}\right)t & \text{if } Y^{min} < \hat{y}^L(\mathbf{x}) < Y^T < \hat{y}^U(\mathbf{x}) < Y^{max}, \hat{y}(\mathbf{x}) > Y^T \\ \min\left(\frac{Y^{max} - \hat{\eta}(\mathbf{x})}{Y^{max} - Y^T}\right)z & \text{if } Y^T < \hat{y}^L(\mathbf{x}), \hat{y}^U(\mathbf{x}) < Y^{max} \\ \tau & \text{if } \hat{y}^L(\mathbf{x}) \leq Y^{min} \text{ or } \hat{y}^L(\mathbf{x}) \geq Y^{max}, \end{cases} \quad (3.9)$$

where $\hat{d}_R^{(h)}$ is the modified robust desirability value of estimated response $\hat{y}(\mathbf{x})$ at h^{th} iteration, τ is a very small positive number, Y^{min} , Y^T , and Y^{max} denote the lower bound, target value, and upper bound of response, $y(\mathbf{x})$, respectively, s , t , and z are the adjustment parameters that determine the shape of $\hat{d}_R^{(h)}$. For any $\mathbf{x}$, $\hat{\eta}(\mathbf{x}) \in [\hat{y}^L(\mathbf{x}), \hat{y}^U(\mathbf{x})]$, where $\hat{y}^L(\mathbf{x})$ and $\hat{y}^U(\mathbf{x})$ are the lower and upper confidence interval limits as functions of design parameters, respectively.

The construction of confidence intervals assumes no correlation among the responses and is based on the individual type I error α . Consequently, the family error of the response surface generated by the simultaneous confidence intervals is $1 - (1 - \alpha)^m$ where m denotes the number of responses, which is larger than the type I error α .

After building the response surface models and selecting the α value, the preference parameters are initialized. These parameters are determined either based on the DM's preferences or by considering the range of the response surface functions. In the latter scenario, the minimum and/or maximum values of the functions are determined by minimizing and/or maximizing them individually across the design parameter space. Subsequently, robust desirability functions are constructed, and the overall desirability is maximized by solving the following

mathematical program,

$$\begin{aligned}
& \text{Maximize} && D_R \\
& \text{subject to} && \\
& && D_R \leq d_{R_i}^h(\mathbf{x}) \quad \forall i \in \{1, 2, \dots, m\} \\
& && D_R \geq 0 \\
& && \mathbf{x} \in \Omega.
\end{aligned} \tag{3.10}$$

where D_R is the minimum robust desirability value with respect to all responses and h is the iteration counter.

The resulting mean response values, along with their corresponding confidence interval limits, are presented to the DM for evaluation. If the confidence interval limits fall within acceptable regions, the associated responses are considered satisfactory. Otherwise, they are considered unsatisfactory. The DM can select one of the unsatisfactory responses for tightening or one of the satisfactory responses for relaxation. Tightening and relaxation are achieved by making adjustments in shape, bound, and target parameters as explained by Jeong and Kim (2009). The desirability functions and Equation (3.10) are updated to reflect the DM's adjustments and a solution for the next iteration is obtained. This iterative process continues until a solution is found where all confidence intervals fall within their respective acceptable bounds.

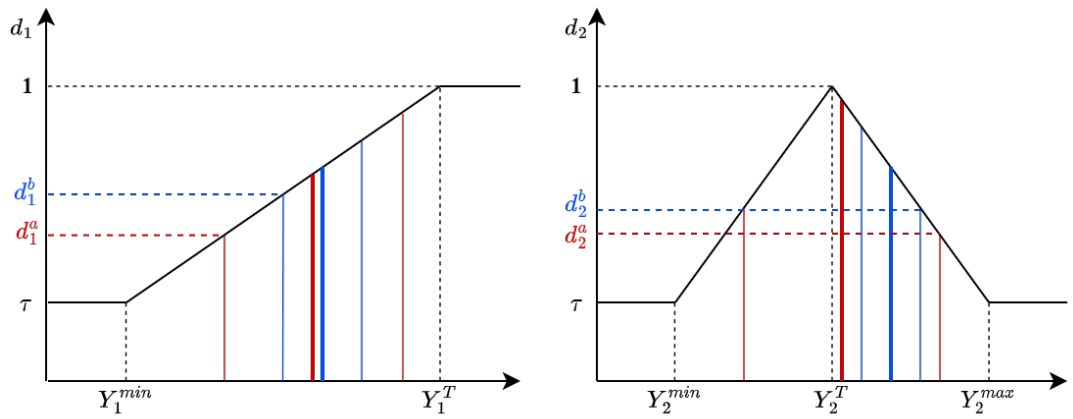


Figure 3.4: Two design parameter settings (a and b) in the design space illustrating robustness measures for the desirability functions

To illustrate how RIDFA works, we assume a two-response case, with one LTB and one NTB response. For simplicity, we set s , t , and z to 1 implying that the desirability functions are linear. In Figure 3.4, the red and blue colored thick lines depict the mean response values for two different settings of the design parameters (*i.e.*, a and b), while the thin lines represent the confidence intervals around the means. Based on the definitions by He et al. (2021), the overall desirability value for the blue setting is d_2^b , while the overall desirability value for the red setting is d_1^a . RIDFA selects the setting b because it yields a higher desirability value (*i.e.*, $d_2^b > d_1^a$).

Issues with RIDFA. RIDFA does not have a mechanism for considering the alternative optimal solutions to the problem formulated in Equation (3.10). In other words, there may be many different solutions with the same optimal value of D_R since the constraints do not differentiate in better values for some of the m constraints, and RIDFA is not capable of considering such solutions. One of the consequences of this deficiency is that the solution by RIDFA may be dominated by some of those alternative optimal solutions. However, every DM is likely to be interested in improving the performance of the responses, if possible, for the given optimal D_R value. Another is that the different DMs may have different preferences among the nondominated ones of those alternative optimal solutions.

Moreover, RIDFA considers model parameter uncertainty in a restricted manner and does not allow the DM to state her/his preferences with respect to model parameter uncertainty. It only searches for the solutions at which all the individual $100(1 - \alpha)\%$ confidence intervals are within the corresponding acceptable limits. When all solutions are within the specified limits, the selection is based on the performance of the worst possible outcome within the confidence regions. However, the DM may not necessarily be interested in the robust solution selected based on the worst-case scenario. The DM may prefer another solution, confidence intervals of which are in the acceptable region, explicitly considering the response means and associated model parameter uncertainty. For instance, in Figure 3.4, although the confidence intervals for the red solution are wider and the worst possible response values are worse than that of the blue solution, a DM still may prefer the red solution. The confidence interval for the second

response covers the target. This means that the red solution is likely to produce more outputs closer to the target compared to the blue solution for the second response. In addition, for the first response, although the red confidence interval has some space above the blue confidence interval. This implies that there is a chance that the red solution generates outputs with better response values for the first response.

Furthermore, He et al. (2021) demonstrate the application of RIDFA by considering both response means and variances in the presence of model parameter uncertainty. They construct response surface models for means and variances using OLS regression, which assumes constant error variance. However, the inclusion of the response variances in the performance measures is motivated by their potential variability across different design parameter settings. Thus, constructing mean models using OLS regression contradicts this motivation. Besides, it may be hard for the DM to make adjustments in desirability functions due to the difficulty of anticipating their consequences, and it becomes even more complex for the DM to additionally consider desirability functions for response variances.

Finally, it may also be a difficult task to determine the value of the type I error, α , prior to the solution procedure. The authors state that this value is determined based on the risk attitude of the DM. However, different α levels may lead the search to different regions in the solution space. In such a case, it may not be easy for a DM to foresee the effect of selecting different α levels on the solutions and their practical implications.

Demonstrations. To demonstrate some of the issues regarding the solution process of RIDFA, we combine the piece-wise definitions in Eq. (3.9) with

Eq. (3.10) by formulating a MINLP as follows,

$$\begin{aligned}
& \max D_R \\
& \text{subject to} \\
& D_R \leq d_{R_i} \quad \forall i \in \{1, 2, \dots, m\} \\
& d_{R_l} \leq \frac{\hat{y}_l^L(\mathbf{x}) - Y_l^{\min}}{Y_l^{\max} - Y_l^{\min}} + M(1 - b_l) \quad \forall l \in L \\
& d_{R_j} \leq \frac{\hat{y}_j^L(\mathbf{x}) - Y_j^{\min}}{Y_j^{\text{target}} - Y_j^{\min}} + M(1 - b_j) \quad \forall j \in J \\
& d_{R_j} \leq \frac{Y_j^{\max} - \hat{y}_j^U(\mathbf{x})}{Y_j^{\max} - Y_j^{\text{target}}} + M(1 - b_j) \quad \forall j \in J \\
& d_{R_i} \leq \tau + Mb_i \quad \forall i \in \{1, 2, \dots, m\} \\
& b_i \in \{0, 1\} \quad \forall i \in \{1, 2, \dots, m\} \\
& D_R \geq 0 \\
& d_{R_i} \geq 0 \quad \forall i \in \{1, 2, \dots, m\} \\
& \mathbf{x} \in \Omega,
\end{aligned} \tag{3.11}$$

where L and J denote the index sets for LTB and NTB responses, respectively. We assume linear desirability functions in our demonstrations similar to the illustrative implementation provided by He et al. (2021), which Eq. (3.11) is able to replicate.

To generate numerical results, we consider the polymer experiment that involves two responses of interest. Eq. (3.11) takes into account LTB and NTB response types, since both the polymer experiment and the example problem considered by He et al. (2021) involve those response types. However, STB responses can easily be accommodated by introducing additional constraints when required.

We assume that RIDFA is at iteration h and the DM sets $LAL_1 = 80$, $LAL_2 = 55$, $UAL_2 = 60$, $Y_1^{\min} = 80$, $Y_1^T = 90$, $Y_2^{\min} = 55$, $Y_2^{\max} = 60$, and $Y_2^T = 57.5$. Then, we solve the following optimization problem,

$$\begin{aligned}
& \max D_R \\
& \text{subject to} \\
& D_R \leq d_{R_i} \quad \forall i \in \{1, 2\} \\
& d_{R_1} \leq \frac{\hat{y}_1^L(\mathbf{x}) - 80}{90 - 80} + M(1 - b_1) \\
& d_{R_2} \leq \frac{\hat{y}_2^L(\mathbf{x}) - 55}{57.5 - 55} + M(1 - b_2) \\
& d_{R_2} \leq \frac{60 - \hat{y}_2^U(\mathbf{x})}{60 - 57.5} + M(1 - b_2) \\
& d_{R_i} \leq \tau + Mb_i \quad \forall i \in \{1, 2\} \\
& b_i \in \{0, 1\} \quad \forall i \in \{1, 2\} \\
& D_R \geq 0 \\
& d_{R_i} \geq 0 \quad \forall i \in \{1, 2\} \\
& 1.68 \geq x_k \geq -1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{3.12}$$

Table 3.10: The solution obtained by solving Eq. (3.12)

i	LAL_i	Y_i^{min}	$\hat{y}_i^L(\mathbf{x})$	$\hat{y}_i(\mathbf{x})$	$\hat{y}_i^U(\mathbf{x})$	Y_i^{max}	UAL_i	d_{R_i}	CI Length
1	80	80	87.1852	92.9708	98.7565	90	-	0.7185	11.5713
2	55	55	56.7963	57.5000	58.2037	60	60	0.7185	1.4075

The obtained solution is presented in Table 3.10. According to He et al. (2021)'s definitions, both responses are considered satisfactory since their confidence intervals fall within the acceptable region. Consequently, RIDFA stops at this step. However, the solution presented in Table 3.10 is, in fact, a dominated solution. That is, there exist solutions that further improve d_{R_1} (d_{R_2}) while maintaining the same level of d_{R_2} (d_{R_1}) and hence the optimal overall desirability value D_R^h . To identify such a solution, we solve the following problem:

$$\begin{aligned}
& \max d_{R_1} + d_{R_2} \\
& \text{subject to} \\
& D_R^h \leq D_R \\
& D_R \leq D_{R_i} \quad \forall i \in \{1, 2\} \\
& d_{R_1} \leq \frac{\hat{y}_1^L(\mathbf{x}) - 80}{90 - 80} + M(1 - b_1) \\
& d_{R_2} \leq \frac{\hat{y}_2^L(\mathbf{x}) - 55}{57.5 - 55} + M(1 - b_2) \\
& d_{R_2} \leq \frac{60 - \hat{y}_2^U(\mathbf{x})}{60 - 57.5} + M(1 - b_2) \\
& d_{R_i} \leq \tau + Mb_i \quad \forall i \in \{1, 2\} \\
& b_i \in \{0, 1\} \quad \forall i \in \{1, 2\} \\
& D_R \geq 0 \\
& d_{R_i} \geq 0 \quad \forall i \in \{1, 2\} \\
& 1.68 \geq x_k \geq -1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{3.13}$$

Table 3.11 presents the obtained results.

Table 3.11: The solution that dominates the one reached by RIDFA

i	LAL_i	Y_i^{min}	$\hat{y}_i^L(\mathbf{x})$	$\hat{y}_i(\mathbf{x})$	$\hat{y}_i^U(\mathbf{x})$	Y_i^{max}	UAL_i	d_{R_i}	CI Length
1	80	80	88.2587	94.7438	101.2289	90	-	0.8259	12.9705
2	55	55	56.7963	57.5000	58.2037	60	60	0.7185	1.4075

Figure 3.5 visualizes the solution by RIDFA (in blue) as well as the improvement in d_{R_1} (in red) as a result of solving Eq. (3.13).

The solution we presented in Table 3.11 maximizes d_{R_1} . However, a DM may not always prefer the maximum value because the intermediate values of d_{R_1} correspond to different confidence interval lengths as illustrated in Table 3.12. DMs may have varying preferences for these intermediate values and their respective confidence interval lengths. RIDFA does not have a mechanism to search among such solutions.

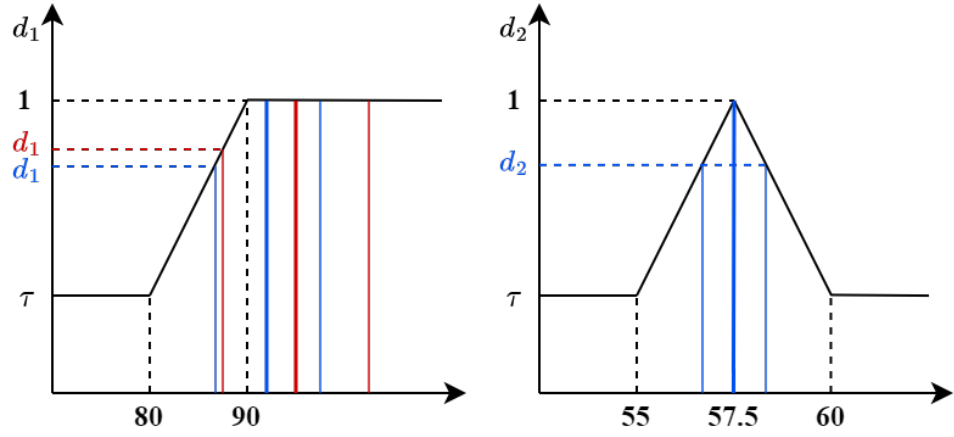


Figure 3.5: Visualization of the solution by RIDFA (in blue) and the improvement in d_{R_i} resulting from solving Eq. (3.13) (in red)

Table 3.12: Alternative nondominated solutions with respect to d_{R_1} and confidence interval lengths for first response

i	LAL_i	Y_i^{min}	$\hat{y}_i^L(\mathbf{x})$	$\hat{y}_i(\mathbf{x})$	$\hat{y}_i^U(\mathbf{x})$	Y_i^{max}	UAL_i	d_{R_i}	CI Length
1	80	80	88.2587	94.7438	101.2289	90	-	0.8259	12.9705
1	80	80	87.8394	94.0197	100.2000	90	-	0.7839	12.3606
1	80	80	87.3130	93.1565	98.9998	90	-	0.7313	11.6868



CHAPTER 4

OVERVIEW OF THE METHODOLOGY

We elaborate in Chapter 2 that many of the existing approaches assume that preferences of the DM are known prior to the solution procedure. This is a strong assumption that is hard to justify in practice. Several other approaches incorporate DM's preferences into the solution process in an interactive manner. Only two of those interactive approaches consider model parameter uncertainty in the empirical functions. However, they consider neither unequal robustness nor possible correlations among responses. They also have other deficiencies we demonstrate in Chapter 3.

Özateş (2015) develops an interactive approach to two-response product and process design optimization problems considering unequal robustness and possible correlations among responses under model parameter uncertainty. However, she uses rough estimates in constructing performance measures, which may lead to unrealistic solutions in practice. Specifically, unequal robustness is ignored in empirical model building although an RPD scenario is assumed.

To overcome the issues with the existing approaches, we develop two interactive optimization approaches considering DM's preferences under model parameter uncertainty for product and process design problems with two responses. Assuming that the data is appropriately collected prior to our solution procedures, we focus on two solution stages: empirical model building and optimization. Main differences between our two approaches arise from the differences in the empirical model building.

We develop and illustrate our approaches in Chapters 5 and 6. In this chapter, our

aim is to overview our methodology and to provide the common methodological background on the developed approaches. First, we briefly explain data collection stage and our assumptions regarding the collected data in Section 4.1. Then, in Section 4.2, we mathematically express and briefly discuss the assumptions of the four regression methods we utilize in building response surface models. We devote Section 4.3 to the optimization stage related matters. In Section 4.3.1, we develop our performance measures. We overview our interactive approaches and provide the mapping between the considered regression methods and our approaches in Section 4.3.2. We also explain how we handle nonlinearity in our mathematical models.

4.1 Data Collection

Designed experiments are conducted as a series of runs in which design parameters are purposefully varied together to observe the changes in responses at the data collection stage of MRO. It is important to properly design an experiment to draw meaningful conclusions. Well-designed experiments often lead to good empirical models of the system (*i.e.*, product or process) under consideration (Montgomery, 2020, p. 430).

Short Review of Existing Designs. Several designs exist for fitting and analyzing response surfaces in the literature. To determine the design parameters significantly affecting the responses of interest, *screening experiments* are conducted, mostly through economical designs with less number of runs. Such designs are known as *first-order designs* which allow fitting first-order response surface models. The most common first-order designs involve full and fractional factorial designs at two levels, Plackett-Burman, and simplex designs.

Once the significant design parameters and the experimental region believed to contain the optimal design parameter setting are determined through a series of screening experiments, an *optimization experiment* is designed. *Second-order designs* are commonly used in conducting optimization experiments as they allow fitting second-order response surface models incorporating curvature. Full

factorial designs at three levels, central composite designs (CCDs), and Box-Behnken designs are among the most frequently used second-order designs.

When robustness of responses is concerned, *crossed array designs* suggested by Taguchi (1986 as cited in Robinson et al., 2004) are widely used to consider the effects of noise factors in data collection. Assuming that noise factors can be controlled for experimentation purposes, such designs are created by crossing two separate designs for noise factors (*i.e.*, outer array) and design parameters (*i.e.*, inner array). We illustrate the experimental layout of a crossed array design in Figure 4.1, respectively.

Inner Array			Outer Array								
x_1	x_2	x_3	z_1	1	-1	1	-1				
			z_2	1	1	-1	-1				
				y_{11}	y_{21}	y_{12}	y_{22}	y_{13}	y_{23}	y_{14}	y_{24}
-1	-1	-1									
1	-1	-1									
-1	1	-1									
1	1	-1									
-1	-1	1									
1	-1	1									
-1	1	1									
1	1	1									
-1.682	0	0									
1.682	0	0									
0	-1.682	0									
0	1.682	0									
0	0	-1.682									
0	0	1.682									
0	0	0									
0	0	0									
0	0	0									
0	0	0									
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0	0	0									
0	0	0									

Figure 4.1: Illustration of a crossed array design layout for 2 responses: The design contains a CCD for 3 design parameters as the inner array and a 2^2 design for 2 noise factors as the outer array, which are formed by transforming natural variables to coded variables. Each design parameter setting in the inner array is performed for all 4 combinations in the outer array, producing the crossed array with 80 experimental runs at which both responses are observed.

Crossed array designs may require a large experiment with too many runs as the number of factors increase (Robinson et al., 2004). Combined arrays, introduced by Welch et al. (1990) and named by Shoemaker et al. (1991), are more

economical alternatives to crossed array designs. They combine noise factors and design parameters in a single experimental design. Therefore, resulting response surface models contain noise factors as regressors together with design parameters. Although combined array designs allow analyzing interactions between design parameters and noise factors, developing empirical models, confidence and prediction regions for the responses or their statistics are challenging since regressors of response surface models involve noise factors, which are, in fact, random variables.

Our Assumptions on the Collected Data. We assume that the data are collected with $r \geq 0$ replications for each experimental run prior to our solution procedure. The number of replications can be determined according to the design of an outer array. When it is not possible to control noise factors during the experiments, runs can be replicated in a random manner without designing an outer array. Even though replicated experiments provide a better insight into approximating response surface models especially when the separate models for variances of the responses are utilized (Kutner et al., 2005, pp. 421-426), it is usually impractical to replicate the runs of an experiment which leads to an extensive number of runs (Box and Meyer, 1986). Therefore, our solution framework does not force experimenters to replicate the runs albeit it can enjoy the advantages of replication when economically allowed.

Regardless of the availability of replications, we assume the following conditions.

- Screening experiments are already conducted and we are provided with the optimization experiment results.
- The order of the experimental runs is completely randomized to prevent serial correlations.
- Measurement system is analyzed prior to data collection and improved if needed. Therefore, measurement errors are minimized.
- Design parameters and noise factors are not combined in a single array so that response surface models do not involve random regressors.
- Responses are continuous.

4.2 Empirical Model Building

We consider two-response product and process design problems in which *quality characteristics*, so-called *responses*, are influenced by the changes in the relevant design parameter values. Similar to the majority of the existing MRO approaches, we assume that the relationship between the i^{th} response, y_i , and the design parameters denoted by $x_1, x_2, \dots, x_k$ is approximated via a second-order response surface model as follows,

$$y_i = \beta_{i0} + \sum_{j=1}^k \beta_{ij} x_j + \sum_{l=1}^{k-1} \sum_{j=l+1}^k \beta_{ijl} x_j x_l + \sum_{j=1}^k \beta_{ijj} x_j^2 + \varepsilon_i, \quad i \in \{1, 2\}. \quad (4.1)$$

Although second-order models have advantages in capturing possibly high degree of curvature in the true response functions, there might be cases where first-order models with only the first two terms of (4.1) better explain the relationship between responses and relevant design parameters. Our approaches can accommodate both models.

Several methods can be used to estimate β parameters in (4.1). The majority of prior MRO approaches (Costa and Lourenço, 2017) and all interactive MRO approaches estimate model parameters by using OLS which is a well studied method with several theoretical justifications. Its finite sample properties are precise and not influenced by the number of observations under certain limiting assumptions (Greene, 2018, pp. 57-63). Specifically, it assumes that responses are uncorrelated and variances of random errors (or variances of responses) are constant over the design parameter space (*i.e.*, equal robustness or homoskedasticity). However, the data obtained at the first stage of MRO may be multivariate in nature. Furthermore, when an RPD problem is of concern, variances of random errors are naturally not constant over design parameter space (*i.e.*, unequal robustness or heteroskedasticity). Ignoring possible correlations among the responses and unequal robustness in building empirical models may result in increased variance of estimated model coefficients (*i.e.*, β estimates with low precision) and correspondingly unrealistic decisions at the optimization stage.

There are other parametric linear regression methods such as multivariate regression (MVR), seemingly unrelated regression (SUR), generalized least squares (GLS) regression, and weighted least squares (WLS) regression, which are commonly used in econometrics literature. These methods extend OLS to more general cases violating some of its assumptions. Yet, they are underused in MRO approaches. Some prior MRO approaches (Fogliatto and Albin, 2000; Ko et al., 2005; Ouyang et al., 2017; Wang et al., 2020) employ SUR with the purpose of producing more precise model parameter estimates when responses are correlated (Shah et al., 2004). However, some of those approaches assume unequal robustness which contradicts the constant variance assumption of SUR. On the other hand, WLS regression is utilized in a few prior MRO approaches (Ribeiro et al., 2000; Lopes et al., 2013) to consider the unequal robustness of responses in building empirical models.

Despite their advantages in extending OLS assumptions, the aforementioned regression methods bring additional difficulties for measuring model parameter uncertainty in MRO problems. Our solution framework aims to overcome those difficulties in considering model parameter uncertainty when some of the OLS assumptions do not hold. To this respect, we consider four parametric linear regression methods: OLS regression, MVR, SUR, and WLS regression to estimate β parameters of response surface models in our interactive approaches. Each of these methods has a different set of assumptions that play a critical role in developing our solution procedures. We mathematically express these assumptions through the formulation of SUR.

We build each response surface model in the following form:

$$\mathbf{y}_i = \mathbf{X}_i \boldsymbol{\beta}_i + \boldsymbol{\varepsilon}_i, \quad i \in \{1, 2\}, \quad (4.2)$$

where $\mathbf{y}_i \in \mathbb{R}^{n \times 1}$ is a vector of observations, $\mathbf{X}_i$ is an $n \times (p_i + 1)$ design matrix specifying values of the regressors as known functions of design parameters such as powers and cross products, p_i denotes the number of regressors, $\boldsymbol{\beta}_i \in \mathbb{R}^{(p_i+1) \times 1}$ is a vector of model coefficients and $\boldsymbol{\varepsilon}_i \in \mathbb{R}^{n \times 1}$ is a random error vector associated with the i^{th} response.

Stacking two response surface models in the form of Eq. (4.2) yields

$$\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_2 \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \end{bmatrix} + \begin{bmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \end{bmatrix} \quad (4.3)$$

or $\mathbf{y} = \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\varepsilon}$ where $\mathbf{y} \in \mathbb{R}^{2n \times 1}$ is a vector of observations, $\mathbf{X}$ is a $2n \times (p+2)$ block diagonal design matrix with $p = \sum_{i \in \{1,2\}} p_i$, $\boldsymbol{\beta} \in \mathbb{R}^{(p+2) \times 1}$ is a vector of model coefficients and $\boldsymbol{\varepsilon} \in \mathbb{R}^{2n \times 1}$ is a random error vector.

We assume that the following conditions hold for all the considered regression methods.

Assumption 4.2.1 $\mathbf{X}_i$ is non-stochastic $\forall i \in \{1, 2\}$.

Assumption 4.2.2 $E(\boldsymbol{\varepsilon}_i) = \mathbf{0} \quad \forall i \in \{1, 2\}$.

Assumption 4.2.3 $\text{Var}(\boldsymbol{\varepsilon}) = \boldsymbol{\Sigma}$, where $\boldsymbol{\Sigma} \in \mathbb{R}^{2n \times 2n}$ is a positive definite matrix in the following form:

$$\boldsymbol{\Sigma} = \begin{bmatrix} \text{Var}(\boldsymbol{\varepsilon}_1) & \text{Cov}(\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2) \\ \text{Cov}(\boldsymbol{\varepsilon}_2, \boldsymbol{\varepsilon}_1) & \text{Var}(\boldsymbol{\varepsilon}_2) \end{bmatrix}. \quad (4.4)$$

Assumption 4.2.4 $\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$.

The estimator of $\boldsymbol{\beta}$ is expressed as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{y}. \quad (4.5)$$

The distinctive property in determining the appropriate linear regression method is the structure of $\boldsymbol{\Sigma}$. We require Assumption 4.2.4 not for estimating $\boldsymbol{\beta}$ but for performing statistical inference through confidence and prediction regions, which we discuss in Section 4.3

Let $\text{Var}(\boldsymbol{\varepsilon}_i) = \sigma_i^2 \mathbf{W}_i \quad \forall i \in \{1, 2\}$, where $\mathbf{W}_i$ is an $n \times n$ diagonal positive definite matrix. Table 4.1 summarizes the assumptions on $\boldsymbol{\Sigma}$ for using OLS, WLS, SUR, and MVR.

Table 4.1: Summary of assumptions for using OLS, WLS, SUR, and MVR

Method	$\mathbf{W}_i$	$\text{Cov}(\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2)$	$\boldsymbol{\Sigma}$
OLS	$= \mathbf{I}_n \forall i \in \{1, 2\}$	$= \mathbf{0}$	$\begin{bmatrix} \sigma_1^2 \mathbf{I}_n & 0 \\ 0 & \sigma_2^2 \mathbf{I}_n \end{bmatrix}$
WLS	$\neq \mathbf{I}_n \forall i \in \{1, 2\}$	$= \mathbf{0}$	$\begin{bmatrix} \sigma_1^2 \mathbf{W}_1 & 0 \\ 0 & \sigma_2^2 \mathbf{W}_2 \end{bmatrix}$
SUR/MVR	$= \mathbf{I}_n \forall i \in \{1, 2\}$	$= \sigma_{12} \mathbf{I}_n$ ($\sigma_{12} = \sigma_{21}$)	$\begin{bmatrix} \sigma_1^2 \mathbf{I}_n & \sigma_{12} \mathbf{I}_n \\ \sigma_{21} \mathbf{I}_n & \sigma_2^2 \mathbf{I}_n \end{bmatrix}$

If correlations exist between the responses and each response surface model has potentially a different set of regressors (*i.e.*, $\mathbf{X}_1 \neq \mathbf{X}_2$), SUR produces more precise estimates than OLS when the variances of responses are constant over the design parameter space (Zellner, 1962; Shah et al., 2004). Similar to OLS, SUR assumes that responses are uncorrelated across observations. That is, ε_{ju} (associated with the u^{th} observation on response j) is not serially correlated to ε_{it} or ε_{jt} , $u \neq t$ so that the off-diagonal elements are zero in $\mathbf{W}_i = \mathbf{I}_n \forall i \in \{1, 2\}$ and $\text{Cov}(\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2)$. SUR has two special cases where its model parameter estimates are identical to the estimates that would be obtained by applying OLS to each individual response. These cases are: (1) no correlations exist between responses (*i.e.*, $\sigma_{12} = \sigma_{21} = 0$), and (2) each response surface model has the same set of regressors (*i.e.*, $\mathbf{X}_s = \mathbf{X}_1 = \mathbf{X}_2$). Instead of using OLS for each response separately with the same set of regressors, MVR can be used in the second case to find the same model parameter estimates while considering the possible correlations between responses and allowing for joint statistical inference under Assumption 4.2.4 (Johnson and Wichern, 2002, pp. 383-398). MVR may yield a large set of regressors; hence, fitted response surface models may involve insignificant regressors, which is a disadvantage of MVR estimator.

When the variances of responses vary by the design parameters (*i.e.*, $\mathbf{W}_i \neq \mathbf{I}_n \forall i \in \{1, 2\}$) and no correlations exist between responses, WLS can be used in separately fitting response surface models. The main idea behind WLS is to gain efficiency by applying OLS to the data "correctly" weighted in a way that less weights are assigned to the observations with larger variances. The main

drawback of WLS is that the resulting estimators may be less efficient than that of OLS when the weights are misspecified. Similar to aforementioned methods, WLS assumes no serial correlation (*i.e.*, the off-diagonal elements in $\mathbf{W}_i$ are zero). OLS regression can be viewed as a special case of WLS regression when $\mathbf{W}_i = \mathbf{I}_n$. Under WLS conditions, it may also be possible to transform the collected data (*i.e.*, log transform) to stabilize variances of responses and then apply OLS instead of using WLS regression. However, it may be difficult to interpret the performance measures in the transformed scale in MRO applications. Finding equivalents of performance measures in the original scale is not straightforward and may lead to additional errors due to back transformation.

In the general case where responses are correlated and their variances vary by design parameters, SUR and generalized least squares (GLS) regression methods can be combined considering particular forms of heteroskedasticity (Mandy and Martins-Filho, 1993; Srivastava and Giles, 1987, pp. 235-254). However, estimation approaches used might not be efficient, especially for small and medium size data. Moreover, further investigation is needed for joint statistical inference (*i.e.*, variance-covariance matrix estimation and construction of confidence and prediction regions of the estimated parameters). For this reason, leaving the consideration of the general case to future research, our approaches consider (i) possible correlations among the responses assuming equal robustness and (ii) unequal robustness assuming no correlations among responses. We discuss the details of incorporating MVR, SUR and WLS regression into our solution procedures in Chapters 5 and 6 where we develop our interactive approaches.

4.3 Optimization

Two questions are addressed in the optimization stage of MRO: “what-to-optimize” and “how-to optimize-it” (Jeong, 2011). Although we conceptually determine “what-to-optimize”, so-called *performance measures*, there are certain conditions under which we cannot easily formulate them to be directly controlled in the optimization due to the limiting assumptions of the utilized regression methods. That is, we cannot answer those two questions as if optimization stage was

independent from empirical model building.

Based upon this, our aim is to conceptually develop our performance measures by motivating their use as well as to interface our interactive optimization procedures with the considered regression methods in this section.

4.3.1 Development of the Performance Measures

Formally defining the *best* solution to an MRO problem is a difficult task, which highly depends on the problem context and the particular DM. In general, specifications play an important role in evaluating the system performance at a given design parameter setting. The common form of specifications are *response targets* (*i.e.*, values or improvement directions) and acceptance limits (*i.e.*, intervals within which the response values are to lie).

Multiple response systems often operate in a conflicting way so that it is typically not possible to simultaneously achieve the response targets or to satisfy the acceptance limits. Moreover, three important statistical properties should be considered in solving MRO problems, which complicates the process of defining and searching the best compromise. Those statistical properties are (1) possible correlations among the responses, (2) quality of response surface models, and (3) robustness of the responses (Jeong, 2011; Costa et al., 2010).

MRO approaches typically seek design parameter settings producing responses close to their respective targets with minimal associated uncertainty. Their performance measures mainly differ with respect to the considered statistical properties as we discuss in Section 2.2.

Our approaches assume that a static target (*i.e.*, response targets are fixed) is specified as a value or an improvement direction (*i.e.*, minimize or maximize) for each response leaving consideration of other forms of specifications to future research. Our main motivation in selecting the performance measures is to consider as many statistical properties as possible while providing the DM with the relevant information on the outcomes of the solutions in a comprehensible way to facilitate the interaction with the DM. To this end, we empower the DM to

consider the distances of estimated response values from their respective targets together with the area of the $100(1 - \alpha)\%$ joint prediction region as performance measures. We take possible correlations among responses into account to the extent allowed by the assumptions of the utilized regression method.

Distance of Response Means to their Respective Targets. Distance-to-target is one of the typical performance measures widely used in the literature and industrial applications (Ribeiro et al., 2000). In evaluating the *location* performance of a solution under consideration, we consider the L_1 -norm of the difference between the estimated expected value of each response and the associated target value as follows:

$$|\hat{y}_i(\mathbf{x}) - t_i|, \quad i \in \{1, 2\} \quad (4.6)$$

where $\hat{y}_i(\mathbf{x}) = \mathbf{f}_i(\mathbf{x})^T \hat{\boldsymbol{\beta}}_i$ is the fitted response surface model for the response i , $\mathbf{x}$ is a $k \times 1$ vector of design parameters, $\mathbf{f}_i(\mathbf{x})$ is the vector of regressors as functions of design parameters in the expanded second order model form given in Eq. (4.1) (*i.e.*, if $k = 2$ and all terms are significant, then $\mathbf{f}_i(\mathbf{x})^T = [1, x_1, x_2, x_1^2, x_2^2, x_1x_2]$), $\hat{\boldsymbol{\beta}}_i$ is the vector of estimated model coefficients, k and t_i denote the number of design parameters and target value for the response i .

100(1 - α)% Joint Prediction Region Area. The three stages of MRO are subject to uncertainty from various sources of errors in the data collection and empirical model building stages. Failure to take these errors into account at the optimization may lead to misleading results and poor design of the product or process of interest. Those error sources include measurement errors (*i.e.*, inaccuracies in measurements due to measurement system), random errors (or intrinsic variation) in response observations due to noise factors (*i.e.*, unknown factors or known but uncontrollable factors), and model uncertainty (*i.e.*, errors in estimating model structure and its parameters). As we mention in Section 4.1, we assume that measurement system is analyzed (*i.e.*, by means of gage repeatability and reproducibility (R&R) or gage calibration studies) and associated errors are minimized prior to data collection stage. Ouyang et al. (2017) state that regardless of how well measurement procedures are designed or maintained, measurement

errors are inevitable. We consider such inevitable errors as part of random errors. Furthermore, we assume that true response surface model structures are selected, they include all appropriate regressor terms, and their assumptions are validated by meaningful statistics. We provide brief discussions and references on validating model assumptions in respective sections of Chapters 5 and 6, where we illustrate each of our approaches under different sets of assumptions.

Even when measurement errors are minimized and the true model structure is selected, there still exists uncertainty associated with model parameters due to estimation errors. Moreover, variances of random errors may differ by design parameter settings. We discuss in Chapter 2 that, to the best of our knowledge, none of the existing interactive MRO approaches appropriately consider the uncertainty due to model parameters and random errors simultaneously. To overcome their deficiencies, we empower the DM to consider the area of the $100(1 - \alpha)\%$ joint prediction region as a measure collectively quantifying the uncertainty due to model parameters and random errors.

To motivate the use of prediction region area, we analyze the *variance of prediction error* assuming a univariate response case. Let $y_i(\mathbf{x})$ be the true response surface model for the response i . We can represent $y_i(\mathbf{x}_0)$, a future observation on response i at a given design parameter setting, $\mathbf{x}_0$, as follows:

$$y_i(\mathbf{x}_0) = \mathbf{f}_i(\mathbf{x}_0)^T \boldsymbol{\beta}_i + \varepsilon_i(\mathbf{x}_0), \quad (4.7)$$

where $\boldsymbol{\beta}_i$ is the vector of true model coefficients and $\varepsilon_i(\mathbf{x}_0)$ is the random error with $\text{Var}[\varepsilon_i(\mathbf{x}_0)] = \sigma_i^2(\mathbf{x}_0)$. The point estimator for $E[y_i(\mathbf{x}_0)]$ is the value of fitted response surface model evaluated at $\mathbf{x}_0$, $\hat{y}_i(\mathbf{x}_0)$, which is also our best estimator for $y_i(\mathbf{x}_0)$. Associated prediction error, $y_i(\mathbf{x}_0) - \hat{y}_i(\mathbf{x}_0)$, is subject to variability due to the two aforementioned uncertainty sources. When this variability is large, the system may not demonstrate the anticipated performance at the selected design parameter setting.

We obtain the variance of the prediction error as

$$\begin{aligned}
\text{Var}[y_i(\mathbf{x}_0) - \hat{y}_i(\mathbf{x}_0)] &= \text{Var}[\mathbf{f}_i(\mathbf{x}_0)^T \boldsymbol{\beta}_i + \varepsilon_i(\mathbf{x}_0) - \hat{y}_i(\mathbf{x}_0)] \\
&= \text{Var}[\varepsilon_i(\mathbf{x}_0)] + \text{Var}[\hat{y}_i(\mathbf{x}_0)] \\
&= \text{Var}[\varepsilon_i(\mathbf{x}_0)] + \text{Var}[\mathbf{f}_i(\mathbf{x}_0)^T \hat{\boldsymbol{\beta}}_i] \\
&= \text{Var}[\varepsilon_i(\mathbf{x}_0)] + \mathbf{f}_i(\mathbf{x}_0)^T \text{Var}(\hat{\boldsymbol{\beta}}_i) \mathbf{f}_i(\mathbf{x}_0),
\end{aligned} \tag{4.8}$$

since $\varepsilon_i(\mathbf{x}_0)$ and $\hat{y}_i(\mathbf{x}_0)$ are independent, *i.e.*, we assume no serial correlation across response observations so that the new observation is independent of the observations used to build the response surface model.

Eq. (4.8) shows that $\text{Var}[y_i(\mathbf{x}_0) - \hat{y}_i(\mathbf{x}_0)]$ has two components representing two different uncertainty sources. The first component, $\text{Var}[\varepsilon_i(\mathbf{x}_0)]$, is associated with the randomness in response observations which can be caused by uncontrollable or unknown factors; that is, it represents robustness performance of the solutions. When it is unequal across design parameter space, it can be included in the optimization as a decision criterion. Otherwise, it is constant over the design parameter space (*i.e.*, $\text{Var}[\varepsilon_i(\mathbf{x}_0)] = \sigma_i^2$) and does not affect the decisions regarding settings of design parameters. Even so, the DM may want to be aware of the variability caused by this source to better understand the uncontrollable consequences of the solutions due to problem nature. The second component, $\text{Var}[\hat{y}_i(\mathbf{x}_0)]$, on the other hand, is a function of design parameters regardless of the behavior of random errors and the regression method used in finding $\hat{\boldsymbol{\beta}}_i$. It is known as *prediction variance* and affected by the design of the optimization experiment conducted at the data collection stage so that it can get larger in certain directions of design parameter space.

We illustrate the behavior of the prediction variance over the CCD, the inner array in Figure 4.1, on a *variance dispersion graph* (VDG) (Giovannitti-Jensen and Myers, 1989) displayed in Figure 4.2. The CCD has eight factorial points, six axial points, and a total of six center points. Under OLS conditions (*i.e.*, $\mathbf{W}_i = \mathbf{I}$), $\text{Var}(\hat{\boldsymbol{\beta}}_i) = \sigma_i^2 (\mathbf{X}_i^T \mathbf{X}_i)^{-1}$ so that $\text{Var}[\hat{y}_i(\mathbf{x})] = \sigma_i^2 \mathbf{f}_i(\mathbf{x})^T (\mathbf{X}_i^T \mathbf{X}_i)^{-1} \mathbf{f}_i(\mathbf{x})$. We plot the prediction variance values divided by σ_i^2 to eliminate the unknown part which is constant over the design parameter space. Figure 4.2 demonstrates that prediction variance increases as the distance from the center of the experimental

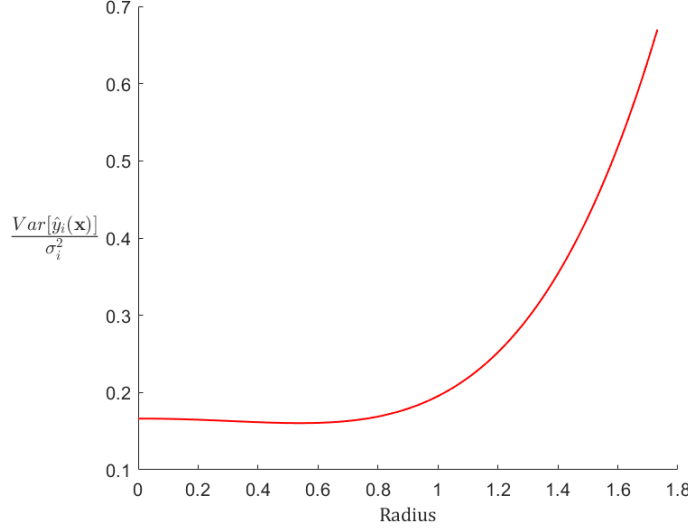


Figure 4.2: Display of $\frac{\text{Var}[\hat{y}_i(\mathbf{x})]}{\sigma_i^2}$ versus the radius of the CCD

region increases. We should note that $\frac{\text{Var}[\hat{y}_i(\mathbf{x})]}{\sigma_i^2}$ is multiplied by n , the number of observations in the design (*i.e.*, the size of the design), to facilitate comparing designs of different sizes, and referred to as *scaled-prediction variance* (SPV) (Montgomery, 2020, pp. 436-437).

Under WLS conditions (*i.e.*, $\mathbf{W}_i \neq \mathbf{I}$), the prediction variance, $\text{Var}[\hat{y}_i(\mathbf{x})]$, is also affected by the behavior of $\mathbf{W}_i$. Let $v_i: \mathbb{R}^{(p_{v_i}+1)} \rightarrow \mathbb{R}_+$ is a nonrandom function, called *skedastic function* (Romano and Wolf, 2017), denoting the known functional form of the heteroskedasticity associated to the i^{th} response, and

$$\begin{aligned} \text{Var}(\boldsymbol{\varepsilon}_i) &= \sigma_i^2 \mathbf{W}_i \\ &= \begin{bmatrix} v_i(\mathbf{X}_{i1}^T) & & & \\ & \ddots & & \\ & & \ddots & \\ & & & v_i(\mathbf{X}_{in}^T) \end{bmatrix} \end{aligned} \quad (4.9)$$

where $\mathbf{X}_{ij}^T$ denotes transpose of the j^{th} row of the design matrix, $\mathbf{X}_i$. Then, $\text{Var}[\hat{\boldsymbol{\beta}}_i] = (\mathbf{X}_i^T \mathbf{W}_i^{-1} \mathbf{X}_i)^{-1}$ so that $\text{Var}[\hat{y}_i(\mathbf{x})] = \mathbf{f}_i(\mathbf{x})^T (\mathbf{X}_i^T \mathbf{W}_i^{-1} \mathbf{X}_i)^{-1} \mathbf{f}_i(\mathbf{x})$.

We observe the behavior of the prediction variance by assuming two different skedastic functions, $v_{i1}(\mathbf{x}) = \exp(3 - x_1^2 - 3x_3^2)$ and $v_{i2}(\mathbf{x}) = \exp(2 + 2x_1^2 - x_3^2)$. As the distance from the center of the experimental region increases, $v_{i1}(\cdot)$ decreases

and $v_{i2}(\cdot)$ increases.

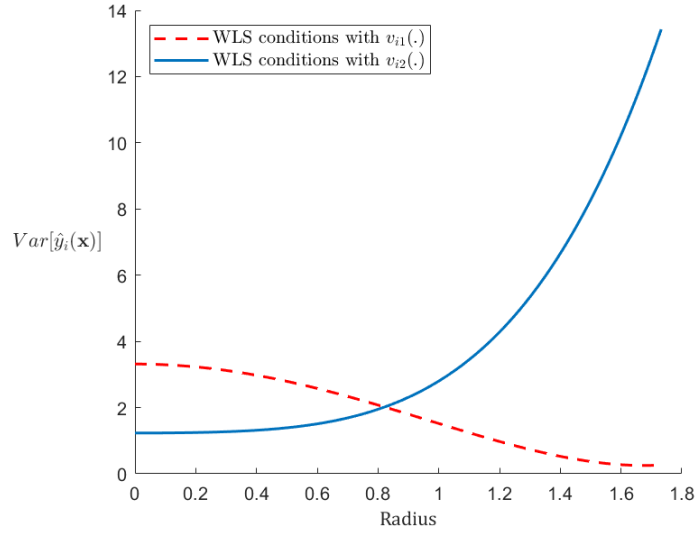


Figure 4.3: Display of $\text{Var}[\hat{y}_i(\mathbf{x})]$ under two different forms of heteroskedasticity versus the radius of the CCD

Figure 4.3 shows that prediction variance may vary over the design parameter space in different manners depending on the form of underlying heteroskedasticity.

The DM may not be aware of the uncertainty associated to the model parameters. S/he should be informed about the fact that the response values presented to her/him are the expected values and subjected to variation due to both model parameters and the random errors. S/he may be interested in more stable settings even if the distances of estimated response values to their respective targets are somewhat larger. Hence, in addition to the mean performance of the responses, we empower the DM to evaluate a solution regarding the associated overall uncertainty. To this end, the variance of the prediction error given in Eq. (4.8)) can be estimated to be included as a decision criterion at the optimization stage. However, when the DM is presented by the variance of the prediction error at a design parameter setting under consideration, s/he may have difficulties in comprehending its consequences, and in expressing her/his preferences. To better interact with the DM, we use prediction region area which is easier to understand for the DM especially when the resulting region is visualized. Prediction region area corresponds to prediction interval length in

the univariate case. Prediction interval length formulation can easily be obtained from prediction interval formulation.

For the future observation on the response i in Eq. (4.7), $100(1 - \alpha)\%$ prediction interval under OLS conditions is

$$\hat{y}_i(\mathbf{x}_0) \pm t_{\alpha/2, n-p_i-1} \sqrt{\hat{\sigma}_i^2 + \hat{\sigma}_i^2 \mathbf{f}_i(\mathbf{x}_0)^T (\mathbf{X}_i^T \mathbf{X}_i)^{-1} \mathbf{f}_i(\mathbf{x}_0)} \quad (4.10)$$

since we assume $\boldsymbol{\varepsilon}_i \sim \mathcal{N}(\mathbf{0}, \sigma_i^2 \mathbf{I})$.

Under WLS conditions with known skedastic function, we derive the $100(1 - \alpha)\%$ prediction interval as follows:

$$\hat{y}_i(\mathbf{x}_0) \pm t_{\alpha/2, n-p_i-1} \sqrt{\hat{\sigma}_i^2 v_i(\mathbf{x}_0) + \hat{\sigma}_i^2 \mathbf{f}_i(\mathbf{x}_0)^T (\mathbf{X}_i^T \mathbf{W}_i^{-1} \mathbf{X}_i)^{-1} \mathbf{f}_i(\mathbf{x}_0)}. \quad (4.11)$$

We give the derivation of Eq. (4.11) in Appendix C.

The main difficulty in the case when WLS conditions apply is that skedastic function is typically unknown and required to be estimated. It should be noted that if an estimator for skedastic function is used, then the underlying statistic may no longer follow a t -distribution. That is, the prediction interval in Eq. (4.11) may be misleading.

The prediction interval formulations in Eqs. (4.10) and (4.11) show that the variance of the prediction error defines the length of the associated prediction interval. Consequently, minimizing the prediction interval length and minimizing the variance of the prediction error result in same solution in the optimization. It can be shown that this property also applies for the two response case, where we are interested in $100(1 - \alpha)\%$ *joint* prediction region that can be constructed either as an ellipse or as a rectangle regarding the assumptions of the utilized empirical model building method. Those assumptions may also affect whether a closed form expression is available for the prediction region area or not.

4.3.2 Overview of the Developed Approaches

Although prior MRO approaches are conceptually easy to understand, it may be difficult for the DM to specify all the required preference information in advance, since it has a complex structure dependent on the particular problem context (Keeney and Raiffa, 1976). On the contrary to prior approaches, we give the DM the opportunity to learn both her/his preferences and the problem characteristics through our interactive solution procedures so that s/he can better understand and develop her/his preferences as the interactions progressed. Fig. 4.4 shows the shared framework of our approaches.

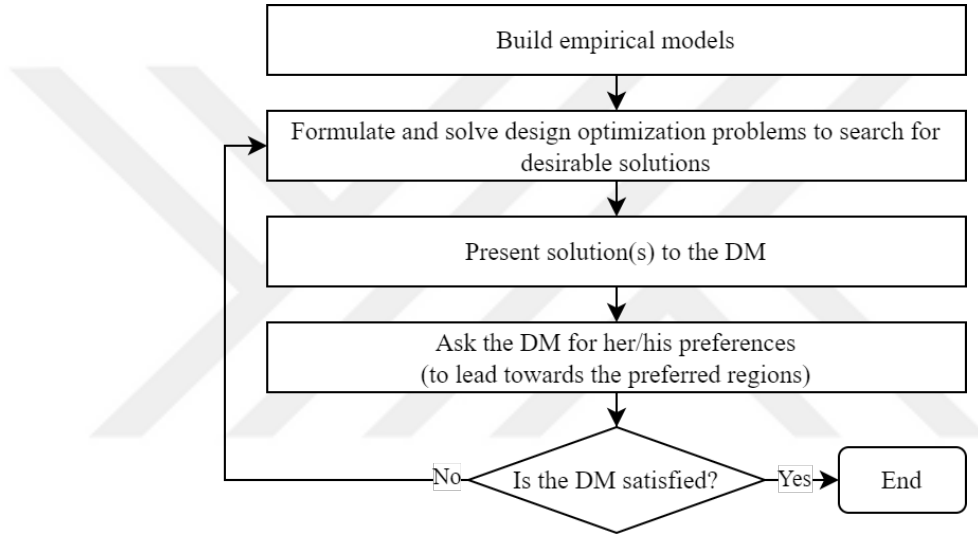


Figure 4.4: Overview of our interactive solution procedures

Both of the developed approaches empower the DM to consider the distances of estimated response values from their target values together with the area of the joint prediction region as performance measures. To facilitate the interaction with the DM, we produce visual aids on performance measures such as joint confidence and prediction regions of the responses at design parameter settings under consideration. At each interaction iteration, DA converts DM's verbal preferences into mathematical expressions and continues searching the solution space. The procedure continues until the DM is satisfied.

None of the regression methods reviewed in Section 4.2 can efficiently model the general case where possible correlations exist among the responses and variances

of random errors are not constant over the experimental region. Consequently, along with DM's preferences and model parameter uncertainty, our approaches can consider either (i) possible correlations among the responses assuming equal robustness or (ii) unequal robustness assuming no correlations among responses.

Main differences between our two approaches arise from the differences in the empirical model building. The first is for the case when the area of the joint prediction region is available as a closed-form function of design parameters, and the second is for the case when it can only be numerically estimated at given design parameter settings. The latter complicates the process of navigating towards desirable solutions. Figure 4.5 schematically shows how the assumptions of utilized regression methods determine which of our approaches to incorporate regarding the problem characteristics.

Built upon Özateş (2015), in the first approach, we fit response surface models by using multivariate regression (MVR) or OLS regression under equal robustness and weighted least squares (WLS) regression under unequal robustness. Closed-form functions for confidence and prediction regions are exactly known for MVR and OLS regressions, while they can be approximated for WLS regression (Romano and Wolf, 2017; Wooldridge, 2016, pp. 264-265). Therefore, we use a closed-form function of prediction region area directly as an objective or a constraint in our mathematical models and visualize the resulting region.

However, as discussed in Section 4.2, none of MVR and OLS regression is appropriate when response surface models contain different set of regressors with the existence of correlations among responses. To consider such cases, we build empirical models by using seemingly unrelated regression (SUR) under equal robustness. Since the exact distribution of the SUR estimator, derived by Phillips (1985), is complicated, it cannot be accommodated in easily formed inferential methods (Riggs et al., 2016). For that reason, we use bootstrapping, a computer-intensive technique, in constructing confidence and prediction regions at a given design parameter setting. To the best of our knowledge, there is no readily available multivariate bootstrap procedure for building confidence region for response means and prediction region for future response observations in SUR

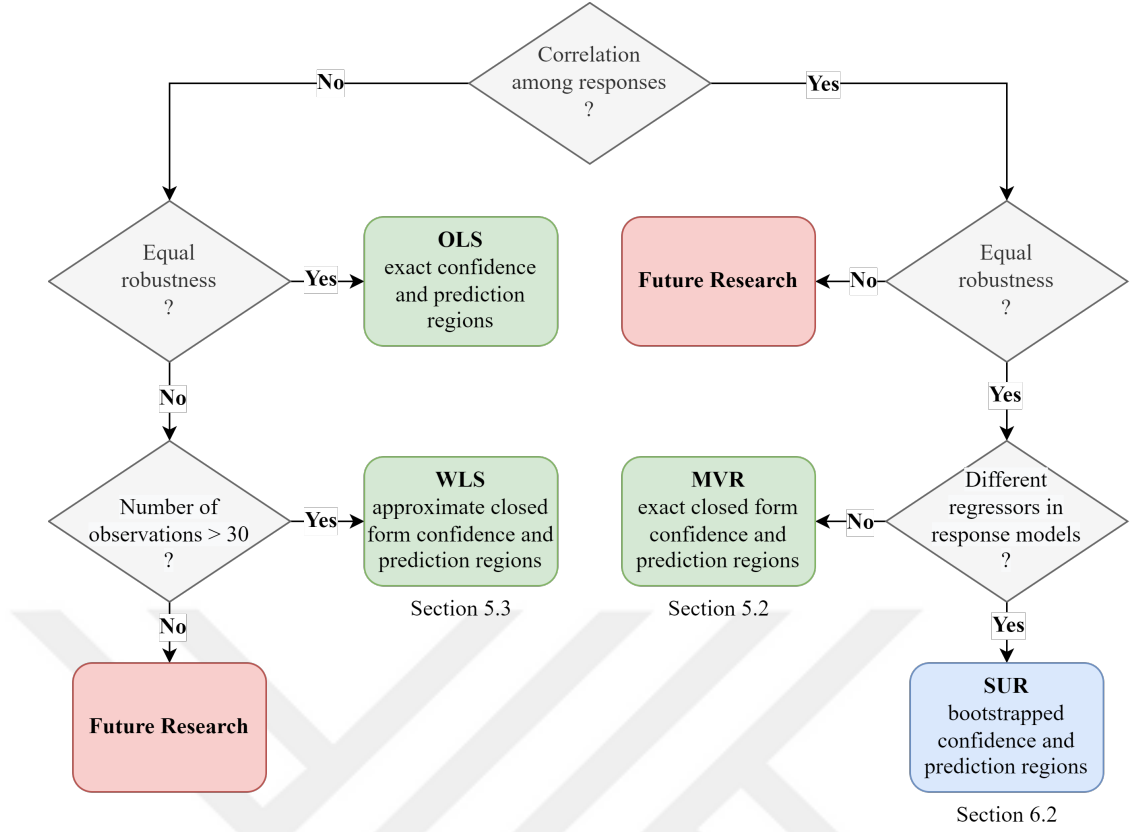


Figure 4.5: Mapping between the developed approaches and the utilized regression methods regarding problem characteristics: The sections of the thesis devoted to the development and illustration of the developed approaches are indicated under the associated green/blue colored cases.

estimation. We adapt a multiparameter approach described by Davidson and Hinkley (1997, pp. 231-233) and the residuals bootstrap (Freedman, 1981) in developing a bootstrapping procedure.

Therefore, in the second approach, we use proxy functions of the joint confidence and/or prediction region area in our mathematical models, while we present values calculated as a result of the associated bootstrapping procedure at the design parameter setting under consideration in interacting with the DM. Although some general knowledge about the effects of changing proxy measures on the prediction region area exists, the exact magnitudes of those effects are not known since they are determined by complex problem characteristics. For this reason, the search process differs from the first approach in that we actively involve

the DA in the search process to help the DM to converge to her/his preferred solutions quickly. At each interaction iteration, using proxy functions, the DA converts the DM's verbal preferences into mathematical expressions that have the potential to lead the search toward regions containing solutions desirable to the DM. The DA identifies the solutions that may be attractive and presents several of them to the DM. The procedure continues until the DM is satisfied.

We illustrate the developed approaches on polymer experiment for the aforementioned two cases: *(i)* possible correlations among the responses assuming equal robustness or *(ii)* unequal robustness assuming no correlations among responses. We consider OLS conditions as a special case of the conditions for WLS with approximate closed-form confidence and prediction intervals; hence, we discuss without illustration in Section 5.2.

Nonlinearity of Mathematical Models. We mention in Section 4.2 that the relationships between responses of interest and relevant design parameters are typically nonlinear in design parameters. That being said, our mathematical models are mostly nonlinear since we consider such relationship functions as objectives and/or constraints in the interactive optimization. To solve those problems, we use BARON (Tawarmalani and Sahinidis, 2005) global optimization solver under MATLAB. Under mild assumptions, BARON guarantees to find the global optimal solution.

In our study, BARON terminated with the global optimal solution in most of the cases. In some rare cases, it did not guarantee global optimality and terminated with "Problem is numerically sensitive" message. It is noted in the BARON users manual that the best possible solution reported on the objective is likely to be correct in such cases.

CHAPTER 5

THE APPROACH UNDER CLOSED-FORM EXPRESSIONS OF CONFIDENCE AND PREDICTION REGIONS

In this chapter, we develop an approach considering the case when a closed form expression is available for the area of $100(1 - \alpha)\%$ joint prediction. We build our approach upon Özateş (2015)'s interactive approach that addresses two-response product and process design optimization problems. Özateş (2015) is the first to consider model parameter uncertainty under unequal robustness and possible correlations among responses through an interactive solution procedure. However, rough estimates are used in constructing performance measures, which may lead to unrealistic solutions in practice. Specifically, MVR is used in building response surface models although unequal robustness is assumed. We extend Özateş (2015) mainly in that we eliminate the contradiction in empirical model building. We separately consider two problem cases, namely, equal robustness and unequal robustness. We use MVR or OLS regression under equal robustness and WLS regression under unequal robustness instead of using MVR for both cases. We incorporate methods from econometrics literature to construct the prediction region under WLS conditions. In addition to the $100(1 - \alpha)\%$ joint prediction region area, we include the lengths of associated *simultaneous* prediction intervals securing the joint confidence level as decision criteria in the optimization to allow the DM to assess dispersion performance of the responses individually.

We develop the general formulation of our approach in Section 5.1. Then, we formulate the performance measures and illustrate our approach under two different sets of assumptions in Sections 5.2 and 5.3.

5.1 Development of the Method

We express the two response design optimization problem as the following MOO program:

$$\begin{aligned}
\text{Min } z_1(\mathbf{x}) &= |\hat{y}_1(\mathbf{x}) - t_1| \\
\text{Min } z_2(\mathbf{x}) &= |\hat{y}_2(\mathbf{x}) - t_2| \\
\text{Min } z_3(\mathbf{x}) &= A(\mathbf{x}) \\
\text{Min } z_4(\mathbf{x}) &= l_1(\mathbf{x}) \\
\text{Min } z_5(\mathbf{x}) &= l_2(\mathbf{x}) \\
&\text{subject to} \\
&\mathbf{x} \in \Omega
\end{aligned} \tag{5.1}$$

where $\hat{y}_i(\mathbf{x})$ is the fitted response surface model for the response i , $A(\mathbf{x})$ denotes the closed form function of the $100(1 - \alpha)\%$ joint prediction region area, and $l_i(\mathbf{x})$ is the length of the $100(1 - \alpha)\%$ *simultaneous* prediction interval for response i (*i.e.*, projection of the prediction region onto the coordinate axis for response i) securing the joint confidence level, $\mathbf{x}$ is the vector of design parameters, t_i is the target value for response i , z_j is the j^{th} objective function bounded over Ω , $i \in \{1, 2\}$, $j \in \{1, 2, \dots, 5\}$, and Ω is the experimental region.

Our interactive solution approach to Eq. (5.1) is based on some concepts of STEP method (STEM) (Benayoun et al., 1971), one of the first interactive approaches originally designed for linear MOO problems. STEM is an algorithm iteratively restricting the feasible region based on the DM's preferences in a manner that the restrictions cannot be withdrawn. Our approach, on the other hand, is rather a learning oriented search procedure enabling the DM to explore the solution space. We use the ideas from STEM due to two main reasons: (1) It is one of those approaches that can reach any nondominated point as it minimizes a weighted Tchebycheff function (a special "achievement scalarizing function") and (2) it requires preference information from a DM that is cognitively easy to provide.

We initialize our solution procedure by finding the ideal objective vector ($\mathbf{z}^*$), the nadir objective vector ($\mathbf{z}^{\text{nad}}$), and the associated weighting vector ($\mathbf{w}$). For

this purpose, we construct a *payoff table*, $\mathbf{Q}$, of the following form,

$$\mathbf{P} = \begin{bmatrix} z_1^* & z_{12} & \dots & z_{15} \\ z_{21} & z_2^* & \dots & z_{25} \\ \vdots & \vdots & \ddots & \vdots \\ z_{51} & z_{52} & \dots & z_5^* \end{bmatrix} \quad (5.2)$$

where the rows denote *criterion vectors* resulting from individually minimizing each of the objectives. We formulate the problem of minimizing the j^{th} objective as the following *lexicographic program*:

$$\begin{aligned} & \text{lex min } \{z_j(\mathbf{x}), \mathbf{1}^T \mathbf{z}(\mathbf{x})\} \\ & \text{subject to} \\ & \mathbf{x} \in \Omega \end{aligned} \quad (5.3)$$

where $\mathbf{1}^T$ is the sum vector of ones. This model first minimizes the j^{th} objective function and then minimizes the sum of the objectives while keeping the j^{th} objective at its minimum value.

Eq. (5.3) ensures that the rows of the payoff table in Eq. (5.2) are nondominated criterion vectors. If the first stage optimization, $\min \{z_j(\mathbf{x}) \mid \mathbf{x} \in \Omega\}$, yields $\mathbf{S}_j$, the set of criterion vectors with the minimal value of the j^{th} objective, with $|\mathbf{S}_j| > 1$, then the second stage optimization, $\min \{\mathbf{1}^T \mathbf{z}(\mathbf{x}) \mid \mathbf{z}(\mathbf{x}) \in \mathbf{S}_j\}$, eliminates weakly nondominated but dominated points and returns a unique nondominated criterion vector. We solve Eq. (5.3) $\forall j \in \{1, 2, \dots, 5\}$ to find the rows of the payoff table.

The ideal objective vector consists of the main diagonal elements of the payoff table which are the optimal values separately reached in each criterion. We estimate the nadir objective vector by choosing the maximum element in each column of the payoff table (Benayoun et al., 1971). Using the ideal and nadir objective vectors, we calculate the weights suggested by Vanderpooten and Vincke (1989) as follows:

$$w_j = \frac{\rho_j}{\sum_{u=1}^5 \rho_u}, \quad \forall j \in \{1, 2, \dots, 5\} \quad (5.4)$$

where

$$\rho_j = \frac{z_j^{\text{nad}} - z_j^*}{\max(|z_j^{\text{nad}}|, |z_j^*|)}, \quad \forall j \in \{1, 2, \dots, 5\}. \quad (5.5)$$

We should note that finding the true nadir objective vector requires information about the entire set of nondominated points, which is not trivial to generate when we have more than two objectives. The nadir objective vector estimated from the payoff table may be an underestimation (overestimation) of the true nadir objective vector when all objectives are to be minimized (maximized) if weakly nondominated but dominated solutions are prevented in finding the payoff table (Korhonen et al., 1997). The resulting errors affect the estimated ranges of the criterion values, and correspondingly the weights. The good news is that the weights are not of outstanding importance in our solution procedure since we do not use them in assessing how the objectives trade off against one another. Their only role is to bring all objective functions into a similar scale such that larger weights are assigned to the objectives farther from their ideal objective vector components.

We employ the *weighted Tchebycheff metric* in measuring the distance of any feasible criterion vector to the ideal objective vector. The following formulation returns the solution closest to the ideal objective vector according to the weighted Tchebycheff distance,

$$\begin{aligned} \min \quad & \max_{j \in \{1, \dots, 5\}} [w_j(z_j(\mathbf{x}) - z_j^*)] \\ \text{subject to} \quad & \\ & \mathbf{x} \in \Omega. \end{aligned} \quad (5.6)$$

To manipulate the minimax objective function we formulate Eq. (5.6) as the following *weighted Tchebycheff program*,

$$\begin{aligned} \min \quad & \alpha \\ \text{subject to} \quad & \\ & \alpha \geq w_j(z_j(\mathbf{x}) - z_j^*) \quad \forall j \in \{1, \dots, 5\} \\ & \mathbf{x} \in \Omega. \end{aligned} \quad (5.7)$$

where $\alpha \in \mathbb{R}$.

We mention in Section 4.2 that the response surface models are mostly nonlinear functions of relevant design parameters. Consequently, unsupported nondominated criterion vectors are likely to occur. Eq. (5.7) is vulnerable to ending up with such vectors. It produces weakly nondominated criterion vectors which may involve some dominated criterion vectors. To overcome this issue and to ensure that the DM is presented by nondominated criterion vectors throughout the solution procedure, we solve *lexicographic weighted Tchebycheff program* (Steuer and Choo, 1983) formulated as

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*)\} \\
& \text{subject to} \\
& \alpha \geq w_j(z_j(\mathbf{x}) - z_j^*) \quad \forall j \in \{1, \dots, 5\} \\
& \mathbf{x} \in \Omega.
\end{aligned} \tag{5.8}$$

Similar to the model in Eq. (5.3), if the optimal solution to first stage optimization, $\min \{\alpha \in \mathbb{R} \mid \alpha \geq w_j(z_j(\mathbf{x}) - z_j^*) \quad \forall j \in \{1, \dots, 5\}, \mathbf{x} \in \Omega\}$, is α^* and there are alternative optimal solutions producing α^* , then the second stage optimization, $\min \{\mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*) \mid \alpha \leq \alpha^*\}$, eliminates weakly nondominated but dominated points and returns a unique nondominated criterion vector.

We start interacting with the DM by presenting the solution of Eq. (5.8). We use the visual aids displayed in Figure 5.1 to help the DM understand the consequences of selecting the design parameter setting ($\mathbf{x}_0$) under consideration and better express her/his preferences. The forms of the joint confidence and prediction regions differ based on the estimation procedure used in building response surface models. MVR produces elliptical regions, while WLS (or OLS) regression results in rectangular Bonferroni regions.

There are also some interactive stochastic programming-based MOO approaches, in domains such as public debt management (Balibek and Köksalan, 2012) and portfolio optimization (Köksalan and Şakar, 2016), that utilize joint confidence regions to provide the DM with information regarding the uncertainty associated with the considered solutions. Unlike our joint prediction region visualizations, these methods find simultaneous confidence intervals and project them onto individual objective axes when presenting them to the DM mainly due to considering

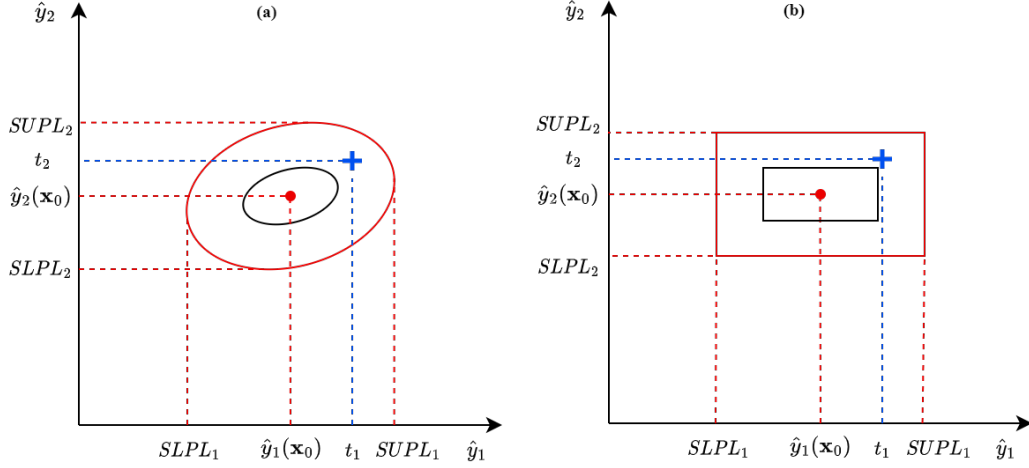


Figure 5.1: Visualization of performance measures at a given design parameter setting, $(\mathbf{x}_0)$: The outer red ellipse (or outer red rectangle) denotes $100(1 - \alpha)\%$ joint prediction region. $SUPL_i$ and $SLPL_i$ are the simultaneous upper and lower prediction limits for the i^{th} response, respectively. The inner black ellipse (or inner black rectangle) denotes $100(1 - \alpha)\%$ joint confidence region. Plus sign marker denotes the target.

more than two objectives. Besides, they construct joint confidence regions by relying on large sample theory to relax Assumption 4.2.4, while we allow finite sample inference.

Adapting the classification idea of STEM, we assume that the DM can indicate the objectives that need further improvement and the ones on which s/he agrees to make a concession. We inform the DM about the fact that it is not possible to improve all objectives simultaneously at a nondominated criterion vector; that is, it is inevitable to sacrifice from at least one other objective to improve any objective.

Let $\mathbf{J}^h$ be the index set of objective values to be improved at h^{th} interaction iteration and Δ_j^h is the amount of relaxation from the current value of the j^{th}

objective $\forall j \notin \mathbf{J}^h$. Then, we update the formulation in Eq. (5.8) as follows,

$$\text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*)\} \quad (5.9a)$$

subject to

$$\alpha \geq w_j(z_j(\mathbf{x}) - z_j^*) \quad \forall j \in \mathbf{J}^h \quad (5.9b)$$

$$z_j(\mathbf{x}^h) + \Delta_j^h \geq z_j(\mathbf{x}) \quad \forall j \notin \mathbf{J}^h \quad (5.9c)$$

$$z_j(\mathbf{x}^h) \geq z_j(\mathbf{x}) \quad \forall j \in \mathbf{J}^h \quad (5.9d)$$

$$\mathbf{x} \in \Omega.$$

At each interaction iteration h , we ask the DM to indicate the objectives that s/he wants to improve, the objectives s/he is willing to relax, and the relaxation amounts. If s/he has difficulty in specifying the relaxation amounts, the DA supports the DM by performing extra search steps in between interaction iterations. We ensure that the objectives in set $\mathbf{J}^h$ do not get worse by adding the constraints in Eq. (5.9d). If an objective j is not in $\mathbf{J}^h$ and the DM does not allow it to be relaxed, then we set $\Delta_j^h = 0$. The procedure continues until the DM is satisfied with the current solution.

Discussions. In MRO problems, the aim is not only to determine the optimal design parameter levels but also to understand the system characteristics. In line with this aim, we do not suggest an algorithm converging within a certain number of steps under some assumptions about the DM's possible preference statements. We rather suggest a search procedure throughout which the DM can learn the system characteristics and learn more about her/his preferences better in conjunction with the available solutions. We do not assume any underlying value function. The convergence of our procedure highly depends on the problem and the preferences of the DM. Unlike STEM, our procedure permits the DM to change her/his mind and to return to a solution previously evaluated to see what would happen if s/he indicated a different set of objectives to be improved/relaxed with different relaxation amounts. We believe that the DM explores the solution space and learns the desirable regions better in time so that the time to reach a satisfactory solution is reasonable.

The MRO problem under consideration may not always produce a satisfactory

solution under the current set-up due to its nature. Consequently, the procedure may stop because the DM is not willing to sacrifice from any of the objective function values although s/he still finds some of the objective values unacceptable or s/he is not satisfied with any of the objective values. We believe that our procedure helps the DM to discover the limitations of the system of interest and justify further efforts such as tolerance design or technological advancements.

In some cases, the DM may have difficulties in predicting the outcomes of her/his choices on the objectives to be relaxed as well as that of the amounts of relaxation. Then, the DA can search for solutions that may be desirable to the DM by relaxing different objectives for different relaxation amounts. In selecting the ones to be presented to the DM, the DA can consider the improvement ratio which is where small sacrifices can create sizeable improvements. Based on our experience, we recommend presenting the DM with at most 3 solutions at an interaction iteration since the DM may not handle more information at once. Even if the DM is able to classify the objectives and determine the relaxation amounts, active involvement of the DA in the search process may still be helpful in navigating the search towards desirable regions. This is because, regardless of the amount of improvement, to improve the objectives in $\mathbf{J}^h$ at least one of the constraints given in Eq. (5.9c) becomes binding. That is to say, even if the objectives in $\mathbf{J}^h$ improve by very small amounts, the formulation in Eq. (5.9) worsens at least one of the other objectives up to its bound defined by the associated relaxation amount. However, it may be possible to achieve a desirable improvement without relaxing that objective until its bound, which may be more desirable for the DM. Without further search, those potentially more desirable solutions may remain undiscovered. The DA may play an important role in discovering such regions by performing additional search steps in which the objective selected by DM for relaxation is relaxed by smaller amounts than that indicated by the DM.

Moreover, the DM may sometimes be conservative in her/his sacrifices. To better learn the problem, the DA can perform intermediate search steps further relaxing some of the objectives to see if there are any interesting solutions with better improvement ratios that may be desirable to the DM.

5.2 MVR under Equal Robustness

In this section, we build our formulations on the following assumptions.

Assumption 5.2.1 *Response variances are constant over the experimental region. That is, $\text{Var}(\boldsymbol{\epsilon}_i) = \sigma_i^2 \mathbf{I}_n \quad \forall i \in \{1, 2\}$.*

Assumption 5.2.2 *Each response surface model has the same model form and involves the same set of regressors. That is, $\mathbf{X}_1 = \mathbf{X}_2 = \mathbf{X}$.*

We use MVR in fitting the response surface models. When estimating $\boldsymbol{\beta}$ is concerned, MVR is an equivalent method to OLS regression which is a special case of SUR under Assumption 5.2.2 as proved by Shah et al. (2004). Therefore, Equation (4.5) is reduced to the following formulation:

$$\hat{\boldsymbol{\beta}}_i = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}_i \quad \forall i \in \{1, 2\}. \quad (5.10)$$

With this simplification, we modify the stacked form given in Equation (4.3) as follows,

$$\mathbf{y} = \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad (5.11)$$

where $\mathbf{y} = [\mathbf{y}_1 : \mathbf{y}_2]$ is $n \times 2$ matrix of response observations, $\boldsymbol{\beta} = [\boldsymbol{\beta}_1 : \boldsymbol{\beta}_2]$ is $(p+1) \times 2$ matrix of model coefficients, $\boldsymbol{\epsilon} = [\boldsymbol{\epsilon}_1 : \boldsymbol{\epsilon}_2]$ is $n \times 2$ matrix of random errors, and p is the number of regressors.

We find the estimated values of the responses at a given design parameter setting, $\mathbf{x}_0$, as

$$\hat{\mathbf{y}}(\mathbf{x}_0) = \hat{\boldsymbol{\beta}}^T \mathbf{f}(\mathbf{x}_0) \quad (5.12)$$

where $\hat{\mathbf{y}}(\mathbf{x}_0) = [\hat{y}_1(\mathbf{x}_0), \hat{y}_2(\mathbf{x}_0)]^T$ is a 2×1 vector and $\hat{\boldsymbol{\beta}} = [\hat{\boldsymbol{\beta}}_1 : \hat{\boldsymbol{\beta}}_2]$ is a $(p+1) \times 2$ matrix of estimated model coefficients.

Unlike OLS regression, MVR allows for joint statistical inference considering possible correlations among the responses. Let $\mathbf{S}$ be the variance-covariance matrix of the responses at a given design parameter setting. Then,

$$\mathbf{S} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}. \quad (5.13)$$

We mention in Section 4.2 that we assume that responses are uncorrelated across experimental runs in MRO. Hence, $\mathbf{\Sigma}$ given in Equation (4.4) simplifies to $\mathbf{S} \otimes I_n$ as shown in the last row of Table 4.1.

Under Assumption 4.2.4, $100(1 - \alpha)\%$ joint prediction region at $\mathbf{x}_0$ is formulated as

$$\begin{aligned} & (\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0))^T \left(\frac{n}{n-p-1} \hat{\mathbf{S}} \right)^{-1} (\mathbf{y}(\mathbf{x}_0) - \hat{\boldsymbol{\beta}}^T \mathbf{f}(\mathbf{x}_0)) \\ & \leq \left((1 + \mathbf{f}(\mathbf{x}_0)^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{f}(\mathbf{x}_0)) \left[\frac{2(n-p-1)}{n-p-2} F_{2,n-p-2}(\alpha) \right] \right) \end{aligned} \quad (5.14)$$

where $\mathbf{y}(\mathbf{x}_0) = [y_1(\mathbf{x}_0), y_2(\mathbf{x}_0)]^T$ is a future observation vector at $\mathbf{x}_0$, n is the number of observations, p is the number of regressors, $F_{2,n-p-2}(\alpha)$ is the upper $(100\alpha)^{\text{th}}$ percentile of the F -distribution with $(2, n-p-2)$ degrees of freedom, and $\hat{\mathbf{S}}$ is the maximum likelihood estimator of $\mathbf{S}$ given by,

$$\hat{\mathbf{S}} = \frac{1}{n} \hat{\boldsymbol{\epsilon}}^T \hat{\boldsymbol{\epsilon}} = \frac{1}{n} (\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}})^T (\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}}) \quad (5.15)$$

where $\hat{\boldsymbol{\epsilon}} = [\hat{\boldsymbol{\epsilon}}_1 : \hat{\boldsymbol{\epsilon}}_2]$ is $n \times 2$ matrix of *residuals* (i.e., $\hat{\boldsymbol{\epsilon}}_i = \mathbf{y}_i - \mathbf{X} \hat{\boldsymbol{\beta}}_i \quad \forall i \in \{1, 2\}$) (Johnson and Wichern, 2002, p.390).

The area of the ellipse defined in Eq. (5.14) is formulated as

$$A(\mathbf{x}_0) = \pi \sqrt{\left| \frac{n}{n-p-1} \hat{\mathbf{S}} \right| \left(1 + \mathbf{f}(\mathbf{x}_0)^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{f}(\mathbf{x}_0) \right) \left[\frac{2(n-p-1)}{n-p-2} F_{2,n-p-2}(\alpha) \right]} \quad (5.16)$$

(Johnson and Wichern, 2002, p. 127).

The length of the $100(1 - \alpha)\%$ simultaneous prediction interval for the i^{th} response at $\mathbf{x}_0$ is formulated as

$$l_i(\mathbf{x}_0) = 2 \sqrt{(1 + \mathbf{f}(\mathbf{x}_0)^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{f}(\mathbf{x}_0)) \left(\frac{n}{n-p-1} \hat{\sigma}_i^2 \right) \left[\frac{2(n-p-1)}{n-p-2} F_{2,n-p-2}(\alpha) \right]} \quad (5.17)$$

where $\hat{\sigma}_i^2$ is the i^{th} diagonal element of $\hat{\mathbf{S}}$ and $i \in \{1, 2\}$. We should note that $l_1(\mathbf{x})$ and $l_2(\mathbf{x})$ have parallel gradients; that is, there exists no trade off between

these two performance measures when MVR is used in building the response surface models. Therefore, we exclude them from the mathematical models while we present their values to the DM at interaction iterations in the illustrative example.

Illustrative Example. We illustrate our solution procedure on polymer experiment presented in Appendix A. We assume that the collected data given in Table A.1 satisfies Assumption 5.2.1 and Assumption 5.2.2. However, in practice, those assumptions should be supported by meaningful statistics. For detailed instructions on validating model assumptions, we refer to Johnson and Wichern (2002, pp. 377-383) and Montgomery (2020, pp. 402-407).

We do not assume an underlying value function in illustrating interaction iterations since it does not help to determine the relaxation amounts. Instead, we play the role of the DM without collaborating with a real DM. We present nondominated criterion vectors to the DM throughout the iterations; thus, s/he knows that improving a particular objective is possible only if at least one other objective gets worse.

In this example, we illustrate a case where the DA supports the DM in her/his decisions by performing some additional search steps between interaction iterations. We assume that the DM is more interested in decreasing the distance between second response mean and its target.

Using the experimental data given in Table A.1 consisting of $n = 20$ observations for each of the responses, we fit the response surface models as follows,

$$\begin{aligned}\hat{y}_1(\mathbf{x}) &= 81.09 + 1.03x_1 + 4.04x_2 + 6.21x_3 - 1.84x_1^2 + 2.95x_2^2 \\ &\quad - 5.20x_3^2 + 2.13x_1x_2 + 11.38x_1x_3 - 3.87x_2x_3 \\ \hat{y}_2(\mathbf{x}) &= 59.85 + 3.59x_1 + 0.26x_2 + 2.23x_3 + 0.84x_1^2 + 0.07x_2^2 \\ &\quad + 0.06x_3^2 - 0.39x_1x_2 - 0.04x_1x_3 + 0.31x_2x_3.\end{aligned}\tag{5.18}$$

We assume that the DM decides to set $\alpha = 0.1$. Then, $A(\mathbf{x})$ and $l_i(\mathbf{x}) \forall i \in \{1, 2\}$ are given by Eq. (5.16) and Eq. (5.17) with $\hat{\sigma}_{12} = \hat{\sigma}_{21} = -0.55$, $\hat{\sigma}_1^2 = 11.12$, $\hat{\sigma}_2^2 = 1.55$, $p = 9$, and $F_{2,9}(0.1) = 3.01$. The objectives are $z_1(\mathbf{x}) = |\hat{y}_1(\mathbf{x}) - 100|$,

$z_2(\mathbf{x}) = |\hat{y}_2(\mathbf{x}) - 57.5|$, and $z_3(\mathbf{x}) = A(\mathbf{x})$.

We initialize the interactive optimization procedure by finding the ideal objective vector, nadir objective vector, and the weighting coefficients, respectively, as $\mathbf{z}^* = [0.00 \ 0.00 \ 200.50]^T$, $\mathbf{z}^{\text{nad}} = [18.57 \ 7.17 \ 307.56]^T$, and $\mathbf{w} = [0.43 \ 0.43 \ 0.15]^T$.

The DA sets $h = 0$ and $\mathbf{J}^0 = \{1, 2, 3\}$. Then s/he solves the following problem,

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& \alpha \geq 0.43(z_1(\mathbf{x}) - 0.00) \\
& \alpha \geq 0.43(z_2(\mathbf{x}) - 0.00) \\
& \alpha \geq 0.15(z_3(\mathbf{x}) - 200.50) \\
& 1.68 \geq x_k \geq -1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{5.19}$$

Table 5.1: Numerical results at $h = 0$

$\hat{y}_1(\mathbf{x}^0)$	$ \hat{y}_1(\mathbf{x}^0) - t_1 $	$\hat{y}_2(\mathbf{x}^0)$	$ \hat{y}_2(\mathbf{x}^0) - t_2 $	$A(\mathbf{x}^0)$	$\text{SPI}_1(\mathbf{x}^0)$	$\ell_1(\mathbf{x}^0)$	$\text{SPI}_2(\mathbf{x}^0)$	$\ell_2(\mathbf{x}^0)$
92.66	7.34	63.91	6.41	221.60	[78.85, 106.46]	27.61	[58.76, 69.07]	10.31

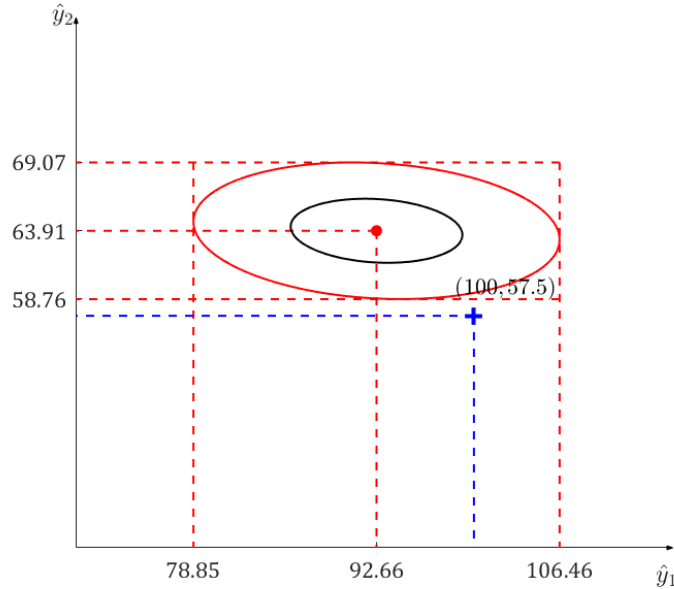


Figure 5.2: Visualization of the solution at $h = 0$

Regarding the visualization in Figure 5.2 and the numerical results in Table 5.1, the DM states that s/he finds the value of $z_2(\mathbf{x}^0)$ unacceptable. S/he wants to improve $z_2(\mathbf{x}^0)$ without sacrificing from $z_3(\mathbf{x}^0)$ and emphasizes that the uncertainty associated with the current solution is already high. S/he is even happier if $z_3(\mathbf{x}^0)$ improves together with $z_2(\mathbf{x}^0)$. S/he is ready to sacrifice from $z_1(\mathbf{x}^0)$ by 2 units. Then, considering the preferences of the DM, the DA sets $h = 1$, $\mathbf{J}^1 = \{2, 3\}$ and updates Eq. (5.19) as follows,

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& \alpha \geq 0.43(z_2(\mathbf{x}) - 0.00) \\
& \alpha \geq 0.15(z_3(\mathbf{x}) - 200.05) \\
& z_1(\mathbf{x}^0) + \Delta_1^1 \geq z_1(\mathbf{x}) \\
& z_j(\mathbf{x}^0) \geq z_j(\mathbf{x}) \quad \forall j \in \mathbf{J}^1 \\
& 1.68 \geq x_k \geq -1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{5.20}$$

The DA searches the solution space by solving Eq. (5.20) for $\Delta_1^1 \in \{1, 2, 3, 4, 5, 6\}$ to explore the solutions for relaxation of less than and greater than 2 units. S/he observes that $z_2(\mathbf{x}^0)$ improves in a decreasing manner for $\Delta_1^1 > 2$ as displayed in Figure 5.3.

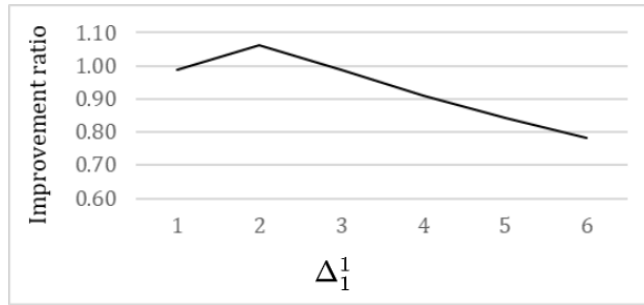


Figure 5.3: Effect of increasing Δ_1^1 on the improvement in $z_2(\mathbf{x}^0)$, where improvement ratio denotes $\frac{z_2(\mathbf{x}^0) - z_2(\mathbf{x}^1)}{\Delta_1^1}$

Figure 5.3 shows that $\frac{z_2(\mathbf{x}^0) - z_2(\mathbf{x}^1)}{\Delta_1^1} < 1$ for $\Delta_1^1 > 3$. Thus, in addition to the solution obtained when $\Delta_1^1 = 2$, the DA decides to present the DM with the solution for $\Delta_1^1 = 3$ at $h = 1$. We should note that the DA does not present

Figure 5.3 to the DM.

Table 5.2: Numerical results at $h = 1$ for $\Delta_1^1 = 2$

$\hat{y}_1(\mathbf{x}^1)$	$ \hat{y}_1(\mathbf{x}^1) - t_1 $	$\hat{y}_2(\mathbf{x}^1)$	$ \hat{y}_2(\mathbf{x}^1) - t_2 $	$A(\mathbf{x}^1)$	$\text{SPI}_1(\mathbf{x}^1)$	$\ell_1(\mathbf{x}^1)$	$\text{SPI}_2(\mathbf{x}^1)$	$\ell_2(\mathbf{x}^1)$
90.66	9.34	61.79	4.29	212.82	[77.13, 104.18]	27.06	[56.74, 66.84]	10.10

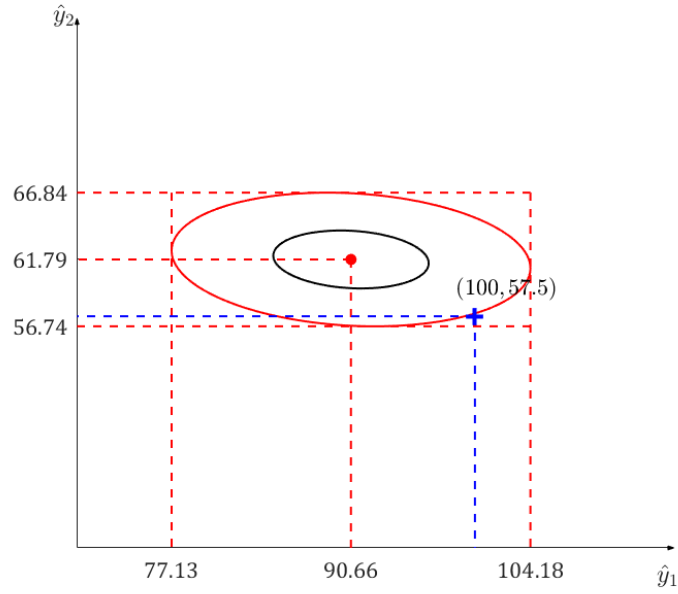


Figure 5.4: Visualization of the solution at $h = 1$ for $\Delta_1^1 = 2$

Table 5.3: Numerical results at $h = 1$ for $\Delta_1^1 = 3$

$\hat{y}_1(\mathbf{x}^1)$	$ \hat{y}_1(\mathbf{x}^1) - t_1 $	$\hat{y}_2(\mathbf{x}^1)$	$ \hat{y}_2(\mathbf{x}^1) - t_2 $	$A(\mathbf{x}^1)$	$\text{SPI}_1(\mathbf{x}^1)$	$\ell_1(\mathbf{x}^1)$	$\text{SPI}_2(\mathbf{x}^1)$	$\ell_2(\mathbf{x}^1)$
89.66	10.34	60.95	3.45	210.40	[76.20, 103.11]	26.90	[55.92, 65.97]	10.04

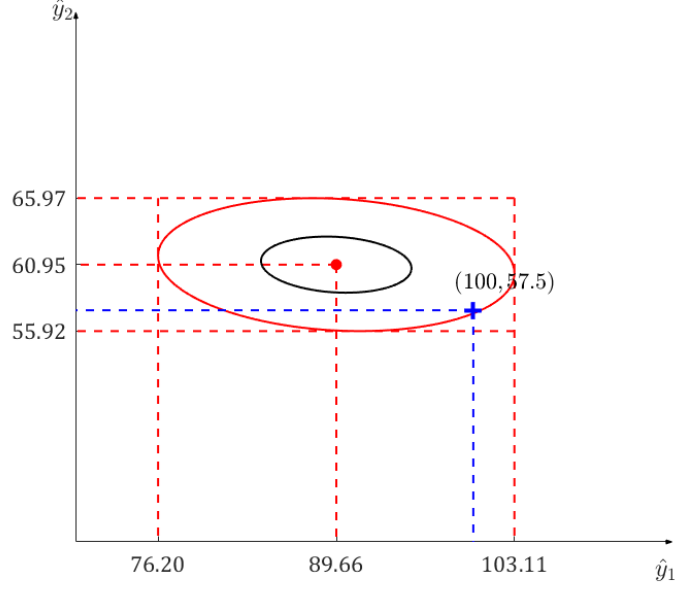


Figure 5.5: Visualization of the solution at $h = 1$ for $\Delta_1^1 = 3$

Given the visualizations in Figures 5.4 and 5.5 and the numerical results in Tables 5.2 and 5.3, the DM states that the value of $z_2(\mathbf{x}^1)$ is still unacceptable and s/he wants to further improve it. At this point, we assume that the DA explains the DM that if $z_1(\mathbf{x}^1)$ is relaxed, then the amount of improvement in $z_2(\mathbf{x}^1)$ will be less than the amount of sacrifice from $z_1(\mathbf{x}^1)$. Based on this information, the DM decides to relax $A(\mathbf{x}^1)$. S/he allows $z_3(\mathbf{x}^1)$ to be as poor as $z_3(\mathbf{x}^0)$. Then, the DA sets $h = 2$ and updates Eq. (5.20) as follows,

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& \alpha \geq 0.43(z_2(\mathbf{x}) - 0.00) \\
& z_1(\mathbf{x}^1) + \Delta_1^2 \geq z_1(\mathbf{x}) \\
& z_3(\mathbf{x}^1) + \Delta_3^2 \geq z_3(\mathbf{x}) \\
& z_j(\mathbf{x}^1) \geq z_j(\mathbf{x}) \quad \forall j \in \mathbf{J}^2 \\
& 1.68 \geq x_k \geq -1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{5.21}$$

where $\mathbf{J}^2 = \{2\}$ and $\Delta_1^2 = 0$.

Based on the DM's preferences, the DA sets $\Delta_3^2 = z_3(\mathbf{x}^0) - z_3(\mathbf{x}^1)$. In addition, the DA further searches the solution space by solving Eq. (5.21) for several Δ_3^2 values and finds out that $z_2(\mathbf{x}^2)$ is almost at its target when $z_3(\mathbf{x}^1)$ is allowed to increase by 15%. As a result, s/he decides to present the DM with two solutions at $h = 2$ for $\Delta_3^2 \in \{z_3(\mathbf{x}^0) - z_3(\mathbf{x}^1), 0.15z_3(\mathbf{x}^1)\}$.

Table 5.4: Numerical results at $h = 2$ for $\Delta_3^2 = z_3(\mathbf{x}^0) - z_3(\mathbf{x}^1)$

$\hat{y}_1(\mathbf{x}^2)$	$ \hat{y}_1(\mathbf{x}^2) - t_1 $	$\hat{y}_2(\mathbf{x}^2)$	$ \hat{y}_2(\mathbf{x}^2) - t_2 $	$A(\mathbf{x}^2)$	$\text{SPI}_1(\mathbf{x}^2)$	$\ell_1(\mathbf{x}^2)$	$\text{SPI}_2(\mathbf{x}^2)$	$\ell_2(\mathbf{x}^2)$
89.66	10.34	59.07	1.57	221.60	[75.85, 103.46]	27.61	[53.92, 64.22]	10.31

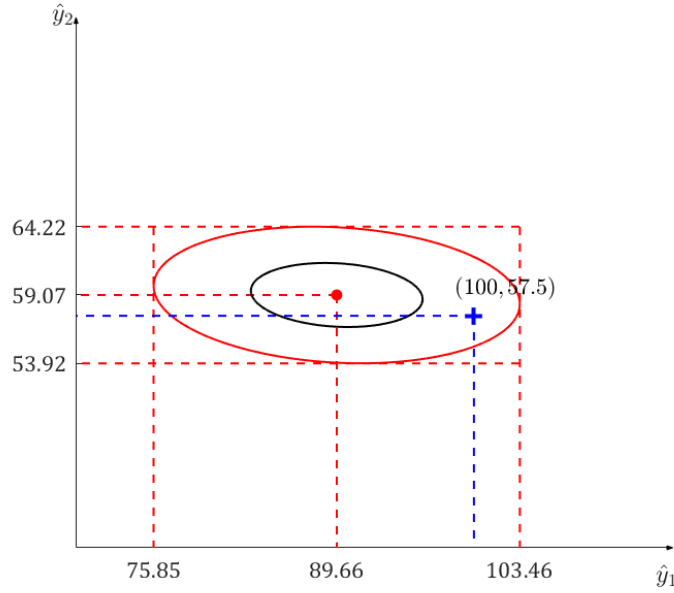


Figure 5.6: Visualization of the solution at $h = 2$ for $\Delta_3^2 = z_3(\mathbf{x}^0) - z_3(\mathbf{x}^1)$

Table 5.5: Numerical results at $h = 2$ for $\Delta_3^2 = 0.15z_3(\mathbf{x}^1)$

$\hat{y}_1(\mathbf{x}^2)$	$ \hat{y}_1(\mathbf{x}^2) - t_1 $	$\hat{y}_2(\mathbf{x}^2)$	$ \hat{y}_2(\mathbf{x}^2) - t_2 $	$A(\mathbf{x}^2)$	$\text{SPI}_1(\mathbf{x}^2)$	$\ell_1(\mathbf{x}^2)$	$\text{SPI}_2(\mathbf{x}^2)$	$\ell_2(\mathbf{x}^2)$
89.66	10.34	57.62	0.12	241.83	[75.23, 104.08]	28.84	[52.24, 63.01]	10.77

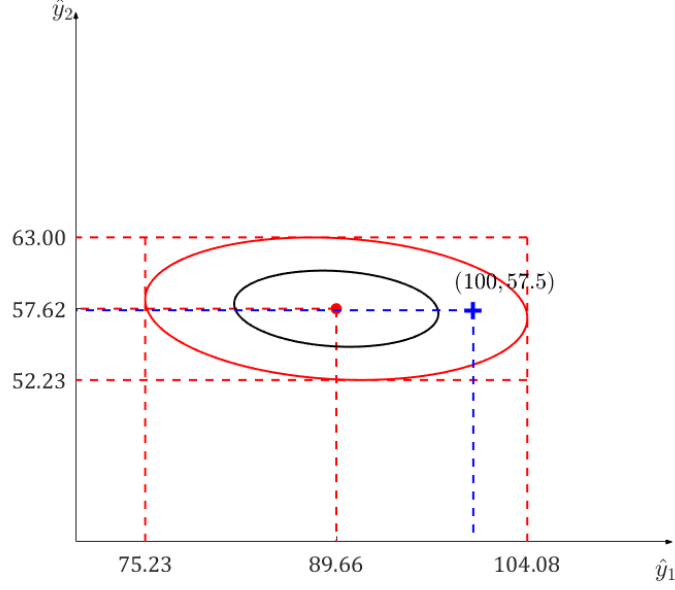


Figure 5.7: Visualization of the solution at $h = 2$ for $\Delta_3^2 = 0.15z_3(\mathbf{x}^1)$

Considering the solutions visualized in Figures 5.6 and 5.7, the DM states that s/he likes the one in Figure 5.7. S/he finds the increase in $l_2(\mathbf{x}^2)$ insignificant in Figure 5.7 since $z_2(\mathbf{x}^2)$ is almost at its target. S/he notes that s/he would prefer smaller prediction interval for $\hat{y}_1(\mathbf{x}^2)$. However, s/he does not want to sacrifice from any of the objectives at this point. Hence, s/he accepts the solution in Figure 5.7.

Although the procedure stops, we may conclude that the DM is not completely satisfied with the predicted outcomes of the selected solution. Such a situation may be encountered when a satisfactory solution does not exist due to the nature of the process influenced by the factors such as technology, methods, and materials used in the process. In such cases, the search procedure can help the DM to discover the difficulty of obtaining satisfactory robust design solutions and justify a tolerance design study.

5.3 WLS Regression with Bonferroni Corrected Approximate t-Intervals under Unequal Robustness

In this section, we build our formulations on the following assumptions while we relax Assumption 5.2.1 and Assumption 5.2.2.

Assumption 5.3.1 *Responses are not correlated. That is, $\sigma_{12} = \sigma_{21} = 0$.*

Assumption 5.3.2 *A nonrandom skedastic function, $v_i: \mathbb{R}^{(p_{v_i}+1)} \rightarrow \mathbb{R}_+$, exists $\forall i \in \{1, 2\}$ and denotes the functional form of the heteroskedasticity associated to the i^{th} response, and*

$$\begin{aligned} \text{Var}(\boldsymbol{\varepsilon}_i) &= \sigma_i^2 \mathbf{W}_i \\ &= \mathbf{V}_i \\ &= \begin{bmatrix} v_i(\mathbf{X}_{i1}^T) & & \\ & \ddots & \\ & & v_i(\mathbf{X}_{in}^T) \end{bmatrix} \end{aligned} \quad (5.22)$$

where $\mathbf{X}_{ij}^T$ denotes transpose of the j^{th} row of $\mathbf{X}_i$.

In the presence of heteroskedasticity in response variances, OLS estimators of model coefficients are still unbiased; yet, they are no longer efficient (*i.e.*, having minimum possible variance), and conventional inference is typically not valid. A remedy to this problem is to use WLS which produces the efficient estimators when the true weights are known. However, the true weights are typically not known in practice. If the weights are poorly estimated due to incorrectly modeling the underlying heteroskedasticity, the resulting WLS estimators may have higher variances than that of OLS estimators. Motivated by this issue, White (1980) promotes retaining OLS estimators with *heteroskedasticity-consistent* (HC) standard errors instead of conventional standard errors. White's HC standard errors ensure valid inference for OLS estimators under heteroskedasticity. On the other hand, Leamer (2010) argues that the heteroskedasticity should be modeled if sensibly reweighting the collected data substantially changes the locations of

the estimates and the widths of the confidence intervals. Agreeing with Leamer (2010), we believe that retaining OLS estimators with HC standard errors is no different than consciously continuing to do the wrong thing because it is possible to measure how much wrongdoing occurred.

In MRO, the performance of the optimization stage can be increased by achieving high precision in estimating the model coefficients and by correctly measuring the associated uncertainty. Thus, we use WLS regression in building response surface models and incorporate HC standard errors to ensure valid inference as suggested by Romano and Wolf (2017). They introduce *adaptive least squares* (ALS) estimator to find the parameters of the response surface models and provide asymptotically valid inference even when the estimated variance model for reweighting the collected data is incorrect. They suggest using WLS regression if heteroskedasticity is significant; otherwise, using OLS regression. The final form of the ALS estimator - OLS or WLS - adapts itself to the collected data. In either case, they suggest using HC standard errors. We utilize their recommendations under Assumption 5.3.2 where WLS regression is utilized with HC standard errors.

We start with estimating the skedastic functions to be used in reweighting the collected data. As recommended by Romano and Wolf (2017), we use the following parametric model,

$$v_i(\mathbf{x}) = e^{\mathbf{g}_i(\mathbf{x})^T \boldsymbol{\theta}_i} \quad (5.23)$$

where $\boldsymbol{\theta} \in \mathbb{R}^{(p_{\boldsymbol{\theta}_i}+1) \times 1}$ is a vector of model coefficients, $\mathbf{g}_i(\mathbf{x})$ is the vector of regressors as functions of design parameters, and $p_{\boldsymbol{\theta}_i}$ is the number of regressors. We assume that Eq. (5.23) nests the case of homoskedasticity (*i.e.*, for every $\sigma_i^2 > 0$ there exists a unique θ_i such that $v_i(\mathbf{x}) \equiv \sigma_i^2 \forall i \in \{1, 2\}$).

To estimate the skedastic functions, we first estimate the model coefficients of Eq. (4.2) by using OLS regression as $\hat{\boldsymbol{\beta}}_{i,ols} = (\mathbf{X}_i^T \mathbf{X}_i)^{-1} \mathbf{X}_i^T \mathbf{y}_i \forall i \in \{1, 2\}$. Then, we estimate $\boldsymbol{\theta}_i$ by the following OLS regression,

$$\log[\bar{\boldsymbol{\varepsilon}}_i] = \mathbf{G}_i \boldsymbol{\theta}_i + \mathbf{u}_i \quad (5.24)$$

where $\bar{\boldsymbol{\varepsilon}}_i$ is an $n \times 1$ vector of modified residuals, $\mathbf{G}_i$ is an $n \times (p_{\boldsymbol{\theta}_i} + 1)$ design matrix specifying values of the regressors as known functions of design parameters such as powers and cross products, $p_{\boldsymbol{\theta}_i}$ denotes the number of regressors, and $\mathbf{u}_i$ is an $n \times 1$ random error vector associated with the i^{th} response. The j^{th} element of $\bar{\boldsymbol{\varepsilon}}_i$ is given by $\bar{\varepsilon}_{ij} = \max(\delta^2, \hat{\varepsilon}_{ij})$ with $\delta^2 > 0$ where $\hat{\varepsilon}_{ij}$ is the j^{th} element of $\hat{\boldsymbol{\varepsilon}}_i = \mathbf{y}_i - \mathbf{X} \hat{\boldsymbol{\beta}}_{i,ols}$.

Romano and Wolf (2017) find the estimated weights for the i^{th} response at a given design parameter setting, $\mathbf{x}_0$, as

$$\hat{v}_i(\mathbf{x}_0) = e^{\mathbf{g}_i(\mathbf{x}_0)^T \hat{\boldsymbol{\theta}}_i} \quad (5.25)$$

which results from the *naive back-transformation* of the estimated values in the log scale. The naive back-transformation is the most commonly used estimator in practice to bring estimated values to the original scale when log models are used in regression. However, the resulting estimator estimates the median of the independent variable. Therefore, the mean is systematically underestimated in the original scale. To decrease such back-transformation errors, we use maximum likelihood (ML) estimator discussed by Shen and Zhu (2008). It is possible to use other estimators demonstrating better performance with respect to bias and/or mean square error (MSE). In this study, our aim is to rather raise awareness on back-transformation errors than search for the best estimator. For further discussions on this issue, we refer to Shen and Zhu (2008).

We reformulate Eq. (5.25) as follows,

$$\hat{v}_i(\mathbf{x}_0) = e^{\left(\mathbf{g}(\mathbf{x}_0)^T \hat{\boldsymbol{\theta}}_i + \frac{\text{RSS}_i}{2n}\right)} \quad (5.26)$$

where $\text{RSS}_i = \bar{\boldsymbol{\varepsilon}}_i^T [\mathbf{I} - \mathbf{G}_i (\mathbf{G}_i^T \mathbf{G}_i)^{-1} \mathbf{G}_i^T] \bar{\boldsymbol{\varepsilon}}_i$.

Let

$$\hat{\mathbf{V}}_i = \begin{bmatrix} \hat{v}_i(\mathbf{X}_{i1}^T) & & \\ & \ddots & \\ & & \hat{v}_i(\mathbf{X}_{in}^T) \end{bmatrix}. \quad (5.27)$$

Considering the form we define for each response surface model in Eq. (4.2), WLS estimator is given by

$$\hat{\boldsymbol{\beta}}_i = (\mathbf{X}_i^T \hat{\mathbf{V}}_i^{-1} \mathbf{X}_i)^{-1} \mathbf{X}_i^T \hat{\mathbf{V}}_i^{-1} \mathbf{y}_i \quad \forall i \in \{1, 2\}. \quad (5.28)$$

The estimated value of the i^{th} response at a given design parameter setting, $\mathbf{x}_0$, is

$$\hat{\mathbf{y}}_i(\mathbf{x}_0) = \hat{\boldsymbol{\beta}}_i^T \mathbf{f}_i(\mathbf{x}_0) \quad \forall i \in \{1, 2\} \quad (5.29)$$

where $\mathbf{f}_i(\mathbf{x}_0)$ is a $(p_i + 1) \times 1$ vector of regressors as functions of design parameters in the expanded form and p_i denotes the number of regressors. Since we build the response surface models separately by Assumption 5.3.1, different set of regressors can be included in the models.

Romano and Wolf (2017) show that the approximate confidence interval for the mean response under Assumption 4.2.4 is formulated as

$$\hat{y}_i(\mathbf{x}_0) \pm t_{n-(p_i+1), 1-\alpha/2} \text{SE}_{\text{HC}}(\hat{\boldsymbol{\beta}}_i) \quad \forall i \in \{1, 2\} \quad (5.30)$$

where $\text{Var}[\hat{y}_i(\mathbf{x}_0)]$ is estimated by $\text{SE}_{\text{HC}}(\hat{\boldsymbol{\beta}}_i)$ denoting heteroskedasticity consistent standard error and $t_{n-(p_i+1), 1-\alpha/2}$ denotes $1 - \alpha/2$ quantile of the t -distribution.

To achieve the overall confidence level of $(1 - \alpha)$, we use Bonferroni simultaneous intervals (Johnson and Wichern, 2002, pp. 232-234). We change $t_{n-(p_i+1), 1-\alpha/2}$ into $t_{n-(p_i+1), 1-\alpha/4}$ since we consider two responses.

We mention in Section 4.3.1 that prediction interval is derived from variance of prediction error which consists of two components representing two different uncertainty sources and give the formulation for the case when WLS regression

is utilized with known skedastic function in Eq. (4.11). Wooldridge (2016, pp. 264-265) discusses that $v(\mathbf{x}_0)$ in Eq. (4.11) can be replaced by its estimator to obtain an approximate interval. Hence, we formulate the prediction interval for the response i based on the discussions in (Wooldridge, 2016, pp. 264-265) as,

$$\hat{y}_i(\mathbf{x}_0) \pm t_{n-(p_i+1), 1-\alpha/4} \sqrt{\text{SE}_{\text{HC}}^2(\hat{\beta}_i) + \hat{v}_i(\mathbf{x}_0)} \quad \forall i \in \{1, 2\} \quad (5.31)$$

where

$$\text{SE}_{\text{HC}}(\hat{\beta}_i) = \sqrt{\frac{1}{n} \mathbf{f}(\mathbf{x}_0)^T \widehat{\text{Avar}}_{\text{HC}}(\hat{\beta}_i) \mathbf{f}(\mathbf{x}_0)}. \quad (5.32)$$

The area of the $100(1 - \alpha)\%$ rectangular prediction region is formulated as

$$A(\mathbf{x}_0) = 4 \times t_{n-(p_1+1), 1-\alpha/4} \sqrt{\text{SE}_{\text{HC}}^2(\hat{\beta}_1) + \hat{v}_1(\mathbf{x}_0)} \times t_{n-(p_2+1), 1-\alpha/4} \sqrt{\text{SE}_{\text{HC}}^2(\hat{\beta}_2) + \hat{v}_2(\mathbf{x}_0)}. \quad (5.33)$$

The length of the $100(1 - \alpha)\%$ simultaneous prediction interval for the i^{th} response at $\mathbf{x}_0$ is formulated as

$$l_i(\mathbf{x}_0) = 2 \times t_{n-(p_i+1), 1-\alpha/4} \sqrt{\text{SE}_{\text{HC}}^2(\hat{\beta}_i) + \hat{v}_i(\mathbf{x}_0)}. \quad (5.34)$$

We mention in Section 4.2 that the idea of conventional WLS regression is to first transform the collected data by using the weights, then apply OLS regression to the weighted data. Romano and Wolf (2017) recommend to find $\text{SE}_{\text{HC}}(\hat{\beta}_i)$ in the same manner. We transform each row of the model in Eq. (4.2) as,

$$\frac{\mathbf{y}_{ij}}{\sqrt{\hat{v}_i(\mathbf{X}_{ij}^T)}} = \frac{\mathbf{X}_{ij}^T}{\sqrt{\hat{v}_i(\mathbf{X}_{ij}^T)}} \beta_i + \frac{\boldsymbol{\varepsilon}_{ij}^T}{\sqrt{\hat{v}_i(\mathbf{X}_{ij}^T)}} \quad (5.35)$$

where $\mathbf{y}_{ij}$ is the j^{th} element of $\mathbf{y}_i$, $\mathbf{X}_{ij}$ is the j^{th} row of $\mathbf{X}_i$, $\beta_i \in \mathbb{R}^{(p_i+1) \times 1}$ is a vector of model coefficients and $\boldsymbol{\varepsilon}_{ij}$ the j^{th} element of $\boldsymbol{\varepsilon}_i$, $i \in \{1, 2\}$, and $j \in \{1, 2, \dots, n\}$.

Eq. (5.35) denotes the j^{th} row of the weighted model given by

$$\tilde{\mathbf{y}}_i = \tilde{\mathbf{X}}_i \beta_i + \tilde{\boldsymbol{\varepsilon}}_i, \quad i \in \{1, 2\} \quad (5.36)$$

where $\tilde{\mathbf{y}}_i \in \mathbb{R}^{n \times 1}$ is a vector of weighted observations, $\tilde{\mathbf{X}}_i$ is an $n \times (p_i + 1)$ design matrix specifying values of the weighted regressors, $\boldsymbol{\beta}_i \in \mathbb{R}^{(p_i+1) \times 1}$ is a vector of model coefficients and $\tilde{\boldsymbol{\varepsilon}}_i \in \mathbb{R}^{n \times 1}$ is a weighted random error vector associated with the i^{th} response.

Using the weighted model, we find $\widehat{\text{Avar}}_{\text{HC}}(\hat{\boldsymbol{\beta}}_i)$ as follows,

$$\widehat{\text{Avar}}_{\text{HC}}(\hat{\boldsymbol{\beta}}_i) = n^2 (\tilde{\mathbf{X}}_i^T \tilde{\mathbf{X}}_i)^{-1} \hat{\mathbf{Q}}_i (\tilde{\mathbf{X}}_i^T \tilde{\mathbf{X}}_i)^{-1} \quad (5.37)$$

where $\hat{\mathbf{Q}}_i = \frac{1}{n} \tilde{\mathbf{X}}_i^T \hat{\boldsymbol{\Psi}}_i \tilde{\mathbf{X}}_i$, $\hat{\boldsymbol{\Psi}}_{ij} = \frac{\hat{\varepsilon}_{ij}^2}{(1 - \hat{H}_{jj})^2}$ is the j^{th} diagonal element of $\hat{\boldsymbol{\Psi}}_i$, and $\hat{H}_{jj}$ is the j^{th} diagonal element of the hat matrix, $\hat{\mathbf{H}} = \tilde{\mathbf{X}}_i (\tilde{\mathbf{X}}_i^T \tilde{\mathbf{X}}_i)^{-1} \tilde{\mathbf{X}}_i^T$. For further discussions on Equation (5.37), we refer to Romano and Wolf (2017).

Illustrative Example. We assume that the collected data satisfies Assumption 5.3.1 and Assumption 5.3.2. However, in practice, the assumptions should be validated by statistical tests. To check if Assumption 5.3.2 holds, we follow the recommendation of Romano and Wolf (2017) and suggest to test the significance of the regression models for the skedastic functions instead of using generic tests for heteroskedasticity.

Similar to the illustration in Section 5.2, we do not assume an underlying value function in illustrating interaction iterations. Instead, we play the role of the DM without collaborating with a real DM. We present nondominated criterion vectors to the DM throughout the iterations; thus, s/he knows that improving a particular objective is possible only if at least one other objective gets worse.

In this example, we aim to illustrate some cases possible to be encountered in using our approach. First, the DM can change her/his mind at an interaction iteration and turn back to an earlier solution to indicate different relaxation amounts. Second, it is not always guaranteed to improve an objective with index $j \in \mathbf{J}^h$ in return to sacrificing from another objective. Last but not least, $z_3(\mathbf{x})$ is multiplication of $z_4(\mathbf{x})$ and $z_5(\mathbf{x})$, which demands particular attention in formulating the mathematical models regarding the associated relaxation amounts. The DA supports the DM in such occurrences. We assume that the DM is more interested in decreasing the distances between response means and

their respective targets.

To obtain meaningful regression models for skedastic functions, we ensure heteroskedasticity in the collected data by generating five replications with the following model (Ko et al., 2005) for each run of the original polymer experiment shown in Table A.1,

$$y_{iju} = y_{ij} + e_{iju} \quad \forall i \in \{1, 2\}, j \in \{1, 2, \dots, 20\} \quad (5.38)$$

where y_{ij} is the j^{th} original observation on the i^{th} response, $e_{iju} \sim \mathcal{N}(0, \sigma_i^2(\mathbf{x}))$, $\sigma_1^2(\mathbf{x}) = e^{(3-x_1^2-3x_3^2)}$, $\sigma_2^2(\mathbf{x}) = e^{(2-2x_1^2-x_3^2)}$, and $u \in \{1, 2, \dots, 5\}$ denotes the number of replications. We should note that replications are not required to fit the regression in Eq. (5.24). We perform this step in our illustration due to the fact that we use the same example problem regardless of the problem assumptions for illustrative purposes.

Using the generated data with $n = 100$ observations for each of the responses, we first estimate the skedastic functions in the original scale as follows,

$$\begin{aligned} \hat{v}_1(\mathbf{x}) &= e^{(2.51-0.43x_1-0.10x_2+1.00x_3-0.78x_1^2-0.50x_3^2-0.53x_3^2+\frac{308.56}{2 \times 100})} \\ \hat{v}_2(\mathbf{x}) &= e^{(1.23-0.33x_1-0.23x_2+0.07x_3-0.86x_3^2+0.52x_1x_2+0.59x_1x_3-0.53x_2x_3+\frac{141.50}{2 \times 100})}. \end{aligned} \quad (5.39)$$

Then, we evaluate the functions in Eq. (5.39) at the design parameter settings in $\mathbf{X}_1$ and $\mathbf{X}_2$ to find the diagonal elements of $\hat{\mathbf{V}}_1$ and $\hat{\mathbf{V}}_2$ as shown in Eq. (5.27). By using the resulting weights, we fit the response surface models as follows,

$$\begin{aligned} \hat{y}_1(\mathbf{x}) &= 82.50 + 0.94x_1 + 4.33x_2 + 5.82x_3 - 2.00x_1^2 + 2.76x_2^2 \\ &\quad - 6.37x_3^2 + 1.42x_1x_2 + 11.20x_1x_3 - 3.53x_2x_3 \\ \hat{y}_2(\mathbf{x}) &= 60.33 + 3.55x_1 + 1.91x_3 + 0.73x_1^2 \end{aligned} \quad (5.40)$$

We assume that the DM decides to set $\alpha = 0.1$. Then, $A(\mathbf{x})$ and $l_i(\mathbf{x}) \forall i \in \{1, 2\}$ are given by Eqs. (5.33) and (5.34) where $p_1 = 9$, $p_2 = 3$, $t_{99-p_1, 0.975} = 1.985$ and $t_{99-p_2, 0.975} = 1.987$.

The objectives are $z_1(\mathbf{x}) = |\hat{y}_1(\mathbf{x}) - 100|$, $z_2(\mathbf{x}) = |\hat{y}_2(\mathbf{x}) - 57.5|$, $z_3(\mathbf{x}) = A(\mathbf{x})$, $z_4(\mathbf{x}) = l_1(\mathbf{x})$, and $z_5(\mathbf{x}) = l_2(\mathbf{x})$.

We initialize the interactive optimization procedure by finding the ideal objective vector, nadir objective vector and the weighting coefficients, respectively, as: $\mathbf{z}^* = [0.00 \ 0.00 \ 5.53 \ 4.06 \ 0.97]^T$, $\mathbf{z}^{\text{nad}} = [76.33 \ 10.45 \ 41.48 \ 13.28 \ 4.52]^T$, and $\mathbf{w} = [0.23 \ 0.23 \ 0.20 \ 0.16 \ 0.18]^T$.

The DA sets $h = 0$ and $\mathbf{J}^0 = \{1, 2, 3, 4, 5\}$. Then s/he solves the following problem,

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& \alpha \geq 0.23 (z_1(\mathbf{x}) - 0.00) \\
& \alpha \geq 0.23 (z_2(\mathbf{x}) - 0.00) \\
& \alpha \geq 0.20 (z_3(\mathbf{x}) - 5.53) \\
& \alpha \geq 0.16 (z_4(\mathbf{x}) - 4.06) \\
& \alpha \geq 0.18 (z_5(\mathbf{x}) - 0.97) \\
& 1.68 \geq x_k \geq -1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{5.41}$$

Regarding the visualization in Figure 5.8 and the numerical results in Table 5.6, the DM states that s/he wants to improve $z_1(\mathbf{x}^0)$ and $z_2(\mathbf{x}^0)$. S/he is willing to sacrifice from the area of the prediction region by 50%.

Table 5.6: Numerical results ($h = 0$)

$\hat{y}_1(\mathbf{x}^0)$	$ \hat{y}_1(\mathbf{x}^0) - t_1 $	$\hat{y}_2(\mathbf{x}^0)$	$ \hat{y}_2(\mathbf{x}^0) - t_2 $	$A(\mathbf{x}^0)$	$\text{SPI}_1(\mathbf{x}^0)$	$\ell_1(\mathbf{x}^0)$	$\text{SPI}_2(\mathbf{x}^0)$	$\ell_2(\mathbf{x}^0)$
78.88	21.12	55.74	1.76	29.91	[76.06, 81.70]	5.64	[53.09, 58.39]	5.30

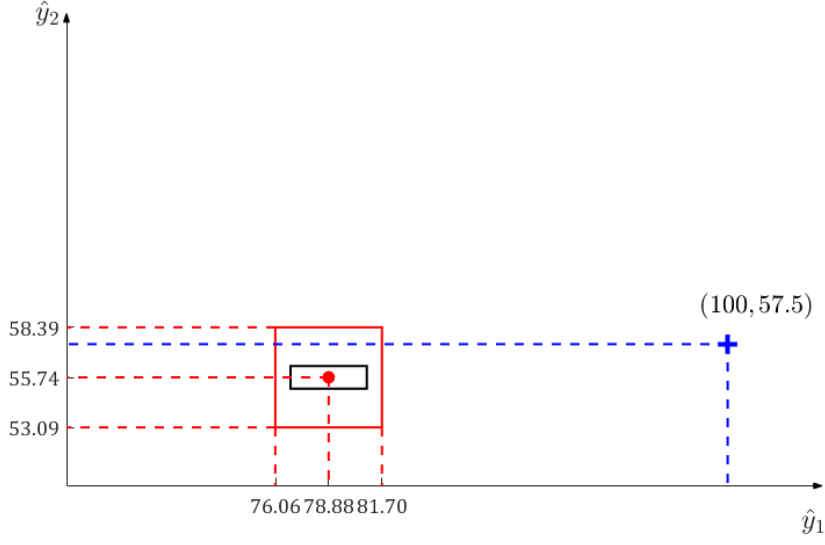


Figure 5.8: Visualization of the solution ($h = 0$)

Considering the preferences of the DM, the DA sets $h = 1$, $\mathbf{J}^1 = \{1, 2\}$ and updates Equation (5.41) as follows,

$$\begin{aligned}
 & \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
 & \text{subject to} \\
 & \alpha \geq 0.23(z_2(\mathbf{x}) - 0.00) \\
 & \alpha \geq 0.23(z_3(\mathbf{x}) - 0.00) \\
 & z_3(\mathbf{x}) \leq z_3(\mathbf{x}^0) + 0.5z_3(\mathbf{x}^0) \\
 & z_l(\mathbf{x}) \leq z_l(\mathbf{x}^0) + M \quad \forall l \in \{4, 5\} \\
 & z_j(\mathbf{x}) \leq z_j(\mathbf{x}^0) \quad \forall j \in \mathbf{J}^1 \\
 & -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\}.
 \end{aligned} \tag{5.42}$$

where M is a sufficiently large number. We should notify that once at least one of $z_3(\mathbf{x})$, $z_4(\mathbf{x})$, and $z_5(\mathbf{x})$ is excluded from $\mathbf{J}^h$, the others should also be removed due to their functional relationship. In such cases, we employ M to prevent $z_3(\mathbf{x}) \leq z_3(\mathbf{x}^0) + 0.5z_3(\mathbf{x}^0)$ from being redundant.

Table 5.7: Numerical results ($h = 1$)

$\hat{y}_1(\mathbf{x}^1)$	$ \hat{y}_1(\mathbf{x}^1) - t_1 $	$\hat{y}_2(\mathbf{x}^1)$	$ \hat{y}_2(\mathbf{x}^1) - t_2 $	$A(\mathbf{x}^1)$	$\text{SPI}_1(\mathbf{x}^1)$	$\ell_1(\mathbf{x}^1)$	$\text{SPI}_2(\mathbf{x}^1)$	$\ell_2(\mathbf{x}^1)$
88.88	11.12	55.74	1.76	44.91	[85.51, 92.26]	6.75	[52.42, 59.07]	6.65

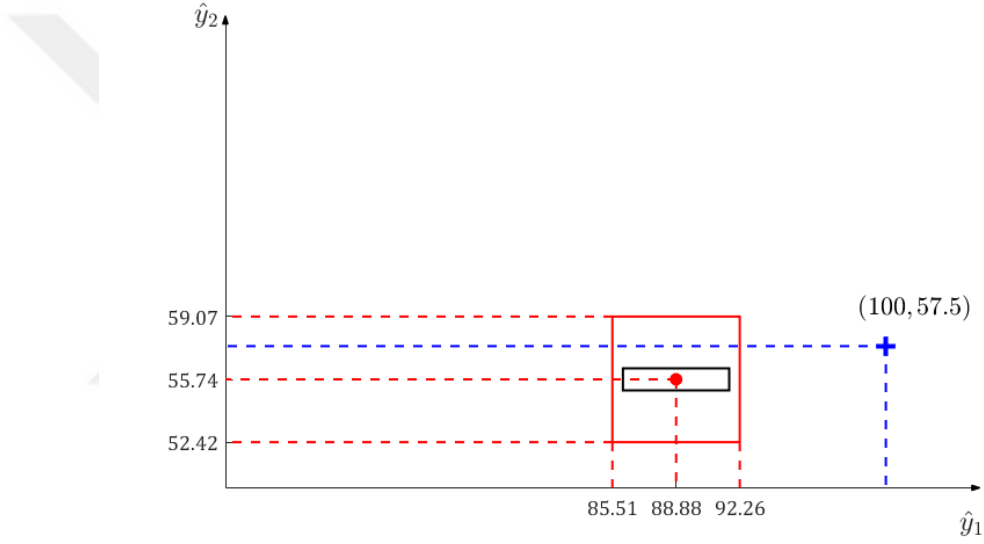


Figure 5.9: Visualization of the solution ($h = 1$)

Given the visualization in Figure 5.9 and the numerical results in Table 5.7, the DM states that s/he finds the increase in $\ell_2(\mathbf{x})$ high. S/he wants to turn back to the previous solution and change her/his decisions. S/he decides to sacrifice from $\ell_1(\mathbf{x}^0)$ and $\ell_2(\mathbf{x}^0)$ by 7 units and 0.5 units instead of indicating the amount of sacrifice for $A(\mathbf{x}^0)$. Then, the DA sets $h = 2$, $\mathbf{J}^2 = \{1, 2\}$ and updates Eq. (5.42)

as follows,

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& \alpha \geq 0.23(z_1(\mathbf{x}) - 0.00) \\
& \alpha \geq 0.23(z_2(\mathbf{x}) - 0.00) \\
& z_3(\mathbf{x}) \leq z_3(\mathbf{x}^0) + M \\
& z_4(\mathbf{x}) \leq z_4(\mathbf{x}^0) + 7 \\
& z_5(\mathbf{x}) \leq z_5(\mathbf{x}^0) + 0.5 \\
& z_j(\mathbf{x}) \leq z_j(\mathbf{x}^0) \quad \forall j \in \mathbf{J}^2 \\
& -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{5.43}$$

Table 5.8: Numerical results ($h = 2$)

$\hat{y}_1(\mathbf{x}^2)$	$ \hat{y}_1(\mathbf{x}^2) - t_1 $	$\hat{y}_2(\mathbf{x}^2)$	$ \hat{y}_2(\mathbf{x}^2) - t_2 $	$A(\mathbf{x}^2)$	$\text{SPI}_1(\mathbf{x}^2)$	$\ell_1(\mathbf{x}^2)$	$\text{SPI}_2(\mathbf{x}^2)$	$\ell_2(\mathbf{x}^2)$
88.92	11.08	57.31	0.19	73.33	[82.60, 95.24]	12.64	[54.41, 60.21]	5.80

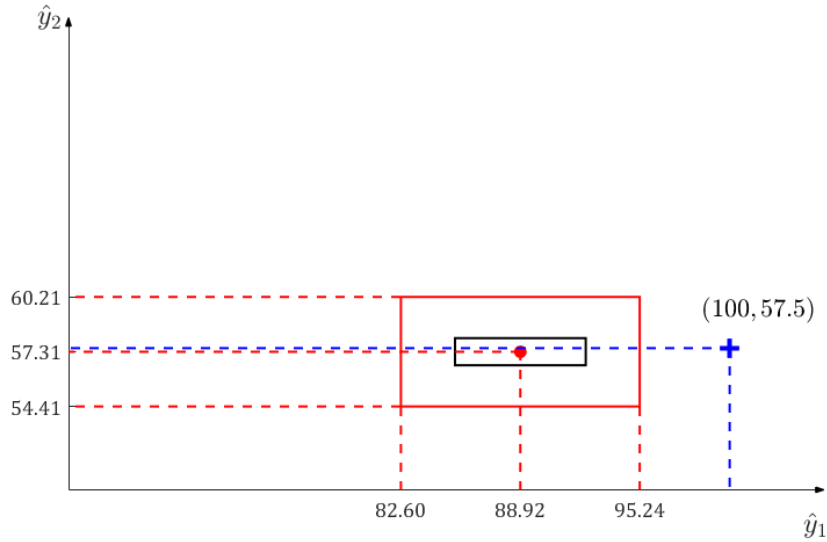


Figure 5.10: Visualization of the solution ($h = 2$)

Considering the visualization in Figure 5.10 and the numerical results in Table 5.8, the DM states that s/he still wants to improve $z_1(\mathbf{x}^1)$. Instead of further relaxing prediction region areas, s/he prefers sacrificing 1 unit from $z_2(\mathbf{x}^1)$. Then, the DA sets $h = 3$, $\mathbf{J}^3 = \{1\}$ and updates Eq. (5.43) as follows,

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& \alpha \geq 0.23(z_1(\mathbf{x}) - 0.00) \\
& z_2(\mathbf{x}) \leq z_2(\mathbf{x}^2) + 1 \\
& z_3(\mathbf{x}) \leq z_3(\mathbf{x}^0) + M \\
& z_4(\mathbf{x}) \leq z_4(\mathbf{x}^0) + 7 \\
& z_5(\mathbf{x}) \leq z_5(\mathbf{x}^0) + 0.5 \\
& z_1(\mathbf{x}) \leq z_1(\mathbf{x}^2) \\
& -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{5.44}$$

The DA observes that the same solution is obtained by Eqs. (5.43) and (5.44). To see if further relaxation on $z_2(\mathbf{x}^2)$ leads to any improvement in $z_1(\mathbf{x}^2)$, s/he solves Eq. (5.44) for $\Delta_2^3 \in \{1, 2, \dots, 10\}$. S/he finds out that $z_1(\mathbf{x}^2)$ improves when $\Delta_2^3 > 8$. S/he informs the DM about her/his observation. The DM does not want to sacrifice from $z_2(\mathbf{x}^2)$ by more than 1 unit; hence, s/he decides to further relax $l_1(\mathbf{x}^2)$ and $l_2(\mathbf{x}^2)$ by 1 and 0.5 units. The DA sets $h = 4$, $\mathbf{J}^4 = \{1\}$ and updates Eq. (5.44) as follows,

$$\begin{aligned}
& \text{lex min } \{\alpha, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& \alpha \geq 0.23(z_1(\mathbf{x}) - 0.00) \\
& z_2(\mathbf{x}) \leq z_2(\mathbf{x}^2) + 1 \\
& z_3(\mathbf{x}) \leq z_3(\mathbf{x}^2) + M \\
& z_4(\mathbf{x}) \leq z_4(\mathbf{x}^2) + 1 \\
& z_5(\mathbf{x}) \leq z_5(\mathbf{x}^2) + 0.5 \\
& z_1(\mathbf{x}) \leq z_1(\mathbf{x}^2) \\
& -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{5.45}$$

Table 5.9: Numerical results ($h = 4$)

$\hat{y}_1(\mathbf{x}^4)$	$ \hat{y}_1(\mathbf{x}^4) - t_1 $	$\hat{y}_2(\mathbf{x}^4)$	$ \hat{y}_2(\mathbf{x}^4) - t_2 $	$A(\mathbf{x}^4)$	$\text{SPI}_1(\mathbf{x}^4)$	$\ell_1(\mathbf{x}^4)$	$\text{SPI}_2(\mathbf{x}^4)$	$\ell_2(\mathbf{x}^4)$
91.39	8.61	57.65	0.15	85.95	[84.57, 98.21]	13.64	[54.50, 60.80]	6.30

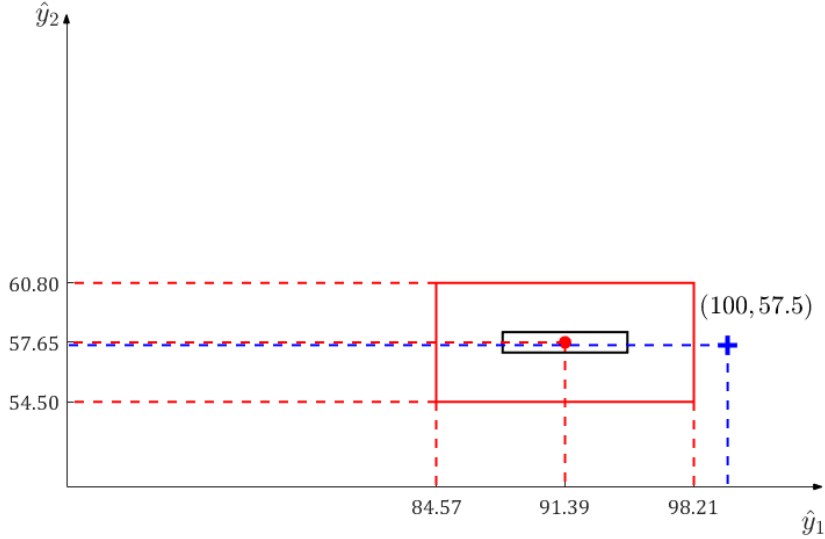


Figure 5.11: Visualization of the solution ($h = 4$)

We assume that the DM likes the solution visualized in Figure 5.11. Thus, the procedure stops at $h = 4$.

Discussions on the OLS Special Case. We consider using OLS regression in building response surface models as a special case of using WLS regression with approximate closed-form confidence and prediction intervals. As we mention earlier, the significance of the regression model for the skedastic function should be tested to check if Assumption 5.3.2 holds. Such a test tells if the form of underlying heteroskedasticity can be represented by the tested regression model. When the regression model is not significant, we cannot conclude that there is no heteroskedasticity in the collected data. That is, we suggest employing a test for homoskedasticity in such cases.

If the regression model is not significant, but the test for homoskedasticity rejects, then we suggest using OLS regression with HC standard errors. In this case, we set the associated $\hat{\mathbf{V}}_i$ to $\mathbf{I}$ and find $\text{SE}_{\text{HC}}(\hat{\beta}_i)$ from the original data without the weighting as in Eq. (5.35).

If the regression model is not significant and the test for homoskedasticity fails to reject, then we suggest using OLS regression with conventional standard errors. To construct joint confidence and prediction regions, we use the formulation of prediction intervals given in Eq. (4.10), respectively. Hence, we formulate Bonferroni corrected $100(1 - \alpha)\%$ rectangular prediction region area at $\mathbf{x}_0$ as

$$A(\mathbf{x}_0) = 4 \times t_{n-p_1-1, \alpha/4} \sqrt{\hat{\sigma}_1^2 + \hat{\sigma}_1^2 \mathbf{f}_1(\mathbf{x}_0)^T (\mathbf{X}_1^T \mathbf{X}_1)^{-1} \mathbf{f}_1(\mathbf{x}_0)} \\ \times t_{n-p_2-1, \alpha/4} \sqrt{\hat{\sigma}_2^2 + \hat{\sigma}_2^2 \mathbf{f}_2(\mathbf{x}_0)^T (\mathbf{X}_2^T \mathbf{X}_2)^{-1} \mathbf{f}_2(\mathbf{x}_0)} \quad (5.46)$$

where $\hat{\sigma}_i^2 = \frac{\epsilon_i^T \epsilon_i}{n} \forall i \in \{1, 2\}$.



CHAPTER 6

THE APPROACH UNDER COMPUTER INTENSIVE CONSTRUCTION OF CONFIDENCE AND PREDICTION REGIONS

The approach developed in Chapter 5 requires all the performance measures to be formulated in closed form so that the DM (and/or the DA) has a direct control over all the objectives in the interactive optimization. Yet, exact closed form expressions for the confidence and prediction regions may not be readily available or easy to employ when finite sample properties of the utilized empirical model building approach are unexplored or highly complicated. Although asymptotic methods formulate approximate regions in closed form, they are known to have poor coverage properties especially in small samples. As a remedy, bootstrap methods are commonly used to construct approximate regions through simulations based on the observed data (Van Aelst and Willems, 2013; Riggs et al., 2016).

In this chapter, we develop an interactive approach for the case when the joint prediction region area at a given design parameter setting is estimated through a bootstrap method. To approximately control uncertainty performance of the solutions in our mathematical models, we use proxy functions of the joint prediction region area and the lengths of the simultaneous prediction intervals. On the other hand, in interacting with the DM at the design parameter setting under consideration, we present the values resulted from the bootstrap procedure. Although some general knowledge about the effects of changing proxy functions on the performance measures exist, the exact magnitudes of those effects are not known due to the randomness in the bootstrap procedure. The potential difficulties that the DM may have in capturing those relations may complicate the

process of navigating towards preferred solutions. To help the DM to converge to her/his preferred solutions quickly, we actively involve the DA in the search process. Even though the DA is assumed to be able to handle more information compared to the DM, the trade-offs among the proxy functions and their effects on the performance measures highly depend on the problem characteristics that are unknown to the DA. Therefore, to be able to help the DM for her/his decisions, the DA needs a systematic framework to extract more information on those relations and to explore the desirable regions in a nonlinear solution space. To this end, we develop a search procedure throughout which the DA progressively observes the relevant parts of the solution space to identify the solutions that are in line with the DM's expressed preferences and presents several of them to the DM within an interactive solution procedure.

We build response surface models by utilizing SUR assuming equal robustness. Since there is no readily available multivariate bootstrap procedure for building confidence region for response means and prediction region for future response observations in SUR estimation, we adapt multiparameter approach described by Davidson and Hinkley (1997, pp. 231-233) and the residuals bootstrap (Freedman, 1981) in developing a bootstrapping procedure.

We develop the general formulation of our approach in Section 6.1. Then, we formulate the performance measures and illustrate our approach under SUR conditions in Section 6.2.

6.1 Development of the Method

We express the two response design optimization problem as the MOO program given in Eq. (5.1). Due to the lack of closed form formulations for $A(\mathbf{x})$ and

$L_i(\mathbf{x}) \forall i \in \{1, 2\}$, we consider the approximate MOO program given by

$$\begin{aligned}
& \text{Min} \quad z_1(\mathbf{x}) = |\hat{y}_1(\mathbf{x}) - t_1| \\
& \text{Min} \quad z_2(\mathbf{x}) = |\hat{y}_2(\mathbf{x}) - t_2| \\
& \text{Min} \quad z_3(\mathbf{x}) = P_A(\mathbf{x}) \\
& \text{Min} \quad z_4(\mathbf{x}) = P_{L_1}(\mathbf{x}) \\
& \text{Min} \quad z_5(\mathbf{x}) = P_{L_2}(\mathbf{x}) \\
& \text{subject to} \\
& \mathbf{x} \in \Omega
\end{aligned} \tag{6.1}$$

where $P_A(\mathbf{x})$ denotes the proxy function for the $100(1 - \alpha)\%$ joint prediction region area, and $P_{L_i}(\mathbf{x})$ is the proxy function for length of the $100(1 - \alpha)\%$ simultaneous prediction interval for response i securing the joint confidence level.

We employ the *e-constraint method* (Haimes et al., 1971) in our interactive solution approach to systematically generate different sets of nondominated solutions to Eq. (6.1). In the *e-constraint method*, one of the objectives is selected to be minimized while all others are converted into constraints each of which is restricted by an upper bound. Thus, the *e-constraint program* for Eq. (6.1) is given by,

$$\begin{aligned}
& \min z_q(\mathbf{x}) \\
& \text{subject to} \\
& z_j(\mathbf{x}) \leq e_j \quad \forall j \in \{1, 2, \dots, 5\}, j \neq q \\
& \mathbf{x} \in \Omega
\end{aligned} \tag{6.2}$$

where $q \in \{1, 2, \dots, 5\}$.

To generate a representative set of nondominated solutions, a series of single objective optimization problems resulted from systematically changing the upper bounds (*i.e.*, e_j values in Eq. (6.2)) are solved.

The *e-constraint method* is one of the methods that have the capability of finding any nondominated solution to any MOO problem regardless of whether the problem is convex or not (Miettinen, 1999, p. 95). Besides its popularity in MOO literature, the *e-constraint method* is utilized by many MRO approaches

both under interactive and prior categories such as Lee et al. (2011); Lee and Lee (2016); Lee et al. (2018) and Moslemi et al. (2018); Bashiri et al. (2020). These approaches configure the problem all at once at the beginning of the solution procedure by determining the objectives to be converted into constraints, their ranges, and the increments of their right-hand side values. Then, they represent the overall Pareto frontier by a set of nondominated solutions from which the final solution is to be selected.

In contrast to those approaches, we adopt the e -constraint method to develop an intermediate search tool that helps the DA to progressively explore the relevant parts of the solution space by utilizing "Pareto frontiers" considering the DM's expressed preferences within an interactive solution procedure. We use the term "Pareto frontier" in a restricted manner based on only the distances of the response means to their respective targets (*i.e.*, $z_1(\mathbf{x})$ and $z_2(\mathbf{x})$) subject to an upper bound on each proxy criterion (*i.e.*, $z_j(\mathbf{x}) \leq u_j \quad \forall j \in \{3, 4, 5\}$). Naturally, changing those upper bounds (*i.e.*, u_j values) produces different Pareto frontiers each of which is a subset of the overall Pareto frontier of Eq. (6.1).

We formulate the optimization scheme of producing a Pareto frontier as the following lexicographic program,

$$\begin{aligned}
& \text{lex min } \{z_q(\mathbf{x}), \mathbf{1}^T \mathbf{z}(\mathbf{x})\} \\
& \text{subject to} \\
& z_r(\mathbf{x}) \leq z_r^* + e_r^\tau \quad r \in \{1, 2\}, r \neq q \\
& z_j(\mathbf{x}) \leq u_j \quad \forall j \in \{3, 4, 5\} \\
& \mathbf{x} \in \Omega.
\end{aligned} \tag{6.3}$$

where $q \in \{1, 2\}$, z_r^* is the r^{th} element of the ideal objective vector found by solving Eq. (5.3) for $j = r$, $\tau \in \{1, 2, \dots, \tau_{\max}\}$ is the counter for the number of solutions on the Pareto frontier, and $\tau_{\max}$ is the number of solutions to appear on the resulting Pareto frontier. The idea is that the DA determines the upper bounds, $u_j \quad \forall j \in \{3, 4, 5\}$, based on the DM's expressed preferences at an interaction iteration, then s/he observes a set of nondominated solutions resulting from solving Eq. (6.3) $\tau_{\max}$ times where $e_r^\tau = e_r^{\tau-1} + \delta_r$ and δ_r denotes the value of increments.

We should note that our formulation in Eq. (6.3) avoids generation of weakly nondominated but dominated solutions unlike Eq. (6.2). If the first stage, optimization yields $\mathbf{S}_q$, the set of criterion vectors with the minimal value of the objective q , with $|\mathbf{S}_q| > 1$, then the second stage optimization eliminates weakly nondominated but dominated points and returns a nondominated criterion vector.

Range of the "Pareto Frontiers". Typically, the range of a Pareto frontier is determined by the ideal objective values in a two objective problem, where a solution achieves the ideal value of one objective corresponds to the nadir value of the other. Then, the bound on the objective converted into a constraint is systematically changed between its ideal and nadir objective values. For this purpose, the DA selects either the number of solutions to be observed on the Pareto frontier ($\tau_{\max}$), which automatically determines the value of increments (δ_r), or the value of increments, leading to the determination of the number of observed solutions accordingly. However, in our solution procedure, the observed Pareto frontiers only consider two objectives while our problem involves more. Therefore, we explore solutions beyond the ideal values of z_1 and z_2 . Although worsening one objective while the other is at its ideal value leads to dominated solutions in a two objective problem, in our problem, such solutions may improve the third objective and provide useful information on the problem nature. These solutions can be desirable for the DM as they are nondominated when all three objectives are considered. To this respect, we establish a stopping rule to support the DA in generating Pareto frontiers without a predetermined range. Algorithm 1 outlines the relevant steps of our procedure for generating a Pareto frontier.

τ_{ext} is the number of iterations for finding solutions beyond z_q^* . We suggest the DA to consider the smallest difference in $z_r(\mathbf{x})$ worth comparing in determining δ_r . We should note that $z_q(\mathbf{x})$ may not reach its ideal value no matter how large the initial value of $\tau_{\max}$ is due to the restrictions on $z_j \forall j \in \{3, 4, 5\}$. If the DA intends to generate solutions beyond z_r^* as well, then s/he can repeat the procedure by swapping the objectives q and r .

Algorithm 1 Outline of the stopping rule in generating a "Pareto frontier"

input $z_r^*, z_q^*, \delta_r, \tau_{\max}, \tau_{\text{ext}}$, and $u_j \forall j \in \{3, 4, 5\}$

$e_r^1 \leftarrow 0$

while $\tau \leq \tau_{\max}$

 solve Eq. (6.3)

$e_r^{\tau+1} \leftarrow e_r^\tau + \delta_r$

if $z_q(\mathbf{x}) = z_q^*$ for the first time

$\tau_{\max} \leftarrow \tau + \tau_{\text{ext}}$

Visualization of the "Pareto Frontiers". We visualize each Pareto frontier on a graph where the axes denotes response means. We mark each solution by a circle such that its relative size is proportional to the area of the respective prediction region obtained by the utilized bootstrap procedure. The aim is to provide the DA with the insights into the tradeoffs among all the performance measures.

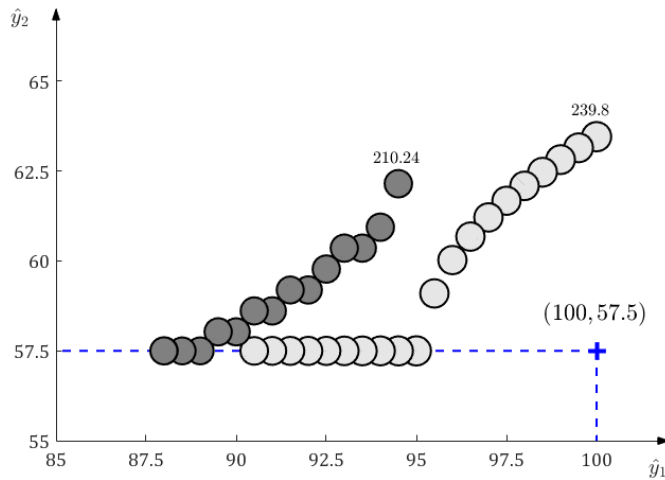


Figure 6.1: Visualization of two "Pareto frontiers" for polymer experiment: The light gray frontier is obtained when there are no bounds on $z_j \forall j \in \{3, 4, 5\}$ while the dark gray frontier results from only restricting $z_3(\mathbf{x})$ by 6. The area values are labeled to the markers indicating the largest regions within their respective frontiers.

Figure 6.1 illustrates the visualization of two different Pareto frontiers generated subject to two different sets of u_j values. The DA can display the Pareto frontiers

in whichever way is more comfortable for her/him, either on the same graph or on separate graphs. The idea is to help the DA to oversee the generated solutions to identify the ones that may be desirable for the DM in addition to reviewing the numerical results of all the solutions that appear on each Pareto frontier. The DA can also evaluate the solutions individually through the visual aids illustrated in Figure 5.1.

It is worth mentioning that, in Figure 6.1, some dark gray solutions may be perceived as dominated by some of the light gray solutions considering the two objectives measuring the distances of the estimated response values to their respective targets. However, in fact, all the visualized solutions are nondominated when all objectives are considered. That is to say, the solutions closer to the target have larger prediction region areas and/or simultaneous prediction interval lengths compared to those that are farther from the target.

Interaction with the DM. We do not present the graph displayed in Figure 6.1 to the DM since the complexity of the underlying structure may mislead her/him. Based on our experience, we recommend to present the DM with at most 3 solutions from the observed Pareto frontiers at an interaction iteration since the DM may not handle more information at once. We utilize the visual aids shown in Figure 5.1 to present the consequences of each of the selected solutions to the DM.

Bounds on the Proxy Criteria. We obtain the initial Pareto frontier by setting no upper bounds on z_j 's $\forall j \in \{3, 4, 5\}$. After interacting with the DM, we update the bounds considering her/his verbal preferences to obtain a new Pareto frontier. We should note that generating a new Pareto frontier after every interaction may not be necessary as previous frontiers may already offer a suitable set of solutions to present to the DM. On the other hand, the DA may need to review multiple Pareto frontiers between interactions until s/he finds a set of solutions that align with the DM's preferences.

Discussions. In MRO problems, the aim is not only to determine the optimal design parameter levels but also to understand the system characteristics. In line with this aim, we do not suggest an algorithm converging within a certain

number of steps under some assumptions about the DM's possible preference statements. We rather suggest a search procedure throughout which both the DA and the DM can learn the system characteristics. Our procedure allows the DM to change her/his mind and past responses, and to return to a solution or a set of solutions for reevaluation. Moreover, the DA's search can prove useful especially when the DM adopts a cautious stance in her/his preferences in exploring interesting solutions. The convergence of our procedure highly depends on the problem, the preferences of the DM, and the DA's ability to navigate towards desirable regions. We believe that, as the process progresses, the DM shapes her/his preferences better and the DA navigates the process towards the DM's desirable regions. Therefore, the effort required to reach a satisfactory solution is expected to be reasonable.

Due to the complexity of the solution space and difficulties in directly controlling some of the objectives, the DA's role in the solution process is important. We believe that incorporating such a search phase into interactive approaches may be an important contribution to solving multiple objective problems that have complex feasible sets and objective functions that cannot be directly controlled.

The MRO problem under consideration may not always produce a satisfactory solution under the current set-up due to its nature. Consequently, the procedure may stop because the DM is not satisfied with any of the presented solutions. We believe that our procedure helps the DM to discover the limitations of the system of interest and justify further efforts such as tolerance design or technological advancements.

6.2 SUR under Equal Robustness

In this section, we relax Assumption 5.2.2 while we remain the following assumption.

Assumption 6.2.1 *Response variances are constant over the experimental region. That is, $\text{Var}(\epsilon_i) = \sigma_i^2 \mathbf{I}_n \quad \forall i \in \{1, 2\}$.*

We use SUR, introduced by Zellner (1962), in fitting the response surface models. We mention in Section 4.2 that if the responses are correlated, SUR produces more precise estimates of response surface model coefficients than OLS regression under Assumption 6.2.1. Besides, unlike MVR, SUR allows for different sets of regressors in the response surface models. Zellner (1962) discusses that the gain in efficiency can be large if the responses are highly correlated and if the regressors in different models are not highly correlated.

We build our formulations upon the stacked model in Eq. (4.3). We use Eq. (4.5) to estimate model coefficients. Since we assume that the responses are uncorrelated across experimental runs in MRO, Σ given in Equation (4.4) simplifies to $\mathbf{S} \otimes \mathbf{I}_n$ as shown in the last row of Table 4.1. $\mathbf{S}$ denotes the variance-covariance matrix of the responses at a given design parameter setting, defined by Eq. (5.13).

For now, we assume that $\mathbf{S}$ is known. Then, the estimated values of the responses at a given design parameter setting, $\mathbf{x}_0$, are given by

$$\hat{\mathbf{y}}(\mathbf{x}_0) = \hat{\boldsymbol{\beta}}^T \mathbf{f}(\mathbf{x}_0) \quad (6.4)$$

where $\hat{\mathbf{y}}(\mathbf{x}_0) = [\hat{y}_1(\mathbf{x}_0) \ \hat{y}_2(\mathbf{x}_0)]^T$, $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T(\mathbf{S} \otimes \mathbf{I}_n)^{-1} \mathbf{X})^{-1} \mathbf{X}^T(\mathbf{S} \otimes \mathbf{I}_n)^{-1} \mathbf{y}$, $\mathbf{f}(\mathbf{x}_0) = [\mathbf{f}_1^T(\mathbf{x}_0) \ \mathbf{f}_2^T(\mathbf{x}_0)]^T$ is a $(p_1 + p_2 + 2) \times 1$ vector of regressors as functions of design parameters in the expanded form, and p_i denotes the number of regressors for each $i \in \{1, 2\}$.

We discuss in Section 4.3.1 that $100(1 - \alpha)\%$ prediction region at $\mathbf{x}_0$ is derived from the variance of prediction error, $\text{Var}[\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)] = \text{Var}[\boldsymbol{\varepsilon}(\mathbf{x}_0)] + \text{Var}[\hat{\mathbf{y}}(\mathbf{x}_0)]$ where $\mathbf{y}(\mathbf{x}_0) = \hat{\mathbf{y}}(\mathbf{x}_0) + \boldsymbol{\varepsilon}(\mathbf{x}_0)$ denotes a future observation vector. The prediction variance, $\text{Var}[\hat{\mathbf{y}}(\mathbf{x}_0)]$, is expressed as

$$\begin{aligned} \text{Var}[\hat{\mathbf{y}}(\mathbf{x}_0)] &= \mathbf{F}^T(\mathbf{x}_0) \text{Var}[\hat{\boldsymbol{\beta}}] \mathbf{F}(\mathbf{x}_0) \\ &= \mathbf{F}^T(\mathbf{x}_0) (\mathbf{X}^T (\mathbf{S} \otimes \mathbf{I}_n)^{-1} \mathbf{X})^{-1} \mathbf{F}(\mathbf{x}_0) \end{aligned} \quad (6.5)$$

where $\mathbf{F}(\mathbf{x}_0) = \begin{bmatrix} \mathbf{f}_1(\mathbf{x}_0) & \mathbf{0} \\ \mathbf{0} & \mathbf{f}_2(\mathbf{x}_0) \end{bmatrix}$.

Under Assumption 4.2.4 and with known $\mathbf{S}$, $\hat{\boldsymbol{\beta}}$ is multivariate normally distributed with mean $\boldsymbol{\beta}$ and covariance matrix $(\mathbf{X}^T (\mathbf{S} \otimes \mathbf{I}_n)^{-1} \mathbf{X})^{-1}$. Furthermore, the

random vector, $\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)$, is multivariate normally distributed with mean $\mathbf{0}$ and covariance matrix $(\mathbf{F}^T(\mathbf{x}_0)(\mathbf{X}^T(\mathbf{S} \otimes I_n)^{-1}\mathbf{X})^{-1}\mathbf{F}(\mathbf{x}_0) + \mathbf{S})$ since $\mathbf{y}(\mathbf{x}_0)$ and $\hat{\mathbf{y}}(\mathbf{x}_0)$ are linear functions of $\boldsymbol{\varepsilon}(\mathbf{x}_0)$ and $\hat{\boldsymbol{\beta}}$, respectively. Consequently, the inequality,

$$(\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0))^T \text{Var}[\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)]^{-1} (\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)) \leq \chi_2^2(\alpha) \quad (6.6)$$

defines the $100(1 - \alpha)\%$ prediction region for the responses in closed form where $\text{Var}[\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)] = (\mathbf{F}^T(\mathbf{x}_0)(\mathbf{X}^T(\mathbf{S} \otimes I_n)^{-1}\mathbf{X})^{-1}\mathbf{F}(\mathbf{x}_0) + \mathbf{S})$. In that event, our first approach illustrated in Sec. 5.2 can be used.

If $\mathbf{S}$ is unknown, as it commonly is, some difficulties arise in the estimation and inference procedures. First, the number of unknowns becomes greater than the number of equations in the regression system so that it is not (so-called) feasible to collectively estimate $\boldsymbol{\beta}$ and $\mathbf{S}$ with the observed data (Greene, 2018, p. 586). Therefore, an estimate of $\mathbf{S}$ is inserted in Equations (6.4) and (6.5). For this purpose, there are two popular approaches each of which is based on residuals obtained by the preliminary application of OLS (Srivastava and Giles, 1987, pp. 13-17). While *unrestricted* residuals are obtained by regressing each of the responses using all the distinct regressors in Eq. (4.3), *restricted* residuals result from regressing each response on its respective $\mathbf{X}_i$. Following the recommendation of Zellner (1963), we use restricted residuals to incorporate more a priori information. The restricted estimator of $\mathbf{S}$ is given by,

$$\hat{\mathbf{S}} = \begin{bmatrix} \frac{1}{n} \hat{\boldsymbol{\varepsilon}}_{1,ols}^T \hat{\boldsymbol{\varepsilon}}_{1,ols} & \frac{1}{n} \hat{\boldsymbol{\varepsilon}}_{1,ols}^T \hat{\boldsymbol{\varepsilon}}_{2,ols} \\ \frac{1}{n} \hat{\boldsymbol{\varepsilon}}_{2,ols}^T \hat{\boldsymbol{\varepsilon}}_{1,ols} & \frac{1}{n} \hat{\boldsymbol{\varepsilon}}_{2,ols}^T \hat{\boldsymbol{\varepsilon}}_{2,ols} \end{bmatrix} \quad (6.7)$$

where $\hat{\boldsymbol{\varepsilon}}_{i,ols} = \mathbf{y}_i - \mathbf{X}_i \hat{\boldsymbol{\beta}}_{i,ols} \forall i \in \{1, 2\}$. We should note that there are other choices to be used in place of the divisor, n . For further discussions, we refer to Srivastava and Dwivedi (1979).

Second, when an estimate of $\mathbf{S}$ is used in estimating $\boldsymbol{\beta}$, the resulting $\hat{\boldsymbol{\beta}}$ involves variability due to both $\hat{\mathbf{S}}$ and $\boldsymbol{\varepsilon}$. Thus, the finite sample properties of $\hat{\boldsymbol{\beta}}$ under known $\mathbf{S}$ are no longer valid. As a remedy, the exact distribution of the SUR

estimator obtained by utilizing unrestricted OLS residuals is derived by Phillips (1985). However, the formulation is so complicated that it cannot be accommodated in easily formed inferential methods (Riggs et al., 2016). We should note that the methods presented by Phillips (1985) are also applicable for the restricted residuals case with more complicated treatment as the author stated. Alternatively, the asymptotic properties of the SUR estimator can be utilized in constructing closed form, but approximate, expressions of confidence and prediction regions. Nonetheless, such regions may have poor coverage properties in small samples (Riggs et al., 2016).

To overcome those issues, we use the bootstrap technique in constructing confidence and prediction regions. The bootstrap technique is a computer intensive statistical method, first proposed by Efron (1979). The idea is to take samples from the original data with replacement then use the resampled data to assess the variability of the statistic of interest. To the best of our knowledge, there is no readily available multivariate bootstrap procedure for building confidence region for response means and prediction region for future response observations in SUR estimation. Thus, we develop a bootstrap procedure by combining the residuals bootstrap and multiparameter approach described by Davidson and Hinkley (1997, pp. 231-233).

Residual bootstrap is a widely used technique in bootstrapping a regression model. In this method, the residuals of a fitted model are resampled with replacement to generate bootstrap samples assuming that variances of error terms are constant. Thus, it is sensitive to the fitted model and its assumptions. On the other hand, the pairs bootstrap, first proposed by Freedman (1981) to accommodate heteroskedasticity, is an alternative approach which resamples cases. However, implicitly assuming that $\mathbf{X}$ is random, the pairs bootstrap does not condition on $\mathbf{X}$ so that each bootstrap sample has a different design matrix. To preserve the structure of the original design matrix, we use residuals bootstrap under Assumption 4.2.1 and Assumption 6.2.1 in generating bootstrap samples. We resample centered residuals (*i.e.*, $\hat{\epsilon}_{i,ols}^c = \hat{\epsilon}_{i,ols} - (\mathbf{1}^T \hat{\epsilon}_{i,ols})/n \forall i \in \{1, 2, \dots\}$) in pairs to consider the possible correlations among the responses.

Algorithm 2 Joint bootstrap confidence and prediction regions at $\mathbf{x}_0$

given $\mathbf{x}_0, \mathbf{f}(\mathbf{x}_0), \hat{\mathbf{y}}(\mathbf{x}_0), \mathbf{X}, \hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\varepsilon}}_{1,ols}^c, \hat{\boldsymbol{\varepsilon}}_{2,ols}^c, \alpha, B$, and D

repeat for $b = 1, 2, \dots, B$

randomly sample $(\boldsymbol{\varepsilon}_1^{(b)} \in \mathbb{R}^n, \boldsymbol{\varepsilon}_2^{(b)} \in \mathbb{R}^n)$ with replacement from $(\hat{\boldsymbol{\varepsilon}}_{1,ols}^c, \hat{\boldsymbol{\varepsilon}}_{2,ols}^c)$

set $\mathbf{y}^{(b)} = \mathbf{X}\hat{\boldsymbol{\beta}} + [\boldsymbol{\varepsilon}_1^{(b)T} \ \boldsymbol{\varepsilon}_2^{(b)T}]^T$

find $\hat{\boldsymbol{\beta}}^{(b)}$ by applying SUR to the bootstrap sample $(\mathbf{y}^{(b)}, \mathbf{X})$

obtain $\hat{\mathbf{y}}^{(b)}(\mathbf{x}_0) = \mathbf{f}(\mathbf{x}_0)^T \hat{\boldsymbol{\beta}}^{(b)}$

estimate $\widehat{\text{Var}}(\hat{\boldsymbol{\beta}}^{(b)}) = (\mathbf{X}^T(\hat{\mathbf{S}}^{(b)} \otimes \mathbf{I}_n)^{-1} \mathbf{X})^{-1}$

estimate $\widehat{\text{Var}}[\hat{\mathbf{y}}^{(b)}(\mathbf{x}_0)] = \mathbf{F}^T(\mathbf{x}_0) \widehat{\text{Var}}(\hat{\boldsymbol{\beta}}^{(b)}) \mathbf{F}(\mathbf{x}_0)$

compute $Q_c^{(b)}$ as:

$$Q_c^{(b)} = (\hat{\mathbf{y}}^{(b)}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0))^T \widehat{\text{Var}}[\hat{\mathbf{y}}^{(b)}(\mathbf{x}_0)]^{-1} (\hat{\mathbf{y}}^{(b)}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0))$$

for $d = 1, 2, \dots, D$

set $b_d = (b-1) \times D + d$

randomly sample one residual pair $(\varepsilon_1^{(b_d)}, \varepsilon_2^{(b_d)})$ from entities of $(\hat{\boldsymbol{\varepsilon}}_{1,ols}^c, \hat{\boldsymbol{\varepsilon}}_{2,ols}^c)$

set $\mathbf{y}^{(b_d)}(\mathbf{x}_0) = \hat{\mathbf{y}}(\mathbf{x}_0) + [\varepsilon_1^{(b_d)} \ \varepsilon_2^{(b_d)}]^T$

estimate $\widehat{\text{Var}}[\mathbf{y}^{(b_d)}(\mathbf{x}_0) - \hat{\mathbf{y}}^{(b)}(\mathbf{x}_0)] = \hat{\mathbf{S}}^{(b)} + \widehat{\text{Var}}[\hat{\mathbf{y}}^{(b)}(\mathbf{x}_0)]$

compute $Q_p^{(b_d)}$ as:

$$Q_p^{(b_d)} = (\mathbf{y}^{(b_d)}(\mathbf{x}_0) - \hat{\mathbf{y}}^{(b)}(\mathbf{x}_0))^T \left(\widehat{\text{Var}}[\hat{\mathbf{y}}^{(b)}(\mathbf{x}_0)] + \hat{\mathbf{S}}^{(b)} \right)^{-1} (\mathbf{y}^{(b_d)}(\mathbf{x}_0) - \hat{\mathbf{y}}^{(b)}(\mathbf{x}_0))$$

find sorting indices such that $Q_c^{(c_1)} < Q_c^{(c_2)} < \dots$ and $Q_p^{(p_1)} < Q_p^{(p_2)} < \dots$

return $Q_c^{(c_{sc})}, Q_p^{(p_{sp})}$ where $sc = (B+1)(1-\alpha)$ and $sp = (BD+1)(1-\alpha)$

Davidson and Hinkley (1997, pp. 231-233) discuss that the question of shape arises in building a joint confidence region for random vectors. We assume that the joint confidence and prediction regions are in elliptical shape due to Assumption 4.2.4. Therefore, for each bootstrap sample, we calculate the bootstrap analogues of the two quadratic quantities originated from the multivariate extension of the

square of the student- t statistic. Their formulations at a given design parameter setting, $\mathbf{x}_0$, are given by

$$Q_c = (\mathbf{f}(\mathbf{x}_0)^T \boldsymbol{\beta} - \hat{\mathbf{y}}(\mathbf{x}_0))^T \widehat{\text{Var}}[\hat{\mathbf{y}}(\mathbf{x}_0)]^{-1} (\mathbf{f}(\mathbf{x}_0)^T \boldsymbol{\beta} - \hat{\mathbf{y}}(\mathbf{x}_0)) \quad (6.8a)$$

$$Q_p = (\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0))^T \widehat{\text{Var}}[\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)]^{-1} (\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)) \quad (6.8b)$$

where $\widehat{\text{Var}}[\hat{\mathbf{y}}(\mathbf{x}_0)]$ is the asymptotic covariance (Zellner, 1962) (*i.e.*, $\mathbf{S}$ is replaced by $\hat{\mathbf{S}}$ in Eq. (6.5)) and $\widehat{\text{Var}}[\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)] = \widehat{\text{Var}}[\hat{\mathbf{y}}(\mathbf{x}_0)] + \hat{\mathbf{S}}$. Q_c and Q_p denote the statistical distance of the estimated response mean vector to the true mean vector and a future observation, respectively. Our aim is to capture the variability in both Q_c and Q_p arising from using an estimate of $\mathbf{S}$ and to approximate their distributions. We simulate the variation in Q_p through an additional resampling within each bootstrap sample. We present the steps of our bootstrap procedure with the associated mathematical formulations in Algorithm 2 where B denotes the number of bootstrap samples and D is the number of predictions simulated in each bootstrap sample.

Based on the discussion in Efron and Tibshirani (1993, pp. 50-52), $\lim_{B \rightarrow \infty} Q_c^{(csc)} = \hat{Q}_c$ and $\lim_{B \rightarrow \infty} Q_p^{(psp)} = \hat{Q}_p$, where $\hat{Q}_c$ and $\hat{Q}_p$ are referred to as the ideal bootstrap estimates. In other words, as B goes to ∞ , the generated population approaches to the complete population composed of all possible samples that can be drawn from the observed data through resampling. Consequently, the variability in the bootstrap estimates decreases. Thus, we suggest selecting B as large as possible considering the computation time. Moreover, we suggest choosing B such that $(B+1)\alpha$ is an integer as discussed by Davidson and Hinkley (1997, pp. 18-19). Accordingly, D can be selected such that $(BD+1)\alpha$ is an integer.

We define the resulting $100(1-\alpha)\%$ bootstrap confidence and prediction regions at $\mathbf{x}_0$ as

$$(\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0))^T \widehat{\text{Var}}[\hat{\mathbf{y}}(\mathbf{x}_0)]^{-1} (\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)) \leq Q_c^{(csc)} \quad (6.9a)$$

$$(\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0))^T (\widehat{\text{Var}}[\hat{\mathbf{y}}(\mathbf{x}_0)] + \hat{\mathbf{S}})^{-1} (\mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0)) \leq Q_p^{(psp)}. \quad (6.9b)$$

We mention in Sec. 4.2 that MVR is a special case of SUR where each response surface model has the same set of regressors. Therefore, in such a case, we expect

our bootstrap procedure and MVR to produce similar confidence and prediction regions. Based upon that we assume same set of regressors for each response surface model and compare the 90% bootstrap confidence and prediction regions to the exact counterparts produced by MVR at various design parameter settings of the polymer experiment.

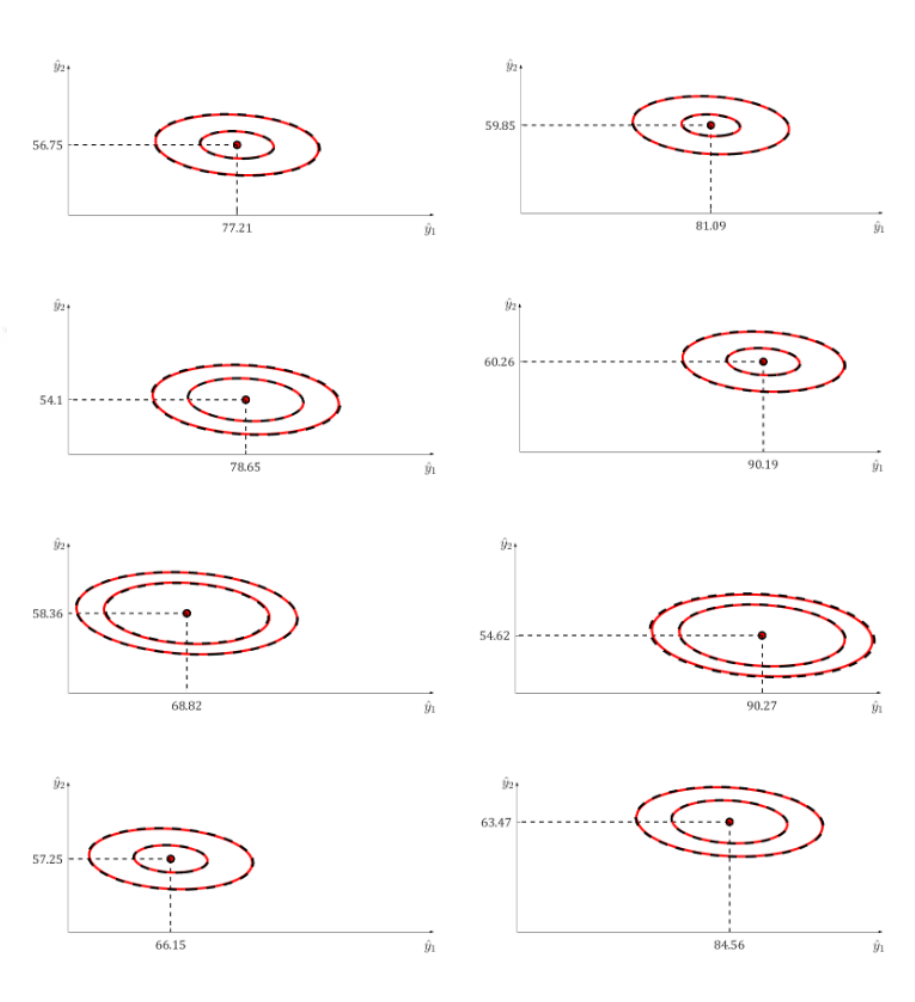


Figure 6.2: Bootstrap SUR regions (black dashed ellipses) vs. exact MVR regions (red solid ellipses) at eight representative design parameter settings selected from the different parts of the design parameter space of the polymer experiment

Fig. 6.2 shows that the bootstrap confidence and prediction regions coincide with the exact MVR regions as anticipated. In this study, our primary aim is to demonstrate our interactive approach when the prediction region cannot be expressed in closed form, rather than developing a state of art bootstrap

algorithm to construct confidence and prediction regions for SUR. Hence, we leave further performance assessment of our bootstrap procedure through Monte Carlo simulations to future research.

The area of the ellipse defined in Eq. (6.9b) at $\mathbf{x}_0$ is formulated as

$$A(\mathbf{x}_0) = \pi \sqrt{\left| \left(\widehat{\text{Var}}[\hat{\mathbf{y}}(\mathbf{x})] + \hat{\mathbf{S}} \right) \right|} Q_p^{(p_{sp})}. \quad (6.10)$$

$A(\mathbf{x}_0)$ can only be evaluated once $Q_p^{(p_{sp})}$ is produced by running Algorithm 2 at $\mathbf{x}_0$. In other words, we have no direct control over the criterion measuring the overall uncertainty at design parameter settings in our mathematical models. Therefore, to approximately control solution performance in terms of the prediction region area, we use the analytically estimated part of $A(\mathbf{x}_0)$ as a proxy criterion in the optimization. We formulate $P_A(\mathbf{x})$ as

$$P_A(\mathbf{x}) = \sqrt{\left| \left(\widehat{\text{Var}}[\hat{\mathbf{y}}(\mathbf{x})] + \hat{\mathbf{S}} \right) \right|}. \quad (6.11)$$

Resulting from the ellipse defined in Eq. (6.9b), the length of the simultaneous prediction interval for i^{th} response at $\mathbf{x}_0$ is formulated as

$$\begin{aligned} L_i(\mathbf{x}_0) &= 2 \sqrt{\left(\widehat{\text{Var}}[\hat{y}_i(\mathbf{x}_0)] + \hat{\mathbf{S}}_i \right) Q_p^{(p_{sp})}} \\ &= 2 \sqrt{\left(\mathbf{f}_i(\mathbf{x}_0)^T \text{Var}(\hat{\beta}_i) \mathbf{f}_i(\mathbf{x}_0) + \hat{\mathbf{S}}_i \right) Q_p^{(p_{sp})}} \end{aligned} \quad (6.12)$$

where $\hat{\mathbf{S}}_i$ is the i^{th} diagonal element of $\hat{\mathbf{S}}$.

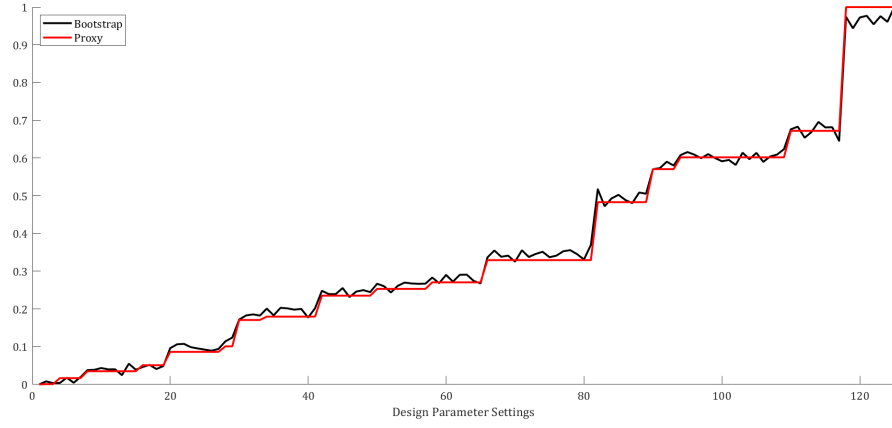
Eq. (6.12) shows that each simultaneous prediction interval is determined by its vector of regressors, $\mathbf{f}_i(\mathbf{x})$. Unlike MVR, SUR allows that different sets of regressors are involved in the response surface models; therefore, the gradients of $L_1(\mathbf{x})$ and $L_2(\mathbf{x})$ may not be parallel. That is, some trade off between the simultaneous prediction interval lengths of the responses may exist when SUR is used in building the response surface models. Therefore, our mathematical models include the proxy functions of simultaneous prediction intervals. We formulate $P_{L_i}(\mathbf{x}) \forall i \in \{1, 2\}$ considering the analytically estimated part of $L_i(\mathbf{x}_0)$ as

$$\begin{aligned} P_{L_i}(\mathbf{x}) &= \sqrt{\left(\widehat{\text{Var}}[\hat{y}_i(\mathbf{x}_0)] + \hat{\mathbf{S}}_i \right)} \\ &= \sqrt{\left(\mathbf{f}_i(\mathbf{x}_0)^T \text{Var}(\hat{\beta}_i) \mathbf{f}_i(\mathbf{x}_0) + \hat{\mathbf{S}}_i \right)}. \end{aligned} \quad (6.13)$$

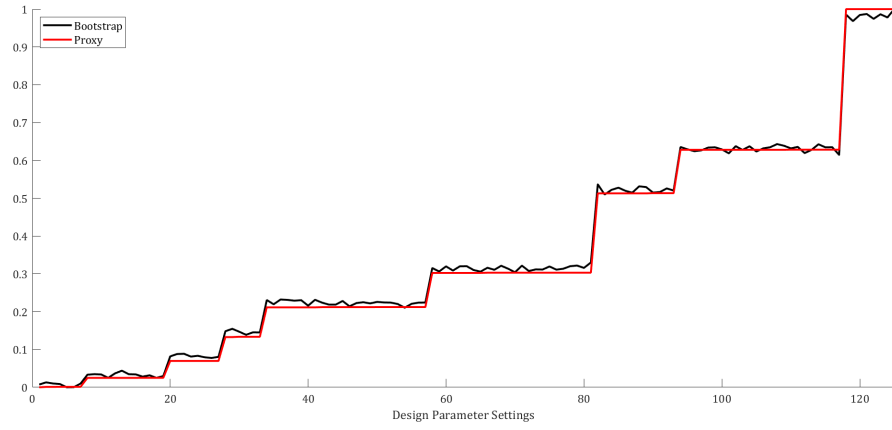
Figure 6.3 demonstrates the performance of the proxy functions given by Eqs. (6.11) and (6.13) in approximating the outcomes of our bootstrap procedure at various design parameter settings of the polymer experiment. We observe that the proxy functions capture the general pattern in the prediction region areas and the lengths of the simultaneous intervals generated by the bootstrap procedure across the design space. Naturally, the proxy function values are constant while the bootstrap prediction interval values vary at the design parameter settings equidistant from the design center in Euclidean distance.

While our demonstrations in Figure 6.3 are specific to the polymer experiment, we anticipate similar results for other problems, given the functional relationships between $A(\mathbf{x}_0)$ and $P_A(\mathbf{x})$ as well as between $L_i(\mathbf{x}_0)$ and $P_{L_i}(\mathbf{x}) \forall i \in \{1, 2\}$. Based on the discussion in Efron and Tibshirani (1993, pp. 50-52), as B approaches to ∞ , both Q_c and Q_p converge to constant values (*i.e.*, $\hat{Q}_c$ and $\hat{Q}_p$). This implies that the parts of $A(\mathbf{x}_0)$ and $L_i(\mathbf{x}_0)$ that varies by $\mathbf{x}$ converge to $P_A(\mathbf{x})$ and $P_{L_i}(\mathbf{x})$, respectively.

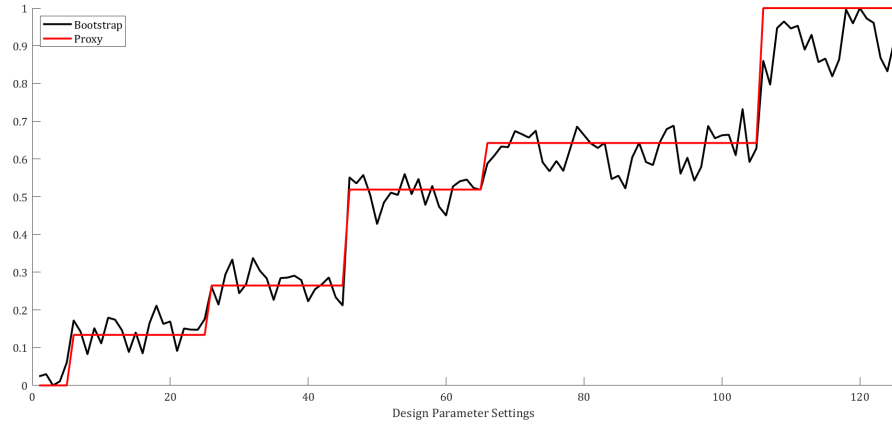
It is also worth mentioning that our interactive procedure can accommodate another computer intensive method replacing Algorithm 2 when constructing confidence and prediction regions for a given design parameter setting. In this situation, other proxy functions may more accurately reflect the results of the utilized bootstrap method into the mathematical models. Therefore, we recommend verifying the consistency between the outcomes of the utilized bootstrap method and associated proxy functions, in a similar manner presented in Figure 6.3.



(a) $A(\mathbf{x}_0)$ vs $P_A(\mathbf{x})$



(b) $L_1(\mathbf{x}_0)$ vs $P_{L_1}(\mathbf{x})$



(c) $L_2(\mathbf{x}_0)$ vs $P_{L_2}(\mathbf{x})$

Figure 6.3: Outcomes of our bootstrap procedure (in black) vs associated proxy function values (in red) at various design parameter settings of the polymer experiment, where y-axes denote the values scaled to the interval $[0, 1]$

Illustrative Example. We illustrate our solution procedure on polymer experiment presented in Appendix A. We assume that the collected data given in Table A.1 satisfies Assumption 6.2.1. However, in practice, the model assumptions should be supported by meaningful statistics. For the instructions on validating model assumptions, we refer to Srivastava and Giles (1987, pp. 346-351).

We do not assume an underlying value function in illustrating our procedure since it does not help us determine the DM's verbal preferences. Instead, we play the role of the DM and the DA. We assume that the DM is aware that improving a particular objective is possible only if at least one other objective gets worse (at a nondominated solution). However, the DA should be aware that there may be exceptions due to use of the proxy functions. For instance, the amount of relaxation in a proxy function may not be directly reflected on the associated performance measure due to the randomness within the bootstrapping procedure.

In this example, we assume that the DM is more interested in decreasing the distance between second response mean and its target.

Using the experimental data given in Table A.1 consisting of $n = 20$ observations for each of the responses, we fit the response surface models as follows,

$$\begin{aligned}\hat{y}_1(\mathbf{x}) &= 80.93 + 1.03x_1 + 4.11x_2 + 6.21x_3 - 1.63x_1^2 + 2.96x_2^2 \\ &\quad - 5.19x_3^2 + 2.03x_1x_2 + 11.37x_1x_3 - 3.80x_2x_3 \\ \hat{y}_2(\mathbf{x}) &= 60.51 + 3.59x_1 + 2.23x_3.\end{aligned}\tag{6.14}$$

$P_A(\mathbf{x})$ and $L_i(\mathbf{x}) \ \forall i \in \{1, 2\}$ are given by Eq. (6.11) and Eq. (6.13) with $\hat{\sigma}_{12} = \hat{\sigma}_{21} = -0.55$, $\hat{\sigma}_1^2 = 11.12$, $\hat{\sigma}_2^2 = 2.20$, $p_1 = 9$, and $p_2 = 2$. The objectives are $z_1(\mathbf{x}) = |\hat{y}_1(\mathbf{x}) - 100|$, $z_2(\mathbf{x}) = |\hat{y}_2(\mathbf{x}) - 57.5|$, $z_3(\mathbf{x}) = P_A(\mathbf{x})$, $z_4(\mathbf{x}) = L_1(\mathbf{x})$, and $z_5(\mathbf{x}) = L_2(\mathbf{x})$. We assume that the DM decides to set $\alpha = 0.1$.

We initialize the interactive optimization procedure by finding the ideal objective vector, $\mathbf{z}^* = [0.00 \ 0.00 \ 29.40 \ 0.00 \ 0.00]^T$.

The DA sets $h = 0$, $q = 2$, $r = 1$, $\delta_1 = 0.5$, $\tau_{\max} = 25$, $\tau_{\text{ext}} = 10$, $B = 9999$, and $D = 11$. Then, s/he generates the first Pareto frontier by solving the following problem,

$$\begin{aligned}
& \text{lex min } \{z_2(\mathbf{x}) - z_2^*, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& z_1(\mathbf{x}) \leq z_1^* + e_1^\tau \\
& -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{6.15}$$

until the stopping condition outlined in Algorithm 1 is satisfied (with no bounds on $z_j(\mathbf{x}) \ \forall j \in \{3, 4, 5\}$).

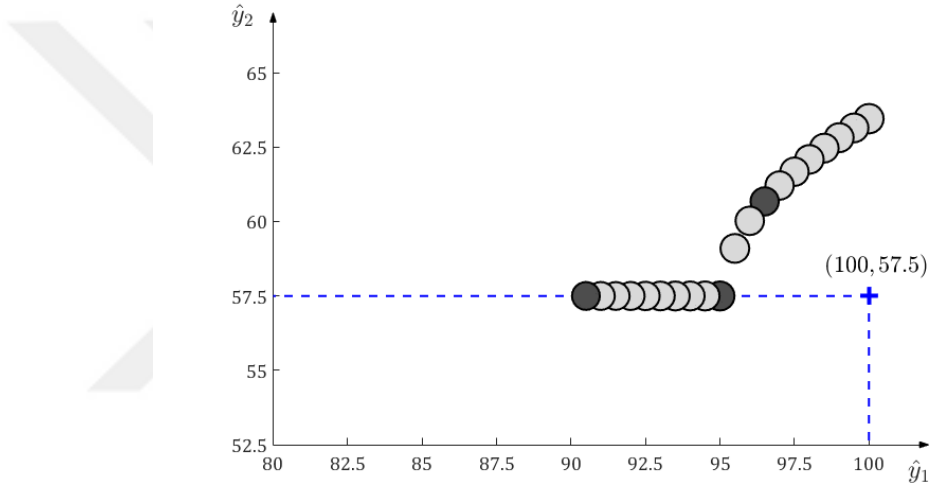


Figure 6.4: Visualization of a set of solutions on the Pareto frontier ($h = 0$): The three solutions selected by the DA to present to the DM are marked in black.

After examining the resulting set of solutions visualized in Figure 6.4, the DA selects three of them (marked in black) to present to the DM. Table 6.1 shows the resulting values of the performance measures associated with the selected solutions visualized in Figure 6.5.

Table 6.1: Numerical results ($h = 0$)

$\hat{y}_1(\mathbf{x}^0)$	$ \hat{y}_1(\mathbf{x}^0) - t_1 $	$\hat{y}_2(\mathbf{x}^0)$	$ \hat{y}_2(\mathbf{x}^0) - t_2 $	$A(\mathbf{x}^0)$	$\text{SPI}_1(\mathbf{x}^0)$	$\ell_1(\mathbf{x}^0)$	$\text{SPI}_2(\mathbf{x}^0)$	$\ell_2(\mathbf{x}^0)$
96.50	3.50	60.68	3.18	226.35	[82.32, 110.68]	28.27	[55.58, 65.78]	10.20
95.00	5.00	57.50	0.00	237.03	[80.23, 109.77]	29.55	[52.37, 62.63]	10.25
90.50	9.50	57.50	0.00	216.32	[77.11, 103.89]	26.78	[52.33, 62.67]	10.33

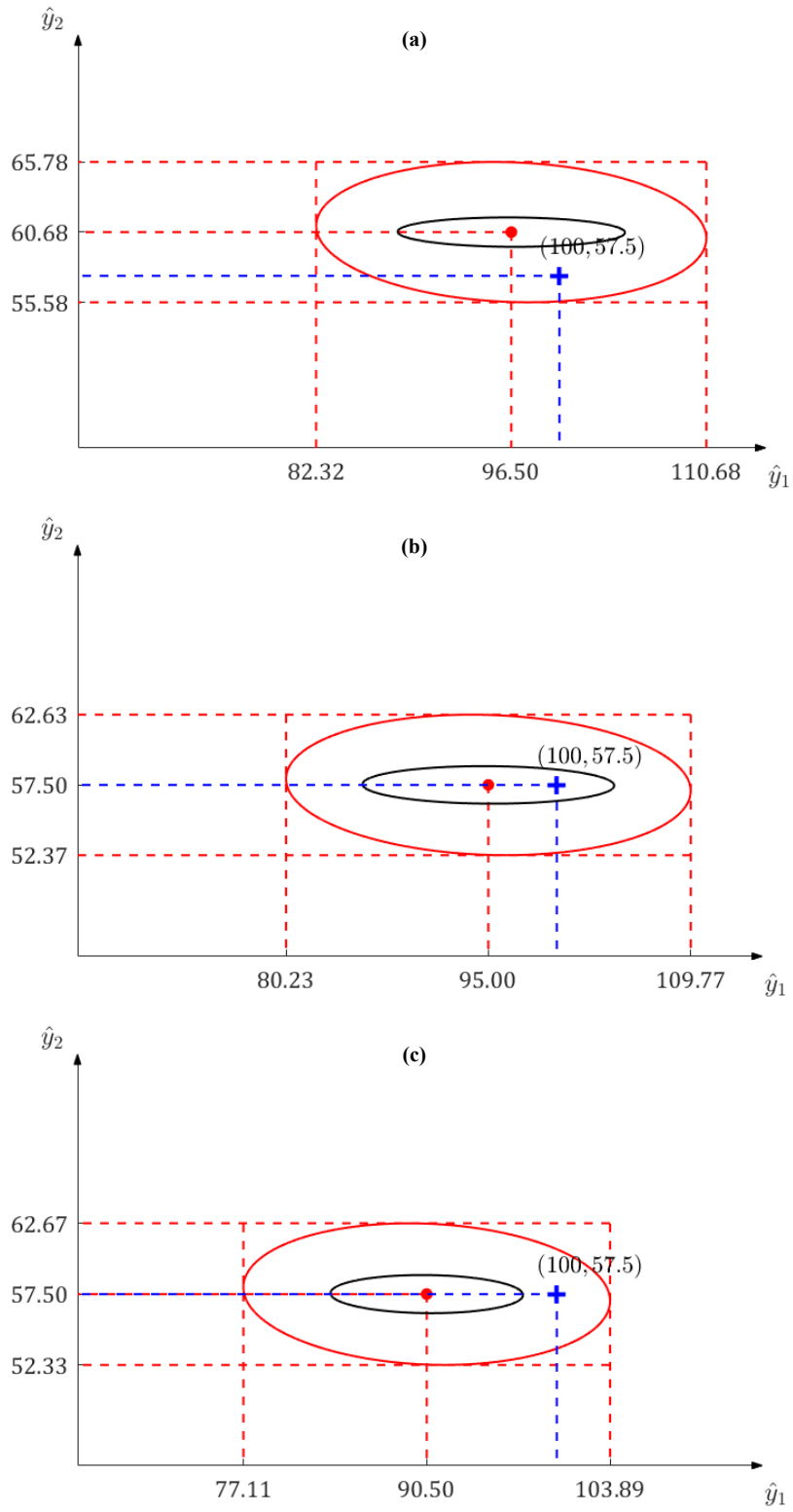


Figure 6.5: Visualization of the selected solutions for $h = 0$

The DA presents Table 6.1 and Figure 6.5 to the DM and informs her/him about the fact that the differences in prediction region areas arise from the uncertainty in response surface model coefficients since robustness is equal over the solution space.

The DM states that $\hat{y}_2$ and $\hat{y}_1$ are far from their targets in solutions (a) and (c) respectively. S/he likes solution (b) in terms of distances to the target. However, s/he adds that the uncertainty around the response means is too high in all solutions and s/he wants to see if solutions with smaller prediction region areas can be found without getting far from the target. Considering the comments of the DM, the DA decides to obtain a new frontier by bounding $P_A(\mathbf{x})$. S/he sets $u_3^1 \leq \min\{P_A(\mathbf{x}_a^0), P_A(\mathbf{x}_b^0), P_A(\mathbf{x}_c^0)\}$ to ensure that the observed solutions are not among the solutions to be generated. Since $\min\{P_A(\mathbf{x}_a^0), P_A(\mathbf{x}_b^0), P_A(\mathbf{x}_c^0)\} = 6.13$, s/he sets $h = 1$ and $u_3^1 = 6$ considering that selecting a smaller value may lead to higher sacrifices from distances to the targets. S/he adds $z_3(\mathbf{x}) \leq u_3^1$ to the initial mathematical model and solves the following problem,

$$\begin{aligned}
& \text{lex min } \{z_2(\mathbf{x}) - z_2^*, \mathbf{1}^T(\mathbf{z}(\mathbf{x}) - \mathbf{z}^*(\mathbf{x}))\} \\
& \text{subject to} \\
& z_1(\mathbf{x}) \leq z_1^* + e_1^T \\
& z_3(\mathbf{x}) \leq u_3^1 \\
& -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\}.
\end{aligned} \tag{6.16}$$

for until the stopping condition is met. S/he obtains a new subset of solutions on the Pareto frontier shown in Figure 6.6.

The DA observes that the response means get far from their targets in return to slight decreases in the prediction region areas. Based on the verbal preferences of the DM, s/he selects the three solutions marked in black in Fig. 6.6. S/he presents the DM with Tab. 6.2 which shows the values of the performance measures associated to the selected solutions and Fig. 6.7 visualizing the selected solutions individually.

The DM does not like solution (a) since s/he finds $\hat{y}_2$ far from its target. On the other hand, s/he likes solutions (b) and (c) for their proximities to the second response target. However, s/he still finds the prediction regions of all the

presented solutions large. In addition, s/he finds it unacceptable to sacrifice from the distance to first response mean in solutions (b) and (c) in return for slightly decreased prediction region areas. The DA informs the DM about that solution (c) is the one at the shortest distance to the first response target among the ones where the second response mean is at its target. That is, it is not possible to obtain solutions closer to the first response mean without sacrificing from the distance to the second response target while remaining the prediction region areas similar to that of the solutions (b) and (c).

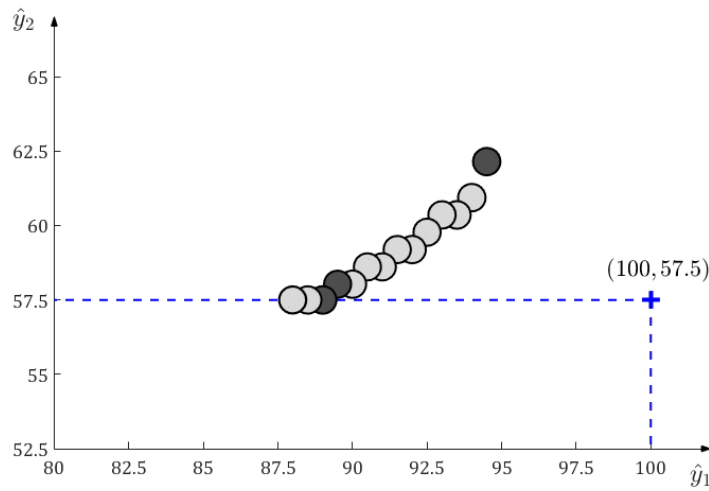


Figure 6.6: Visualization of a set of solutions on the Pareto frontier ($h = 1$): The three solutions selected by the DA to present to the DM are marked in black.

Table 6.2: Numerical results ($h = 1$)

$\hat{y}_1(\mathbf{x}^1)$	$ \hat{y}_1(\mathbf{x}^1) - t_1 $	$\hat{y}_2(\mathbf{x}^1)$	$ \hat{y}_2(\mathbf{x}^1) - t_2 $	$A(\mathbf{x}^1)$	$\text{SPI}_1(\mathbf{x}^1)$	$\ell_1(\mathbf{x}^1)$	$\text{SPI}_2(\mathbf{x}^1)$	$\ell_2(\mathbf{x}^1)$
94.50	5.50	62.15	4.65	208.70	[81.37, 107.63]	26.25	[57.06, 67.23]	10.17
89.50	10.50	58.03	0.53	205.91	[76.63, 102.37]	25.75	[52.91, 63.15]	10.24
89.00	11.00	57.50	0.00	208.39	[76.05, 101.95]	25.91	[52.35, 62.65]	10.30

We assume that DM selects solution (b) from the initial solution set and the procedure ends. S/he decides that s/he is not willing to sacrifice much from the distances of the response means to their respective targets since the prediction region areas are not improving much in return. Besides, in solution (b) of the initial solution set, the confidence region covers the target.

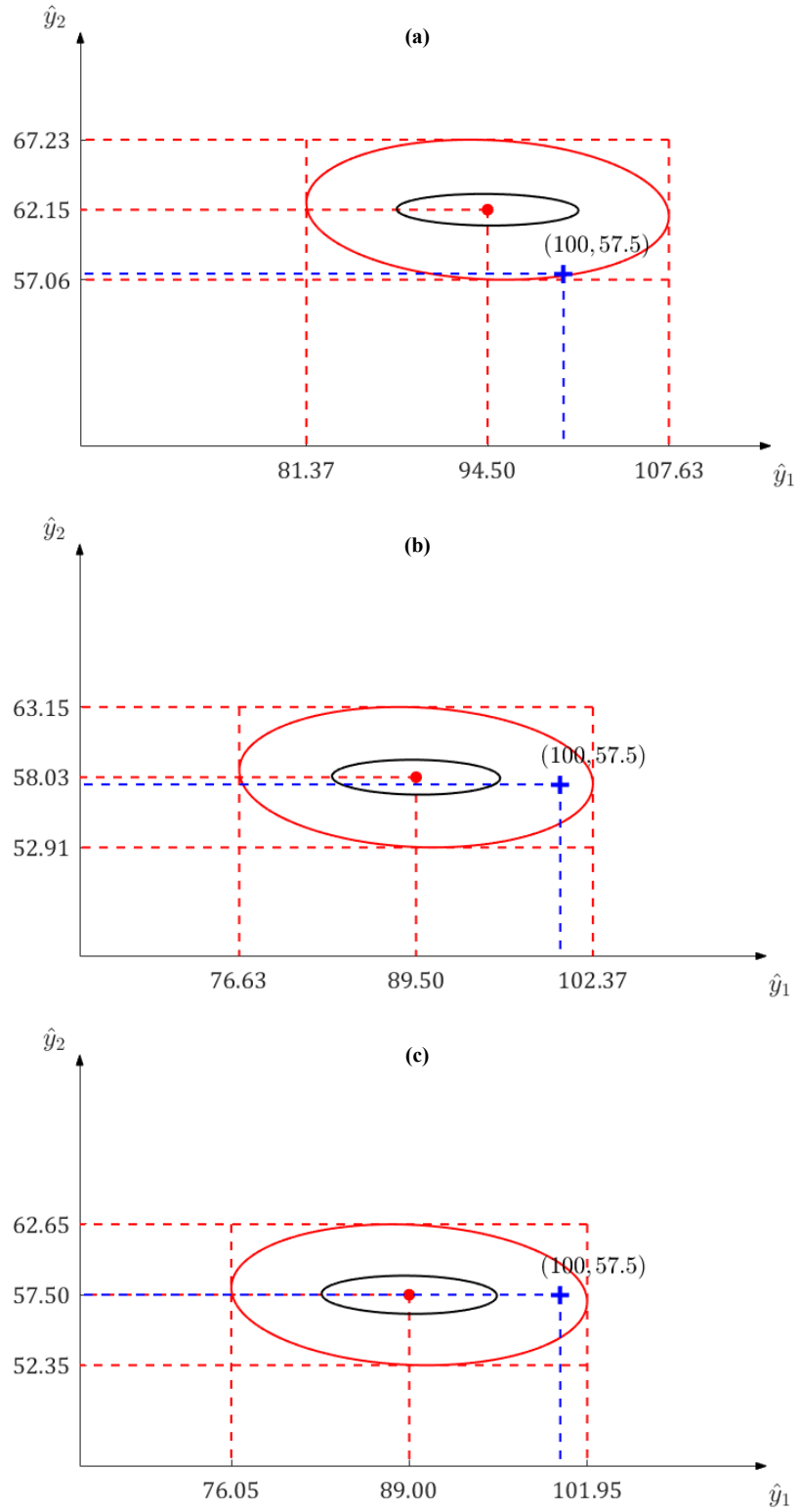


Figure 6.7: Visualization of the selected solutions for $h = 1$



CHAPTER 7

CONCLUSIONS AND FUTURE RESEARCH DIRECTIONS

In this study, we address product and process design optimization problems with two responses. Our extensive literature review shows that the majority of the existing MRO approaches assume that the preferences of the DM are known prior to the solution procedure. This is a strong assumption that is hard to justify in practice. Moreover, the three-stage MRO methodology involves uncertainty arising from various sources of errors during the data collection and empirical model building stages, which propagate to the optimization stage and affect the precision of the expected outcomes of the decisions. Assuming that the measurement errors are minimized, the selected model structure is correct, and the variance of the random errors is constant over the design parameter space, we analyze the variance of a predicted response. Our analysis shows that, despite the aforementioned simplifications, the predictions are affected by the variability in the coefficients of the empirical model. Disregarding this issue may result in selecting design parameter settings where responses perform worse than anticipated.

Addressing the challenge of extracting the DM's preferences beforehand, several approaches incorporate DM's preferences into the solution process in an interactive manner. Only two of those interactive approaches (Park and Kim, 2005; He et al., 2021) consider model parameter uncertainty in the empirical functions, while the rest use the point estimates of the responses in searching for the desirable design parameter settings in the optimization stage.

We evaluate the two interactive MRO approaches taking model parameter uncertainty into account from a MOO perspective to point out their limitations in

addressing model parameter uncertainty effectively in their interactive search procedures. Our demonstrations show that those interactive MRO approaches may fail to guide the search towards the desired regions for the DM, primarily due to the issues in how they consider the model parameter uncertainty in their interactive search procedures.

In addition to the demonstrated deficiencies, Park and Kim (2005) completely ignores RPD problems which are not uncommon to encounter in practice. He et al. (2021) illustrate an RPD scenario by involving empirical models for variances of responses as functions of relevant design parameters. However, the response surface models are built by assuming constant variances of responses which ignores the heteroskedasticity of response variances that naturally arise in RPD problems.

To overcome the issues with the existing approaches, we develop two interactive approaches considering DM's preferences under model parameter uncertainty for product and process design problems with two responses. Assuming that the data is appropriately collected prior to our solution procedures, we focus on two solution stages: empirical model building and optimization.

Our approaches empower the DM to consider the area of the joint prediction region, which represents uncertainty due to model parameters and random errors, and the distances of estimated response values from their target values as performance measures. To facilitate the interaction with the DM, we produce visual aids on the performance measures such as joint confidence and prediction regions of the responses at design parameter settings under consideration. At each interaction iteration, the DA supports the DM in converting her/his verbal preferences into mathematical expressions and searching the solution space. The procedure continues until the DM is satisfied with a solution.

The main differences between our two approaches arise from the differences in the empirical model building. In the first approach (Sec. 5.1), we fit response surface models by using MVR or OLS regression under equal robustness (Sec. 5.2) and WLS regression under unequal robustness (Sec. 5.3). We use closed-form functions of the prediction region area directly as an objective in our mathematical

models and visualize the resulting region. For this purpose, we incorporate the developments in econometrics literature on approximate closed form confidence and prediction interval formulations for WLS regression, while we use the widely known exact closed-form formulations for MVR and OLS regression.

None of MVR, OLS regression, and WLS regression is appropriate when response surface models contain different sets of regressors with the existence of correlations among responses. To consider such cases, we build empirical models by using SUR under equal robustness in the second approach (Ch. 6). To overcome the difficulty in the utilization of the exact distribution of the SUR estimator, we develop a bootstrapping procedure that estimates the resulting joint confidence and prediction regions at a given design parameter setting. Therefore, in the second approach, we use proxy functions of the joint confidence and/or prediction region area in our mathematical models, while we present the values calculated as a result of the associated bootstrapping procedure at the design parameter setting under consideration in interacting with the DM. Although some general knowledge about the effects of changing proxy measures on the prediction region area exists, the exact magnitudes of those effects are not known since they are determined by complex problem characteristics. For this reason, the search process differs from the first approach in that we actively involve the DA in the search process to help the DM to converge to her/his preferred solutions quickly. Our approach supports the DA's search by generating visual aids on which the DA progressively observes the relevant parts of the solution space to identify the ones that may be attractive to the DM.

We illustrate our approaches using the polymer experiment, which is a well-known two response problem in the MRO literature, under three scenarios. The illustrations provide practical guidance on both empirical model building and the interactive search process, and demonstrate the effectiveness of our approaches.

The contributions of this study to the MRO literature are mainly threefold. First, we are the first to properly consider the possible correlations among the responses under model parameter uncertainty in an interactive procedure through the first and second approaches under MVR and SUR conditions, respectively. Second,

the first approach under WLS conditions (Sec. 5.3) is the first interactive MRO procedure considering an RPD scenario without ignoring the resulting heterogeneity in building response surface models under model parameter uncertainty. It is worth mentioning that DRO problems become a special case of our first approach under WLS conditions, which implies that it can be effortlessly adapted and applied to those problems as well. Third, our discussions and demonstrations on the issues with the existing two interactive MRO approaches considering model parameter uncertainty not only point out their issues but also inspire future developments. Some additional contributions include the construction of a bootstrapping procedure to measure the uncertainty associated with the SUR predictions for illustrative purposes and the incorporation of developments from econometrics literature in considering an RPD scenario.

Compared to the existing interactive MRO approaches considering model parameter uncertainty, we present the uncertainty associated with the solutions to the DM in a way that eases its interpretation. Our visual aids also help the DM in improving her/his perception. Moreover, we allow the DM to change her/his mind and past responses, and to return to a solution or a set of solutions for reevaluation so that the DM learns about the possible solutions throughout the solution procedure and better understands her/his preferences. Our approaches not only aim to converge to a final solution but also to help the DM discover the limitations of the system of interest and justify further efforts such as tolerance design or technological advancements if needed. The role of the DA and her/his search is important, especially in the second approach (Ch. 6) due to the difficulties in directly controlling some of the objectives. We believe that incorporating such a search phase into interactive approaches may be an important contribution to solving multiple objective problems that have complex feasible sets and objective functions that cannot be directly controlled.

Our approaches have some limitations that we consider as rooms for future research. One limitation is that our framework, presented as a flow chart in Figure 4.5, does not address situations where the variances of uncorrelated responses exhibit heteroskedasticity and the number of observations is small. This limitation arises because our first approach under WLS conditions (Sec. 5.3) relies

on approximate confidence and prediction interval formulations. The coverage of these approximate regions in WLS estimation is often below the nominal level, particularly when there is a small number of observations. DiCiccio et al. (2019) show that a bootstrap approximation allows for inference with improved finite-sample properties. Therefore, when it is not practical to collect a large number of observations, constructing confidence intervals with the wild bootstrap technique may be a better approach. However, the construction of the prediction intervals deserves more research.

Figure 4.5 also indicates another potential direction of future research, referred to as the general case. The regression methods we consider in this thesis have certain assumptions that limit their effectiveness in modeling the general case where the variances of correlated responses vary by the design parameter settings. The remedy for the construction of joint confidence and prediction regions may not be readily available in the statistics and/or econometrics literature. One possibility may be investigating semi-parametric and nonparametric methods. These methods typically provide other advantages due to their distribution-free assumptions.

Furthermore, more than two responses may be of interest in practice. To extend our approaches to those cases, we mainly need to reconsider the visualization of the performance measures in interacting with the DM. For three-response problems, we may still use the current framework by presenting the joint confidence and prediction regions to the DM as ellipsoids and providing their volumes. For problems with more than three responses, we may use binary combinations of the responses to obtain the confidence and prediction regions and we may use parallel coordinate plots to visualize the response values on the same graph. If the large number of responses increases the DM's cognitive burden, it may be useful to define additional performance measures, such as multivariate capability indices, to facilitate communication with the DM.

We only consider target specifications of the responses while quality characteristics are also evaluated with respect to interval forms of the specifications referred to as specification limits, within which the response values are to lie. Process

fallout probability may be an appropriate performance measure to consider specification limits in our approaches. To formulate the process fallout probability, the cumulative distribution function approximation of bivariate normal distribution is required in closed form. However, to the best of our knowledge, an appropriate function approximation is not available in the literature. Hence, some proxy functions such as multivariate capability indices may be incorporated in approximating the fallout probability to be considered our approaches.

The responses may be bounded in MRO problems such as the first response in the polymer experiment that measures the yield in percent; therefore, its physical upper bound is 100. Similar to all the existing studies using the polymer experiment in their illustrations, our approaches ignore the bounded structure of the first response in building the corresponding response surface model. Therefore, the confidence and prediction regions unrealistically extend beyond 100 in the visualizations. For modeling such responses, β -regression (Ferrari and Cribari-Neto, 2004) is appropriate. Incorporating β -regression into our approaches requires further efforts on the construction of the joint prediction regions, which can be an interesting direction for future research.

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Appendix A

ILLUSTRATIVE EXAMPLE: POLYMER EXPERIMENT

We illustrate our approaches on polymer experiment, a two-response problem widely used in the literature.

Polymer experiment is a chemical process originally presented in Box et al. 1978 and transformed into a multi response problem example in Myers and Montgomery 1995. The problem has been used in many studies in MRO literature including Köksalan and Plante 2003; Park and Kim 2005; Ko et al. 2005; Costa and Lourenço 2017; Ouyang et al. 2017; Wang et al. 2020.

In this problem, responses of interest are conversion of a polymer and thermal activity, which are larger-the-better (LTB) and nominal-the-best (NTB) type responses, respectively. The aim of the experiment is to determine the settings of the design parameters; reaction time, reaction temperature, and the amount of catalyst, to maximize the conversion and to achieve a target value of 57.5 for the thermal activity.

The conducted experiment is a CCD with eight factorial points, six axial points and a total of six center points. The experimental runs are not replicated, *i.e.*, $r = 0$. The original data of the experiment is given in Table A.1.

Table A.1: The Results of Polymer Experiment

x_1	x_2	x_3	y_1	y_2
-1	-1	-1	74.0	53.2
1	-1	-1	51.0	62.9
-1	1	-1	88.0	53.4
1	1	-1	70.0	62.6
-1	-1	1	71.0	57.3
1	-1	1	90.0	67.9
-1	1	1	66.0	59.8
1	1	1	97.0	67.8
-1.682	0	0	76.0	59.1
1.682	0	0	79.0	65.9
0	-1.682	0	85.0	60.0
0	1.682	0	97.0	60.7
0	0	-1.682	55.0	57.4
0	0	1.682	81.0	63.2
0	0	0	81.0	59.2
0	0	0	75.0	60.4
0	0	0	76.0	59.1
0	0	0	83.0	60.6
0	0	0	80.0	60.8
0	0	0	91.0	58.9

Appendix B

SUPPLEMENTARY MATERIAL FOR THE EVALUATIONS ON THE REVISED GDF PROCEDURE

B.1 Iterations for $\omega = (0.15, 0.15, 0.35, 0.35)$ and $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$

Table B.1: Determination of the optimal step size, $t^{(1)*}$, once solved to optimality

t	0.00	0.10	0.20	0.2363	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	1.32	0.89	0.66	0.61	0.56	0.56	0.66	0.88	1.30	2.01	3.13	4.83
v_2	0.18	0.12	0.08	0.07	0.05	0.05	0.07	0.11	0.17	0.25	0.35	0.46
d_1	0.79	0.76	0.75	0.76	0.78	0.84	0.93	0.00	0.00	0.00	0.00	0.00
d_2	0.00	0.27	0.96	0.79	0.35	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.79	95.13	95.08	95.22	95.65	96.83	98.62	101.02	104.03	107.66	111.90	116.76
y_2	53.96	55.68	57.40	58.02	59.12	60.84	62.55	64.27	65.99	67.71	69.43	71.15
$U \times 10^2$	-19.40	-1.83	-0.06	-0.03	-0.28	-1.51	-1.53	-3.75	-14.00	-89.20	-455.37	-1839.83

Table B.2: Determination of the optimal step size, $t^{(2)*}$, once solved to optimality

t	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.61	0.70	0.82	1.00	1.23	1.54	1.94	2.44	3.08	3.86	4.83
v_2	0.07	0.08	0.10	0.13	0.16	0.20	0.24	0.29	0.34	0.40	0.46
d_1	0.76	0.76	0.77	0.79	0.81	0.84	0.88	0.93	0.98	0.00	0.00
d_2	0.79	0.86	0.51	0.16	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.22	95.22	95.39	95.70	96.18	96.81	97.59	98.53	99.62	100.87	102.28
y_2	58.02	57.15	56.28	55.41	54.54	53.67	52.80	51.93	51.06	50.18	49.31
$U \times 10^2$	-0.03	-0.10	-0.60	-3.11	-10.44	-29.67	-78.87	-192.39	-434.05	-918.85	-1839.83

B.2 Iterations for $\omega = (0.35, 0.35, 0.15, 0.15)$ and $\mathbf{x}^{(1)} = (-1.0, 1.6, -0.9)$

Table B.3: Determination of the optimal step size, $t^{(1)*}$, where t is discretized

t	0.00	0.10	0.20	0.30	0.32	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	1.32	0.89	0.66	0.56	0.55	0.56	0.66	0.88	1.30	2.01	3.13	4.83
v_2	0.18	0.12	0.08	0.05	0.05	0.05	0.07	0.11	0.17	0.25	0.35	0.46
d_1	0.79	0.76	0.75	0.78	0.79	0.84	0.93	0.00	0.00	0.00	0.00	0.00
d_2	0.00	0.27	0.96	0.35	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.79	95.13	95.08	95.65	95.83	96.83	98.62	101.02	104.03	107.66	111.90	116.76
y_2	53.96	55.68	57.40	59.12	59.46	60.84	62.55	64.27	65.99	67.71	69.43	71.15
$U \times 10^2$	-530.60	-41.73	-1.60	-0.33	-0.32	-0.37	-1.06	-22.17	-326.22	-2555.17	-13409.33	-54447.31

Table B.4: Determination of the optimal step size, $t^{(2)*}$, where t is discretized.

t	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.55	0.60	0.69	0.82	1.02	1.30	1.68	2.19	2.86	3.73	4.83
v_2	0.05	0.06	0.08	0.10	0.13	0.17	0.21	0.26	0.32	0.39	0.46
d_1	0.79	0.78	0.77	0.78	0.79	0.82	0.86	0.91	0.96	0.00	0.00
d_2	0.22	0.62	0.97	0.57	0.16	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.83	95.53	95.43	95.55	95.88	96.41	97.16	98.13	99.30	100.68	102.28
y_2	59.46	58.45	57.43	56.42	55.40	54.39	53.37	52.36	51.34	50.33	49.31
$U \times 10^2$	-0.32	-0.49	-1.74	-12.15	-73.29	-333.04	-1206.79	-3689.26	-9915.02	-24137.72	-54447.31

Table B.5: Determination of the optimal step size, $t^{(1)*}$, once solved to optimality

t	0.00	0.10	0.20	0.30	0.3244	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	1.32	0.89	0.66	0.56	0.55	0.56	0.66	0.88	1.30	2.01	3.13	4.83
v_2	0.18	0.12	0.08	0.05	0.05	0.05	0.07	0.11	0.17	0.25	0.35	0.46
d_1	0.79	0.76	0.75	0.78	0.79	0.84	0.93	0.00	0.00	0.00	0.00	0.00
d_2	0.00	0.27	0.96	0.35	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.79	95.13	95.08	95.65	95.88	96.83	98.62	101.02	104.03	107.66	111.90	116.76
y_2	53.96	55.68	57.40	59.12	59.54	60.84	62.55	64.27	65.99	67.71	69.43	71.15
$U \times 10^2$	-530.60	-41.73	-1.60	-0.33	-0.32	-0.37	-1.06	-22.17	-326.22	-2555.17	-13409.33	-54447.31

Table B.6: Determination of the optimal step size, $t^{(2)*}$, once solved to optimality

t	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.55	0.60	0.68	0.81	1.01	1.29	1.67	2.18	2.85	3.72	4.83
v_2	0.05	0.06	0.08	0.10	0.13	0.17	0.21	0.26	0.32	0.39	0.46
d_1	0.79	0.78	0.77	0.78	0.79	0.82	0.86	0.91	0.96	0.00	0.00
d_2	0.19	0.59	1.00	0.59	0.18	0.00	0.00	0.00	0.00	0.00	0.00
y_1	95.88	95.55	95.44	95.55	95.86	96.40	97.14	98.11	99.28	100.67	102.28
y_2	59.54	58.51	57.49	56.47	55.45	54.43	53.40	52.38	51.36	50.34	49.31
$U \times 10^2$	-0.32	-0.47	-1.57	-11.01	-68.19	-316.60	-1165.54	-3605.93	-9781.28	-23989.64	-54447.31

B.3 Iterations for $\omega = (0.15, 0.15, 0.35, 0.35)$ and $\mathbf{x}^{(1)} = (1.3, -0.6, -1.4)$

Table B.7: Determination of the optimal step size, $t^{(1)*}$, where t is discretized

t	0.00	0.10	0.20	0.30	0.40	0.50	0.56	0.60	0.70	0.80	0.90	1.00
v_1	1.12	0.56	0.31	0.22	0.21	0.24	0.30	0.36	0.68	1.37	2.65	4.83
v_2	0.32	0.21	0.13	0.08	0.05	0.05	0.07	0.08	0.14	0.22	0.33	0.46
d_1	0.92	0.65	0.41	0.21	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.00	0.00	0.00	0.00	0.00	0.36	0.83	0.86	0.07	0.00	0.00	0.00
y_1	98.40	92.97	88.27	84.30	81.05	78.53	77.37	76.74	75.67	75.33	75.71	76.83
y_2	68.89	66.93	64.97	63.02	61.06	59.10	57.93	57.14	55.19	53.23	51.27	49.31
$U \times 10^2$	-285.46	-38.67	-4.10	-2.11	-2.71	-1.75	-1.51	-1.56	-5.88	-49.71	-353.11	-1839.83

Table B.8: Determination of the optimal step size, $t^{(2)*}$, where t is discretized

t	0.00	0.10	0.20	0.22	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.30	0.33	0.39	0.40	0.49	0.66	0.92	1.30	1.83	2.56	3.54	4.83
v_2	0.07	0.07	0.08	0.08	0.10	0.13	0.16	0.20	0.26	0.32	0.39	0.46
d_1	0.00	0.00	0.03	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.83	0.87	0.92	0.93	0.96	0.99	0.95	0.90	0.86	0.82	0.77	0.73
y_1	77.37	79.50	80.68	80.79	80.88	80.12	78.39	75.69	72.03	67.40	61.81	55.25
y_2	57.93	57.82	57.70	57.68	57.59	57.48	57.37	57.26	57.15	57.04	56.93	56.82
$U \times 10^2$	-1.51	-1.51	-1.35	-1.34	-1.56	-3.28	-10.00	-33.95	-106.61	-300.55	-771.27	-1838.34

Table B.9: Determination of the optimal step size, $t^{(3)*}$, where t is discretized

t	0.00	0.07	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.40	0.38	0.38	0.40	0.46	0.58	0.79	1.13	1.63	2.37	3.41	4.83
v_2	0.08	0.07	0.07	0.07	0.08	0.10	0.13	0.17	0.23	0.30	0.37	0.46
d_1	0.04	0.08	0.10	0.18	0.29	0.41	0.55	0.71	0.89	0.00	0.00	0.00
d_2	0.93	0.55	0.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	80.79	81.62	82.04	83.68	85.71	88.14	90.96	94.18	97.79	101.80	106.20	110.99
y_2	57.68	58.63	59.03	60.38	61.72	63.07	64.41	65.76	67.11	68.45	69.80	71.15
$U \times 10^2$	-1.34	-1.14	-1.19	-2.17	-1.92	-1.95	-3.72	-14.32	-59.13	-213.55	-661.39	-1839.83

Table B.10: Determination of the optimal step size, $t^{(4)*}$, where t is discretized

t	0.00	0.04	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.38	0.41	0.47	0.59	0.76	1.00	1.32	1.73	2.27	2.94	3.79	4.83
v_2	0.07	0.08	0.09	0.11	0.14	0.17	0.20	0.25	0.29	0.34	0.40	0.46
d_1	0.08	0.09	0.08	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.55	0.58	0.62	0.69	0.77	0.84	0.91	0.98	0.94	0.87	0.80	0.73
y_1	81.62	81.72	81.69	81.16	80.03	78.29	75.96	73.02	69.48	65.33	60.59	55.25
y_2	58.63	58.55	58.44	58.26	58.08	57.90	57.72	57.54	57.36	57.18	57.00	56.82
$U \times 10^2$	-1.14	-1.13	-1.20	-1.87	-4.47	-12.00	-32.98	-84.75	-201.10	-444.33	-925.41	-1838.34

Table B.11: Determination of the optimal step size, $t^{(5)*}$, where t is discretized

t	0.00	0.01	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.41	0.41	0.41	0.45	0.54	0.68	0.92	1.27	1.79	2.51	3.50	4.83
v_2	0.08	0.08	0.07	0.07	0.09	0.11	0.14	0.19	0.24	0.31	0.38	0.46
d_1	0.09	0.09	0.16	0.25	0.35	0.47	0.61	0.76	0.94	0.00	0.00	0.00
d_2	0.58	0.53	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	81.72	81.85	83.15	84.90	87.00	89.42	92.18	95.28	98.70	102.47	106.56	110.99
y_2	58.55	58.68	59.81	61.07	62.33	63.59	64.85	66.11	67.37	68.63	69.89	71.15
$U \times 10^2$	-1.13	-1.12	-1.87	-2.01	-1.89	-2.41	-6.11	-22.45	-80.14	-254.79	-715.64	-1839.83

Table B.12: Determination of the optimal step size, $t^{(6)*}$, where t is discretized

t	0.00	0.01	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.41	0.41	0.45	0.53	0.65	0.84	1.11	1.50	2.02	2.72	3.64	4.83
v_2	0.08	0.08	0.08	0.09	0.11	0.14	0.17	0.22	0.27	0.33	0.39	0.46
d_1	0.09	0.09	0.06	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.53	0.57	0.90	0.72	0.35	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	81.85	81.78	81.17	80.53	79.93	79.37	78.85	78.37	77.92	77.52	77.15	76.83
y_2	58.68	58.59	57.74	56.81	55.87	54.93	54.00	53.06	52.12	51.19	50.25	49.31
$U \times 10^2$	-1.12	-1.12	-1.23	-1.54	-2.60	-6.56	-16.42	-47.06	-131.03	-338.94	-814.56	-1839.83

Table B.13: Determination of the optimal step size, $t^{(7)*}$, where t is discretized

t	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.41	0.51	0.64	0.82	1.07	1.39	1.80	2.34	3.00	3.82	4.83
v_2	0.08	0.09	0.12	0.14	0.17	0.21	0.25	0.30	0.35	0.40	0.46
d_1	0.09	0.08	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.57	0.64	0.71	0.78	0.85	0.92	0.99	0.94	0.87	0.80	0.73
y_1	81.78	81.66	80.98	79.73	77.92	75.55	72.62	69.12	65.06	60.43	55.25
y_2	58.59	58.41	58.23	58.05	57.88	57.70	57.52	57.35	57.17	56.99	56.82
$U \times 10^2$	-1.12	-1.29	-2.27	-5.58	-14.77	-38.89	-95.70	-218.66	-467.88	-948.01	-1838.34

Table B.14: Determination of the optimal step size, $t^{(1)*}$, once solved to optimality

t	0.00	0.10	0.20	0.30	0.40	0.50	0.5577	0.60	0.70	0.80	0.90	1.00
v_1	1.12	0.56	0.31	0.22	0.21	0.24	1.12	0.36	0.68	1.37	2.65	4.83
v_2	0.32	0.21	0.13	0.08	0.05	0.05	0.32	0.08	0.14	0.22	0.33	0.46
d_1	0.92	0.65	0.41	0.21	0.05	0.00	0.92	0.00	0.00	0.00	0.00	0.00
d_2	0.00	0.00	0.00	0.00	0.00	0.36	0.00	0.86	0.07	0.00	0.00	0.00
y_1	98.40	92.97	88.27	84.30	81.05	78.53	98.40	76.74	75.67	75.33	75.71	76.83
y_2	68.89	66.93	64.97	63.02	61.06	59.10	68.89	57.14	55.19	53.23	51.27	49.31
$U \times 10^2$	-285.46	-38.67	-4.10	-2.11	-2.71	-1.75	-285.46	-1.56	-5.88	-49.71	-353.11	-1839.83

Table B.15: Determination of the optimal step size, $t^{(2)*}$, once solved to optimality

t	0.00	0.10	0.20	0.2210	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.30	0.32	0.38	0.30	0.49	0.66	0.92	1.29	1.83	2.56	3.54	4.83
v_2	0.07	0.07	0.08	0.07	0.10	0.13	0.16	0.20	0.26	0.32	0.39	0.46
d_1	0.00	0.00	0.03	0.00	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.81	0.86	0.90	0.81	0.95	1.00	0.96	0.91	0.87	0.82	0.77	0.73
y_1	77.41	79.53	80.69	77.41	80.89	80.12	78.39	75.69	72.03	67.40	61.80	55.25
y_2	57.97	57.86	57.74	57.97	57.63	57.51	57.39	57.28	57.16	57.05	56.93	56.82
$U \times 10^2$	-1.51	-1.51	-1.35	-1.51	-1.55	-3.25	-9.95	-33.87	-106.49	-300.44	-771.20	-1838.34

Table B.16: Determination of the optimal step size, $t^{(3)*}$, once solved to optimality

t	0	0.0713	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.40	0.40	0.38	0.40	0.46	0.59	0.80	1.13	1.64	2.37	3.41	4.83
v_2	0.08	0.08	0.07	0.07	0.08	0.10	0.13	0.17	0.23	0.30	0.37	0.46
d_1	0.04	0.04	0.10	0.19	0.29	0.41	0.55	0.71	0.89	0.00	0.00	0.00
d_2	0.91	0.91	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y_1	80.81	80.81	82.07	83.71	85.75	88.18	91.00	94.22	97.82	101.82	106.21	110.99
y_2	57.72	57.72	59.06	60.40	61.75	63.09	64.43	65.77	67.12	68.46	69.80	71.15
$U \times 10^2$	-1.33	-1.33	-1.21	-2.17	-1.92	-1.96	-3.79	-14.58	-59.88	-215.08	-663.47	-1839.83

Table B.17: Determination of the optimal step size, $t^{(4)*}$, once solved to optimality

t	0.00	0.0373	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.38	0.38	0.47	0.59	0.76	1.00	1.32	1.73	2.27	2.94	3.79	4.83
v_2	0.07	0.07	0.09	0.11	0.14	0.17	0.20	0.25	0.29	0.34	0.40	0.46
d_1	0.08	0.08	0.09	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.53	0.53	0.60	0.68	0.75	0.83	0.90	0.98	0.95	0.87	0.80	0.73
y_1	81.67	81.67	81.72	81.18	80.03	78.29	75.95	73.01	69.47	65.33	60.59	55.25
y_2	58.67	58.67	58.49	58.30	58.12	57.93	57.74	57.56	57.37	57.19	57.00	56.82
$U \times 10^2$	-1.15	-1.15	-1.20	-1.87	-4.47	-12.02	-33.05	-84.91	-201.39	-444.77	-925.86	-1838.34

Table B.18: Determination of the optimal step size, $t^{(5)*}$, once solved to optimality

t	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
v_1	0.41	0.50	0.64	0.82	1.06	1.39	1.80	2.34	3.00	3.82	4.83
v_2	0.08	0.09	0.12	0.14	0.17	0.21	0.25	0.30	0.35	0.40	0.46
d_1	0.09	0.08	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
d_2	0.56	0.63	0.70	0.77	0.84	0.92	0.99	0.94	0.87	0.80	0.73
y_1	81.76	81.61	80.90	79.64	77.82	75.45	72.52	69.03	64.99	60.40	55.25
y_2	58.60	58.43	58.25	58.07	57.89	57.71	57.53	57.35	57.17	56.99	56.82
$U \times 10^2$	-1.13	-1.32	-2.34	-5.72	-15.12	-39.64	-97.06	-220.78	-470.64	-950.58	-1838.34

B.4 Nondominance Check for the Solution of the Revised GDF

We solve Eq. (B.1) to find solutions further improving at least one of the objectives without deteriorating their values in the solution of the revised GDF if there are any.

$$\begin{aligned}
& \max d_1(\mathbf{x}) + d_2(\mathbf{x}) - v_1(\mathbf{x}) - v_2(\mathbf{x}) \\
& \text{subject to} \\
& d_1 \geq 0.0891 \\
& d_2 \geq 0.5660 \\
& v_1 \geq 0.0764 \\
& v_2 \geq 0.4144 \\
& d_1 \leq \frac{y_1(\mathbf{x}) - 80}{100 - 80} + M(1 - b_1) \\
& \frac{y_1(\mathbf{x}) - 80}{100 - 80} \leq 1 + M(1 - b_1) \\
& d_2 \leq \frac{y_2(\mathbf{x}) - 55}{57.5 - 55} + M(1 - b_2) \\
& d_2 \leq \frac{60 - y_2(\mathbf{x})}{60 - 57.5} + M(1 - b_2) \\
& d_i \leq Mb_i \quad \forall i \in \{1, 2\} \\
& b_i \in \{0, 1\} \quad \forall i \in \{1, 2\} \\
& -1.68 \leq x_k \leq 1.68 \quad \forall k \in \{1, 2, 3\},
\end{aligned} \tag{B.1}$$

B.5 Comparison with Random Selection of n Nondominated Solutions

Table B.19: Comparisons for $\mathbf{x}^{(1)} = (1.3, -0.6, 1.4)$

ω	$U_{\text{worst}} \times 10^4$	$U_{\text{best}} \times 10^4$	$U_{\text{pk}} \times 10^4$	$U_{\text{norm}} \times 10^2$	$P_s \times 10^2$	$P_{f(3)} \times 10^2$	$P_{f(5)} \times 10^2$
(0.05, 0.05, 0.45, 0.45)	-820.22	-0.65	-244.78	70.21	29.87	97.33	99.76
(0.15, 0.15, 0.35, 0.35)	-308.19	-2.87	-111.50	64.42	25.44	98.35	99.89
(0.25, 0.25, 0.25, 0.25)	-140.35	-3.08	-40.42	72.79	28.16	97.77	99.82
(0.35, 0.35, 0.15, 0.15)	-283.88	-1.16	-5.80	98.36	62.22	75.92	90.68
(0.45, 0.45, 0.05, 0.05)	-775.72	-0.04	-0.14	99.99	82.42	44.02	61.97

Table B.20: Comparisons for $\mathbf{x}^{(1)} = (0.3, -1.2, -0.5)$

ω	$U_{\text{worst}} \times 10^4$	$U_{\text{best}} \times 10^4$	$U_{\text{pk}} \times 10^4$	$U_{\text{norm}} \times 10^2$	$P_s \times 10^2$	$P_{f(3)} \times 10^2$	$P_{f(5)} \times 10^2$
(0.05, 0.05, 0.45, 0.45)	-820.22	-0.65	-246.19	70.04	29.62	97.40	99.77
(0.15, 0.15, 0.35, 0.35)	-308.19	-2.87	-99.23	68.44	27.05	98.02	99.86
(0.25, 0.25, 0.25, 0.25)	-140.35	-3.08	-37.65	74.81	32.04	96.71	99.66
(0.35, 0.35, 0.15, 0.15)	-283.88	-1.16	-6.77	98.02	56.57	81.89	94.20
(0.45, 0.45, 0.05, 0.05)	-775.72	-0.04	-1.04	99.87	71.34	63.70	81.53

B.6 Implementation of the Original GDF Method

In this section, we provide a detailed explanation of the overall utility function and the objective functions used in the implementation of the original GDF method. Additionally, we explain the specific steps taken to generate Table 3.9.

We assume the following objective functions in maximization form,

$$\begin{aligned} f_1(x_1, x_2) &= -x_1^2 - x_2^2 \\ f_2(x_1, x_2) &= 10 - (x_1 - 1)^2 - (x_2 - 2)^2 \end{aligned} \tag{B.2}$$

where their Hessian matrices are given by,

$$H_1 = H_2 = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix}$$

negative definite, implying f_1 and f_2 are concave.

The gradients of f_1 and f_2 are given by,

$$\nabla_{\mathbf{x}} f_1 = \begin{bmatrix} -2x_1 \\ -2x_2 \end{bmatrix}, \quad \nabla_{\mathbf{x}} f_2 = \begin{bmatrix} -2x_1 + 2 \\ -2x_2 + 4 \end{bmatrix} \quad (\text{B.3})$$

from which we obtain their ideal point (x_{i1}^*, x_{i2}^*) for each objective i and the corresponding objective values as,

$$f_1(x_{11}^*, x_{12}^*) = 0 \text{ where } (x_{11}^*, x_{12}^*) = (0, 0)$$

and

$$f_2(x_{21}^*, x_{22}^*) = 10 \text{ where } (x_{21}^*, x_{22}^*) = (1, 2).$$

We assume that the overall utility function is $U(f_1, f_2) = -(f_1^* - f_1)^2 - (f_2^* - f_2)^2$.

Note that its Hessian $H_U = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix}$ implies U is concave over the objective space.

For given $f_1^{(1)} < f_1^{(2)}$ and $f_2^{(1)} < f_2^{(2)}$, we consider:

$$\begin{aligned} U(f_1^{(1)}, f_2^{(1)}) &= -\overbrace{(f_1^* - f_1^{(1)})^2}^{c_1} - \overbrace{(f_2^* - f_2^{(1)})^2}^{c_2} \\ U(f_1^{(2)}, f_2^{(2)}) &= -\underbrace{(f_1^* - f_1^{(2)})^2}_{c'_1} - \underbrace{(f_2^* - f_2^{(2)})^2}_{c'_2} \end{aligned} \quad (\text{B.4})$$

Note that $c_1 < c'_1$ as well as $c_2 < c'_2$, implying $-(c_1 + c_2) > -(c'_1 + c'_2)$, hence $U(f_1^{(1)}, f_2^{(1)}) > U(f_1^{(2)}, f_2^{(2)})$, U is increasing. Therefore, the assumed functions satisfy the assumptions of the GDF method.

In our implementation, we arbitrarily select $\mathbf{x}^{(1)} = (-1, 1)$ as the initial solution and consider f_1 as the reference objective. Substituting the ideal values of the objectives, we obtain $U(f_1, f_2) = -f_1^2 - f_2^2 + 20f_2 - 100$ and find the tradeoff weights at $(-1, 1)$, based on U as,

$$w_1 = 1, \quad w_2 = \frac{\partial U / \partial f_2}{\partial U / \partial f_1} = \frac{-2f_2(-1, 1) + 20}{-2f_1(-1, 1)} = 2.5.$$

Then, we consider the following maximization problem with the obtained weights, $\mathbf{w} = (w_1, w_2)$,

$$\mathbf{g}^{(1)} = \arg \max_{\substack{-2 \leq g_1 \leq 2 \\ -2 \leq g_2 \leq 2}} \mathbf{w}^T(\mathbf{x}^{(1)}) \nabla_{\mathbf{x}} \mathbf{f}^T(\mathbf{x}^{(1)}) \mathbf{g} \quad (\text{B.5})$$

where $\mathbf{f}(\mathbf{x}^{(1)})$ denotes the vector of objective values at $\mathbf{x}^{(1)} = (-1, 1)$. Expanding the sum and the dot product, the problem becomes

$$\mathbf{g}^{(1)} = \arg \max_{\substack{-2 \leq g_1 \leq 2 \\ -2 \leq g_2 \leq 2}} (-2x_1 + w_2(-2x_1 + 2)) g_1 + (-2x_2 + w_2(-2x_2 + 4)) g_2 .$$

Then, we evaluate $\mathbf{f}(\mathbf{x}^{(1)} + t^{(1)}g(1))$ for $t \in \{0.0, 0.1, 0.2, \dots, 1.0\}$ to generate Table 3.9. We visualize the evaluations on the assumed objective functions, the overall underlying utility function in both $\mathbf{f}$ and $\mathbf{x}$ spaces in Figure B.1.

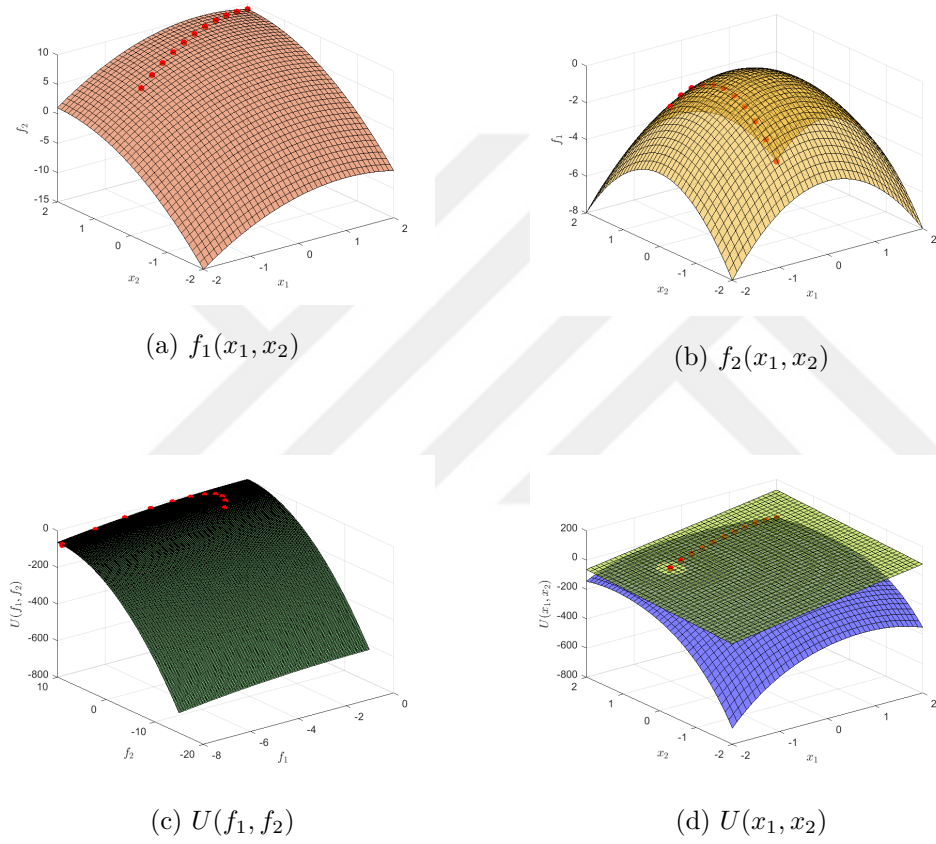


Figure B.1: Visualizations of the Objective Functions and the Overall Utility Function. The red dots denote the solutions observed for $t > 0$ in Table 3.9

Appendix C

DERIVATION OF EQUATION (4.11)

C.1 Derivation of the Confidence Intervals (CIs)

We consider $y = X\beta + \varepsilon$, assuming that $\varepsilon_i \sim N(0, \sigma^2 v(x_i))$, where $v(\cdot)$ is the variance function, $x_i \in \mathbb{R}^n$ is the i^{th} column of $X \in \mathbb{R}^{n \times r}$, and $y \in \mathbb{R}^n$, $\beta \in \mathbb{R}^r$,

$\varepsilon \in \mathbb{R}^n$. We know that $V = \begin{bmatrix} v(x_1) & & \\ & \ddots & \\ & & v(x_n) \end{bmatrix}$ can be decomposed as $V = P^\top P$

and P can be selected as $V^{1/2}$ since V is a positive semi-definite diagonal matrix, and $(V^{1/2})^\top = V^{1/2}$.

We consider the transformed scale as:

$$\begin{aligned} \underbrace{V^{-1/2}y}_g &= \underbrace{V^{-1/2}X}_Z \beta + \underbrace{V^{-1/2}\varepsilon}_u \quad \text{where} \quad \frac{\varepsilon_i}{\sqrt{v(x_i)}} = u_i \sim N(0, \sigma^2) \\ g &= Z \beta + u \end{aligned}$$

Upon applying OLS, we obtain $\hat{\beta} = (Z^\top Z)^{-1} Z^\top g$ then:

$$\text{Var}(z_0^\top \hat{\beta}) = z_0^\top \text{Cov}(\hat{\beta}) z_0 = \sigma^2 z_0^\top (Z^\top Z)^{-1} z_0.$$

Hence, we know that

$$z_0^\top \hat{\beta} \sim N(z_0^\top \beta, \sigma^2 z_0^\top (Z^\top Z)^{-1} z_0),$$

where σ^2 is not known and estimated by $s^2 = \hat{u}^\top \hat{u} / (n-r-1)$. Then, we write:

$$\frac{(z_0^\top \hat{\beta} - z_0^\top \beta) / \sqrt{\sigma^2 z_0^\top (Z^\top Z)^{-1} z_0}}{\sqrt{s^2 / \sigma^2}} \sim t_{n-r-1} = \frac{z}{\sqrt{\chi_{n-r-1}^2 / (n-r-1)}}.$$

Thus, $z_0^\top \hat{\beta} \pm t_{n-r-1, 1-\frac{\alpha}{2}} \sqrt{s^2 z_0^\top (Z^\top Z)^{-1} z_0}$ is $100(1 - \alpha)\%$ CI.

CI for $x_0^\top \hat{\beta}$ can be found in the same manner as follows.

We need to expand $\text{Var}(x_0^\top \hat{\beta}) = x_0^\top \text{Cov}(\hat{\beta}) x_0$. Substituting $\text{Cov}(\hat{\beta}) = \sigma^2 (Z^\top Z)^{-1}$ and $Z = V^{-1/2} X$, we have:

$$\sigma^2 x_0^\top \left((V^{-1/2} X)^\top (V^{-1/2} X) \right)^{-1} x_0.$$

Rearranging the terms, we get:

$$\text{Var}(x_0^\top \hat{\beta}) = \sigma^2 x_0^\top (X^\top V^{-1} X)^{-1} x_0.$$

Thus, $x_0^\top \hat{\beta} \sim N(x_0^\top \beta, \sigma^2 x_0^\top (X^\top V^{-1} X)^{-1} x_0)$, where σ^2 is not known and estimated by $s^2 = \hat{u}^\top \hat{u} / (n-r-1)$. Then, we write:

$$\frac{(x_0^\top \hat{\beta} - x_0^\top \beta) / \sqrt{\sigma^2 x_0^\top (X^\top V^{-1} X)^{-1} x_0}}{\sqrt{s^2 / \sigma^2}} \sim t_{n-r-1} = \frac{z}{\sqrt{\chi_{n-r-1}^2 / (n-r-1)}}.$$

Thus, $x_0^\top \hat{\beta} \pm t_{n-r-1, 1-\frac{\alpha}{2}} \sqrt{s^2 x_0^\top (X^\top V^{-1} X)^{-1} x_0}$ is $100(1-\alpha)\%$ CI.

C.2 Derivation of the Prediction Intervals (PIs)

We first express:

$$\begin{aligned} \text{Var}(G_0 - z_0^\top \hat{\beta}) &= \text{Var}(z_0^\top \beta + u_0 - z_0^\top \hat{\beta}) \\ &\stackrel{(a)}{=} \text{Var}(u_0) + \text{Var}(z_0^\top \hat{\beta}) \\ &\stackrel{(b)}{=} 1 + z_0^\top (Z^\top Z)^{-1} z_0 \end{aligned}$$

where we rely on statistical independence of u_0 and $\hat{\beta}$ in (a), and for (b), we use $u_0 \sim N(0, 1)$ that is independent of u and we substitute $\text{Var}(z_0^\top \hat{\beta}) = z_0^\top (Z^\top Z)^{-1} z_0$.

Then, we write:

$$\frac{(G_0 - z_0^\top \hat{\beta}) / \sqrt{1 + z_0^\top (Z^\top Z)^{-1} z_0}}{\sqrt{s^2 / 1}} \sim t_{n-r-1}.$$

Thus, $z_0^\top \hat{\beta} \pm t_{n-r-1, 1-\frac{\alpha}{2}} \sqrt{1 + z_0^\top (Z^\top Z)^{-1} z_0}$ is PI for transformed data.

For y_0 , we similarly express:

$$\begin{aligned} \text{Var}(y_0 - z_0^\top \hat{\beta}) &= \text{Var}(y_0^\top \beta + \varepsilon_0 - x_0^\top \hat{\beta}) \\ &\stackrel{(a)}{=} \text{Var}(\varepsilon_0) + \text{Var}(x_0^\top \hat{\beta}) \\ &\stackrel{(b)}{=} \sigma^2 v(x_0) + \sigma^2 x_0^\top (X^\top V^{-1} X)^{-1} x_0 \end{aligned}$$

where we rely on statistical independence of ε_0 and $\hat{\beta}$ in (a), and for (b), we use $\varepsilon_0 \sim N(0, v(x_0))$ that is independent of ε and we substitute $\text{Var}(x_0^\top \hat{\beta}) = \sigma^2 x_0^\top (X^\top V^{-1} X)^{-1} x_0$.

Note that $y_0 - x_0^\top \hat{\beta}$ is normal since it can be expressed as a linear combination of $\hat{\beta}$ and ε both of which follow normal distribution. Therefore, we have:

$$\frac{(y_0 - x_0^\top \hat{\beta}) / \sqrt{\sigma^2 v(x_0) + \sigma^2 x_0^\top (X^\top V^{-1} X)^{-1} x_0}}{\sqrt{s^2 / \sigma^2}} \sim t_{n-r-1}.$$

Thus, $x_0^\top \hat{\beta} \pm t_{n-r-1, 1-\frac{\alpha}{2}} \sqrt{s^2(v(x_0) + x_0^\top (X^\top V^{-1} X)^{-1} x_0)}$ is PI for the regressed output.





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3. International Conference on Multiple Criteria Decision Making, Istanbul, Turkey, June 2019
"Incorporating Robustness in Interactive Multi-Response Surface Optimization of Product Design Parameters"
4. EURO, Valencia, Spain, July 2018
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¹ National conferences are excluded.

5. INFORMS Annual Meeting, Houston, TX, USA, October 2017
"An Interactive Approach for Product and Process Design Parameter Optimization under Model Uncertainty"
6. International Conference on Multiple Criteria Decision Making, Ottawa, Canada, July 2017
"An Interactive Approach for Product and Process Design Parameter Optimization under Model Uncertainty"
7. INFORMS Annual Meeting, Nashville, TN, USA, November 2016
"An Interactive Approach to Design Parameter Optimization Considering Response Surface Prediction Errors"
8. INFORMS Annual Meeting, Philadelphia, PA, USA, November 2015
"Interactive Mean-variance-covariance Optimization for Two Responses"
9. International Conference on Multiple Criteria Decision Making, Hamburg, Germany, August 2015
"An Interactive Approach for Two-Response Product and Process Design Parameter Optimization"
10. INFORMS Annual Meeting, San Francisco, CA, USA, November 2014
"An Interactive Approach to Two-Response Design Optimization Problem"

Journal Publications

Özateş, M., M. Şahin, S. Şenol, F. Terzi, S. Yörükoğlu, G. Köksal, and Y. Serin, "Designing a Quality Control System for Short Run Manufacturing Environment" *Journal of Industrial Engineering (Turkish Chamber of Mechanical Engineers)*, 23(3). 40-58, 2015.

Seminars

Department of Industrial Engineering, Middle East Technical University, December 2018, December 2015

"Two-Response Product and Process Design Optimization"

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