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Development of the D-Optimality-Based Coordinate-Exchange Algorithm for an Irregular Design Space and the Mixed-Integer Nonlinear Robust Parameter Design Optimization

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DEVELOPMENT OF THE *D*-OPTIMALITY-BASED COORDINATE-EXCHANGE ALGORITHM FOR AN IRREGULAR DESIGN SPACE AND THE MIXED-INTEGER NONLINEAR ROBUST PARAMETER DESIGN OPTIMIZATION

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ABSTRACT

Robust parameter design (RPD), originally conceptualized by Taguchi, is an effective statistical design method for continuous quality improvement by incorporating product quality into the design of processes. The primary goal of RPD is to identify optimal input variable level settings with minimum process bias and variation. Because of its practicality in reducing inherent uncertainties associated with system performance across key product and process dimensions, the widespread application of RPD techniques to many engineering and science fields has resulted in significant improvements in product quality and process enhancement. There is little disagreement among researchers about Taguchi's basic philosophy. In response to apparent mathematical flaws surrounding his original version of RPD, researchers have closely examined alternative approaches by incorporating well-established statistical methods, particularly the response surface methodology (RSM), while accepting the main philosophy of his RPD concepts. This particular RSM-based RPD method predominantly employs the central composite design technique with the assumption that input variables are quantitative on a continuous scale.

There is a large number of practical situations in which a combination of input variables is of real-valued quantitative variables on a continuous scale and qualitative variables such as integer- and binary-valued variables. Despite the practicality of such cases in real-world engineering problems, there has been little research attempt, if any, perhaps due to mathematical hurdles in terms of inconsistencies between a design space in the experimental phase and a solution space in the optimization phase. For instance, the

design space associated with the central composite design, which is perhaps known as the most effective response surface design for a second-order prediction model, is typically a bounded convex feasible set involving real numbers due to its inherent real-valued axial design points; however, its solution space may consist of integer and real values.

Along the lines, this dissertation proposes RPD optimization models under three different scenarios. Given integer-valued constraints, this dissertation discusses why the Box-Behnken design is preferred over the central composite design and other three-level designs, while maintaining constant or nearly constant prediction variance, called the design rotatability, associated with a second-order model. Box-Behnken design embedded mixed integer nonlinear programming models are then proposed. As a solution method, the Karush-Kuhn-Tucker conditions are developed and the sequential quadratic integer programming technique is also used. Further, given binary-valued constraints, this dissertation investigates why neither the central composite design nor the Box-Behnken design is effective. To remedy this potential problem, several 0-1 mixed integer nonlinear programming models are proposed by laying out the foundation of a three-level factorial design with pseudo center points. For these particular models, we use standard optimization methods such as the branch-and-bound technique, the outer approximation method, and the hybrid nonlinear based branch-and-cut algorithm.

Finally, there exist some special situations during the experimental phase where the situation may call for reducing the number of experimental runs or using a reduced regression model in fitting the data. Furthermore, there are special situations where the experimental design space is constrained, and therefore optimal design points should be generated. In these particular situations, traditional experimental designs may not be appropriate. *D*-optimal experimental designs are investigated and incorporated into nonlinear programming models, as the design region is typically irregular which may end up being a convex problem. It is believed that the research work contained in this dissertation is the initial examination in the related literature and makes a considerable contribution to an existing body of knowledge by filling research gaps.

DEDICATION

This doctoral dissertation is dedicated to the following: Foremost, my parents, Memis and Firdevs Ozdemir, and my sister, Burcu Nur Ozdemir, who always believe in me. They never let me alone during my doctoral study at Clemson University. Their support, love, patience, encouragement, and understanding have also sustained me throughout my whole life. I would also like to dedicate this dissertation to my grandmother, Zekiye Ozdemir, who was always supportive.

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CHAPTER ONE

INTRODUCTION TO RESEARCH

Introductory Remarks

Continuous quality improvement is a disciplined, data-driven, process-based approach to improving the quality of a product or service which often lies in the intersection between statistics and operations research in various engineering settings. The response surface methodology (RSM) is a significant branch of continuous quality improvement. The general RSM approach is an accumulation of mathematical and statistical methods for the modeling and analysis of problems in which a response variable is affected by several input variables and the objective is to maximize or minimize the response problems. In addition, it has many applications in the development of new product designs, as well as in the improvement of existing product designs. Further, reduction of variability and enhanced product and process performance may be achieved directly using the RSM approach. Variation in a key performance characteristic may result in poor quality. Therefore, Taguchi (1986) introduced the term robust parameter design (RPD) for industrial problems. Robust means that the product or process performs on target and is relatively insensitive to environmental conditions. The RPD philosophy strives to reduce variation by selecting levels of input variables that make the system robust (insensitive). The RPD philosophy also incorporates many useful concepts within the RSM framework. The RSM-based RPD approaches may be an effective tool to determine optimum operating conditions for input variables with minimum product or process variation. In this chapter, we present the problem statements and approaches of this dissertation, research goals and significance, and outline of this dissertation.

Problem Statements and Approaches

A careful investigation of the RSM-based RPD literature reveals that the vast majority of the research works has assumed that input variables are quantitative and that both input variables and robust parameter design solutions are allowed to be any real numbers on a continuous scale. It is unfortunate, however, that there has been little attempt to extend the RSM-based RPD research to several real-life situations encountered by engineers and scientists, where (1) some of the input variables are qualitative, (2) some of the input variables and robust design solutions are restricted to be other than real numbers, and (3) standard response surface designs may not work for quantitative input variables due to safety concerns, the scarcity of resources and cost considerations. The main goal of this dissertation is to develop customized the RSM-based RPD models to address these special situations. In addition, Table 1.1 summarizes the current status of statistical modeling and optimization issues in the RSM-based RPD methodology.

In this dissertation, the method of least squares for mean and variance responses is considered for data from a Box-Behnken design to integer-constrained RPD optimization problems. The Box-Behnken design is rotatable (or nearly so) and it is fewer design points than the central composite design. Box-Behnken design embedded nonlinear integer models are developed using the sequential quadratic programming and the Karush-Kuhn-

Tucker conditions. JMP software is used for statistical modeling data analyses. In addition, optimization problems are utilized in the Maple nonlinear programming solver package.

Table 1.1: Problem Statements and Approaches of This Dissertation

Modeling			Optimization		
Experimental Design technique	Design points	Design space	Solution space	Solutions	Operations research technique
Central composite design	± 1, ±α	Circle, sphere	Bounded convex set (BCS)	Real numbers	Nonlinear Programming (Available in the literature)
				Pure or mixed integers	Unexplored but may not be valid
Box-Behnken design	0, ±1	Cube	BCS	Pure or mixed integers	Nonlinear integer programming (Unexplored)
Factorial design with pseudo center points for the combination of qualitative and quantitative input variables	Pseudo center points, ±1	Square, cube	BCS	Pure or mixed integers, binary	0-1 nonlinear integer programming (Unexplored)
Optimal experimental designs	Non-standard	Irregular	BCS	Real numbers	Nonlinear programming (Unexplored due to a nonlinearly-constrained irregular experimental design space)

Further, it is elaborated on why traditional response surface designs may not be effective with the two different types of input variables and lay out the statistical foundation by embedding those input variables into a factorial design with pseudo-center points. A 0-

1 mixed integer nonlinear programming model is then developed and compared the solutions using the three optimization tools, such as the outer approximation method, the branch-and-bound technique, and the hybrid branch-and-cut algorithm, with traditional counterparts. In addition, JMP and BONMIN (basic open-source nonlinear mixed integer programming) software packages are used for statistical data analyses and the optimization phase, respectively.

Finally, the experimental design space may not be a cube or a sphere due to safety concerns, physical processing constraints and the scarcity of resources; therefore, traditional experimental design techniques are not appropriate. In these particular situations, an optimal experimental design may be the best choice for a linearly- or nonlinearly-constrained irregular experimental design space to conduct experiments. While several iterative exchange algorithms for *D*-optimal experimental designs are available for a linearly-constrained irregular design space, it has not been clearly understood how *D*-optimal experimental design points need to be generated when the design space is nonlinearly constrained. Therefore, a selection scheme of *D*-optimal experimental design points is then proposed for a nonlinearly-constrained irregular experimental design space. *D*-optimal experimental design embedded robust parameter design models are proposed to obtain optimal operating conditions for real-valued variables. JMP and MATLAB software packages are used to generate design points and MAPLE software is used to obtain optimal robust parameter design solutions.

Research Goals and Significance

The RSM-based RPD aims at process improvement by obtaining optimal factor level settings, also known as robust parameter design solutions, which minimize the deviation of process mean from the target value of interest and a product variation. Because of the significant potential for industrial applications, the RSM-based RPD approaches have been identified as one of the most important research topics by many federal funding agencies, including the National Science Foundation (NSF). Consequently, hundreds of research papers have been published. In addition, the expected benefits of each chapter are summarized as follows:

In Chapter III, the Box-Behnken design is preferred over the central composite design and other three-level designs to integer-constrained robust parameter design problems. The central composite design (CCD) may not be appropriate for integer-valued input variables due to axial points. Other three-level designs are not rotatable designs and they may give poor pure quadratic coefficients over entire design spaces. In addition, we investigate the rotatability property for maintaining predicted responses. The integer-valued solution space is also developed. Then, a nonlinear integer programming approach is proposed for solving the Box-Behnken design embedded robust parameter design optimization problem for potential application areas of automotive, electronic, mechanical, and process industries. In addition, analytical and numerical solution methods are proposed. The proposed model may also be useful for practitioners and researchers if variance reduction is more significant than meeting the target value.

In Chapter IV, the Box-Behnken design is not capable of assessing binary-valued design points because of three-level design points. Similarly, traditional response surface designs are not appropriate due to binary-valued design points. Therefore, a factorial design with pseudo-center points is offered in order to optimize binary-constrained RPD problems considering the combination of binary qualitative and quantitative input variables with two coded levels. A 0-1 mixed integer nonlinear programming model is proposed for binary-constrained robust parameter design problems to solve the RSM-based RPD optimization problems. The three different solution methods are also performed to obtain optimal operating conditions when the optimization model is either convex or nonconvex. Finally, the proposed model may result in better solutions than the traditional models.

In Chapter V, factorial designs and other traditional response surface designs are no longer effective if an experimental design space is constrained due to the physical infeasibility, safety reasons, and cost considerations. For these situations, optimal designs are also good alternatives to overcome the limitations of traditional experimental designs. Therefore, a selection scheme of optimal design points is a significant issue for a nonlinearly-constrained irregular experimental design space. In addition, the proposed exchange algorithm is proposed to find global solutions of optimal design points. Then, *D*-optimal experimental design incorporated robust parameter design models are offered in order to find global optimal solutions for real-valued variables. The proposed models may have an important advantage while the variance reduction is more significant than attaining the target value.

Finally, this doctoral dissertation lays out the theoretical foundations of the RSM-based RPD and have the potential to impact a wide range of many other engineering science problems and, ultimately leading to process and quality improvement.

Outline of Dissertation

Table 1.2 shows the structure of this dissertation. Chapter I introduces research concepts, including the problem statements and approaches of this dissertation, research goals and significance. In Chapter II, we present a review of the relevant research studies in the literature. Response surface based robust parameter design models are discussed in Chapter III, IV, and V, respectively. Each of these chapters consists of a statistical design phase, an optimization modeling phase, and a comparison phase. Finally, conclusions and future study are presented in Chapter VI.

Table 1.2: Outline of Dissertation

Chapter	Outline
I	Problem statements and approaches, research goals and significance
II	Literature review of the relevant research studies
III	Proposed RPD optimization models for integer-valued input variables using the Box-Behnken design
IV	Proposed RPD optimization models for integer- and binary-valued input variables using the factorial design with pseudo-center points
V	Proposed RPD optimization models for nonlinearly-constrained irregular experimental design spaces using the *D*-optimality criterion for real-valued input variables
VI	Conclusions and Further Studies

CHAPTER TWO

LITERATURE REVIEW

In this chapter, we present an overview of relevant literature review of response surface methodology, Taguchi's robust parameter design, response surface methodology based robust parameter design optimization models, optimization techniques to solving robust parameter design models, pseudo-center points based experimental designs, and optimal experimental designs.

Response Surface Methodology

The response surface methodology (RSM) approach was introduced in the early 1950s. This approach includes major experimental designs, such as central composite designs for fitting linear response surface models and the determination of optimal operating conditions. In particular, the work by Box and Wilson (1951) is considered seminal. They also addressed the determination of the optimal settings for chemical processes with considerable success. The RSM approach was further developed by Box and Hunter (1957). In addition to these works, Box and Draper (1987), Khuri and Cornell (1996), and Myers et al. (2009) also discussed more detailed techniques of the RSM approach, including Taguchi's RPD and its response surface approach. Furthermore, Khuri and Mukhopadhyay (2010) provided a comprehensive discussion of the various steps in the development of the RSM approach. They also discussed generalized linear models, graphical methods for comparing response surface designs, and response surface models with random effects in the modern RSM approach.

Considerable attention has been focused on the Taguchi's approach, and a number of flaws in his methodology have been identified. In addition, there are many research attempts to incorporate the RPD approach within the RSM framework.

Taguchi's Robust Parameter Design

Taguchi (1986) introduced the basic concept of RPD by formulating, which was formulated as the nominal-the-best (N-type) into the concept of the signal-to-noise ratio (SNR), to optimize input variables. The goal is to maximize the SNR. Taguchi's fundamental idea is that the mean of the response should be brought to the desired target value while keeping the variance of the response as small as possible. On the other hand, Leon et al. (1987), Box (1988), Box et al. (1988), Nair (1992), and Tsui (1992) discussed Taguchi's main idea and criticized quality characteristics involving both the mean and variance of a response variable. Steinberg and Bursztyn (1998) also made a wide spectrum investigation on the Taguchi's offline quality control method. In addition, Grize (1995), Robinson et al. (2004), Park et al. (2006), and Arvidsson and Gremyr (2008) also provided comprehensive reviews of the RPD approaches.

Response Surface Methodology Based Robust Parameter Design Optimization Models

Vining and Myers (1990) formulated Taguchi's main idea using an N-type nonlinear programming (NLP) model with the RSM principles. Their model, called the dual response model (DRM), was formulated in the way that the estimated standard deviation of the response is minimized when the estimated mean of the response strictly equals to the target value. They also used the Lagrange multiplier, quadratic response functions, and spherical regions. In addition, a full second-order model is necessary for this approach. On the contrary, we observe that there is a main disadvantage using the dual response approach. The main disadvantage is that the estimated mean response is strictly equal to the target value; therefore, feasible solutions of the model may not exist for input variables. Fathi (1991) and Del Castillo and Montgomery (1993) conducted the further developments of the dual response model, and they reformulated the model with an inequality form of the constraint instead of using the equality form of it. An optimal solution of the dual response model may be suboptimal because the zero-bias assumption forces to make the mean value at the target value. Therefore, Cho (1994) and Lin and Tu (1995) proposed relaxed zero-bias assumption models based on the mean squared error (MSE) criterion. These MSE models have equal priorities for the bias and variance response functions; in addition, they have symmetric quality loss functions and allow the bias. These models may provide less variance while attaining little bias. Lin and Tu (1995) also expressed two further improvements that their proposed approach can be used more realistic models than polynomial models. They also conveyed that the DRM would not work when the responses (e.g., the mean and variance) are dependent. As an extension of the DRM approach, Copeland and Nelson (1996) proposed a model based on a desired upper bound for the bias. Further, Cho et al. (1996) and Koksoy and Doganaksoy (2003) developed weighted mean square error models with a different weight assigned to each quality characteristic. In addition, Koksoy and Doganasksoy (2003) also used Pareto optimal solutions for generating more alternative solutions.

There were several research attempts made in developing more flexible RPD models. For example, Kim and Lin (1998) proposed a fuzzy model to optimize the dual response model, and their approach has a flexible model based on the preference and obtains a better balance between the variance and bias functions. Further, Cho et al. (2000) made further modifications of the mean square error model by incorporating the priority concept. Similarly, Tang and Xu (2002) developed an extended dual response model with different weights for the bias and variance. Kim and Cho (2002) saw the concept of priorities in balancing mean and variability as a critically important research issue and introduced a priority-based RPD model. Romano et al. (2004) then proposed a modified RPD model using the quality loss function concept. They also introduced the multivariate problem when a combined array is used for data collection, and they also included the total quadratic loss function based on maximum and minimum criteria for multiple responses. Formal multi-objective optimization methods were used for solving RPD problems. In particular, the works by Ding et al. (2004) and Shin et al. (2011) are considered seminal. In addition, they used the weighted sum methods in multi-objective optimization, and they proposed weighted MSE approaches. They also reach that the optimal solution to the DRM has to be found in the curve where the different weights clearly get dissimilar solutions for all feasible solution set. Shin and Cho (2005) offered another relaxed zero-bias approach by proposing a bias-specified model while keeping variability at minimum. They also used the epsilon-constrained method to the process bias. Robinson et al. (2006) introduced generalized linear mixed models for estimated fitted functions of the mean and variance. Koksoy (2006) and Park et al. (2012) conducted further studies in the weighted mean square model in the multi-objective optimization context. Further, Shaibu and Cho (2009) considered higher-order polynomial models to improve the predictive of the RSM for the mean and standard deviation functions. Costa (2010) offered a variant model using the mean and standard deviation of a response to optimize associated quality characteristics, and the model minimizes an objective function with the deviation of each quality characteristic from specified target values to a specified range. As an extension, Goethals and Cho (2011) tried to enhance the regression methods using dynamic characteristics for building the model, and they used time-oriented dynamic approach with normal distribution by incorporating consideration of economic criteria on the model.

The pharmaceutical field is one of the new application areas of the RPD. In particular, the determination of optimal pharmaceutical formulations using RPD concepts was studied by Li et al. (2012a, 2012b, 2013). Many products are subject to inspection to weed out defects based on specified specification limits. Chan and Cho (2013a, 2013b) noted that the mean and variance of a product quality characteristic would change after truncating the original process distribution and they incorporated truncated statistics into RPD models. Park (2013) provided another view of the RSM based RPD model using the bootstrap technique based on the concept of Bonferroni joint confidence regions. Another issue is in the multi-objective models is that a number of gaps could occur during a multi-objective model technique applied to weighted sums as a trade-off method; therefore, Brito et al. (2014) offered a normal boundary intersection approach conjugated with the mean square error equations. Time series response models were first introduced to the RPD research community by Shin et al. (2014) in which they formulated the pharmaceutical RPD model. Further, Yang and Du (2014) introduced a new RPD approach that applied to the maximum quality loss among multiple quality characteristics for associated quality problems in which the quality loss is not different regardless which quality characteristics or how many quality characteristics are imperfect.

Recent RPD papers by Nha et al. (2013), Elsayed and Lacor (2014), Hu et al. (2014), Fang et al. (2015), Bao et al. (2016), Brito et al. (2016), Quyang et al. (2016), Hot et al. (2017), and Lu et al. (2017) illustrated a wide spectrum of application areas, including a lexicographical dynamic goal programming approach within the pharmaceutical environment, a multi-objective optimization with surrogate models, a hydrokinetic turbine system, an application from nanomanufacturing, the surface roughness in end milling process, the fatigue life of a product and machine parts, and a case study in automobile manufacturing, respectively.

Optimization Techniques to Solving Robust Parameter Design Models

Myers et al. (1992), Engel and Huele (1996a, 1996b), and Lee and Nelder (2003) studied a generalized linear modeling technique. Along the same line, Myers et al. (2005) proposed a modified dual response model using the generalized linear model. Vining and Myers (1990) used the Lagrange multiplier to obtain robust design solutions. Fathi (1991) also referred conventional optimization techniques, such as the successive quadratic variance approximation method for solving the RPD problems. In addition, Del Castillo and Montgomery (1993) used a generalized reduced gradient algorithm with inequality constraints. The Nelder-Mead simplex search method is another viable solution method, which was used by Copeland and Nelson (1996). Genetic algorithms were also considered as another solution method (see Parkinson (2000), Koksoy and Doganaksoy (2003), and Koksoy and Yalcinoz (2008)). Xu et al. (2004) proposed a goal attainment method for multi-response systems using the sequential quadratic programming technique to solve RPD problems. The epsilon method with Karush-Kahn-Tucker conditions was developed by Shin and Cho (2005). Kovach et al. (2008) introduced physical programming techniques to improve flexibility in the development stage of the experiment. Tang and Xu (2002), Kim and Cho (2002), Kovach and Cho (2008a, 2008b), Kovach and Cho (2009), and Kovach et al. (2009) used nonlinear programming solution methods. Further, special optimization methods are necessary to optimize for the multiple response processes when there exists more than one quality characteristic from consideration. For instance, He et al. (2012) and Brito et al. (2014) proposed multi-objective optimization models using the desirability function and the normal boundary intersection approach, respectively.

Pseudo-Center Points Based Experimental Designs

There are a number of situations in which some variables should be qualitative input variables. However, center points are not employed when some input variables are qualitative. In these situations, pseudo-center points may be employed. Therefore, there exist some research attempts involving pseudo-center points in the current literature and they are summarized in Table 2.1. Note that coded levels of qualitative input variables in these studies are (-1) and (+1) for low and high levels, respectively. In addition, the RSM-based RPD approaches were not considered in these studies in order to find optimal operating conditions.

Table 2.1: Pseudo-Center Points Based Studies in the Literature

Studied by	Approach	Application area
Kim et al. (2002)	Full factorial design	Ultraviolet curable coatings
Li and Rasmussen (2003)	Packett-Burman design	Pharmaceutical experiments
Marengo et al. (2005)	Full factorial design	Textile polyster fibers
Passos et al. (2006)	Full factorial design	Batch adsorption procedure conditions
Anderson-Cook and Robinson (2009)	*D*-optimal design	Screening designs
Rajendran et al. (2011)	Full factorial design	Laccase fermentations

Optimal Experimental Designs

The field of optimal designs has been in the literature for many years. Smith (1918) firstly studied optimal designs for prediction purposes. Wald (1943) then introduced a measure of the efficiency of the design by investigating the quality of parameter estimates. In addition, Wald (1943) first offered the criterion of *D*-optimality, which is the notion of maximizing the determinant of the information matrix. Later, Kiefer and Wolfowitz (1959) developed computational procedures for finding optimal designs, such as *D*-optimality and *E*-optimality, in regression problems of estimation, testing hypotheses, and so on. Similarly, Kiefer (1959) studied certain fundamental assumptions, such as the non-optimality of the balanced designs for hypothesis testing, and certain specific optimality criteria in the spirit of Wald’s decision theory. Next, Kiefer (1961) extended the results of the previous studies to the determination of *D*-optimal designs for several problems in the setting of simplex designs. Then, Fedorov (1972) further developed the research in optimal designs in order to solve numerical optimal design using the exchange algorithm. In particular, John and Draper (1975) reviewed the *D*-optimality for regression designs and examined the procedures for obtaining *D*-optimal designs. Along the same line, Cook and Nachtsheim (1980) provided a comparison of algorithms for the computer generation of *D*-optimal designs. On the other hand, computer-generated designs, such as *D*-optimal designs, have been criticized for being too independent based on statistical models. DuMouchel and Jones (1994) addressed this criticism and developed a modification of the *D*-optimal design with the Bayesian paradigm for reducing dependence on an assumed statistical model. DuMouchel and Jones (1994) also investigated that increasing the determinant of the range of information matrix usually decreased the error variance of the regression coefficients. Orthogonality is also useful in experimental designs due to the mutual independence of the model coefficients; therefore, de Augiar et al. (1995) expressed that a closer orthogonality is accomplished with a higher determinant for a constant size design. In addition to these research works, Cook and Fedorov (1995) also discussed several approaches proposed in experimental designs when some constraints, such as total cost of an experiment, a location of the supporting points and the value of the auxiliary objective functions are imposed.

Another alphabetic design, *I*-optimality, was proposed by Box and Draper (1959). The *I*-optimality criterion is also called the I_V-, *Q*-, and *V*-optimality criteria in the literature. In addition, Box and Draper (1959, 1963) defined as the integrated variance function over a selected design region. Furthermore, Draper (1982) offered an integrated variance criterion to specify the number of center points in response surface designs. In addition, Borkowski (2003) reviewed the different prediction variance measures and developed an evaluation of the *I*-optimality criterion. Allen and Tseng (2011) conducted the further research study in the field of optimal experimental designs and developed variance plus bias optimal experimental designs for stem choice modelling.

In addition to these studies, Myers et al. (2009) and Toro Diaz et al. (2012) provided comprehensive discussions on more theoretical aspects of optimal designs. In Table 2.2, we outline the key application areas utilizing optimal (non-standard) experimental designs, including the most recent studies.

Table 2.2: Review of Application Areas for Optimal Experimental Designs

Studied by	Optimality	Evaluation strategy	Application area
Welch (1984)	*D*-optimality	Mitchell's DETMAX	Leaching experiments
Bezeau and Endrenyi (1986)	*D*-optimality	Hill model	Dose-response parameters
DuMouchel and Jones (1994)	*D*-optimality	Bayesian paradigm	Gasoline blends
Broudiscou et al. (1996)	*D*-optimality	Genetic algorithm	Antigen and antibody tests
Gianchandani and Crary (1998)	*D*- and *I*-optimality	Parametric modelling	Micro accelerometer examples
Reeves and Wright (1999)	*D*-optimality	Genetic algorithm	Design of hydraulic systems
Lee et al. (2000)	*I*-optimality	Simulation	Five-factor micro accelerometer examples
Duffull et al. (2001)	*D*-optimality	Fisher information matrix	Population pharmacodynamics experiments
Kincaid and Padula (2002)	*D*-optimality	Tabu search approach	Optimal location of sensors and actuators to

			control noise and variation
Han and Chaloner (2003)	*D*-optimality	Bayesian optimal designs	Viral dynamics models
Gadkar et al. (2005)	*D*-optimality	Maximizing the accuracy of the parameter estimates in subsequent iterations	Model identification of biological networks
Kovach and Cho (2006)	*D*-optimality	Robust design	A new design for six sigma tools
Sexton et al. (2006)	*D*-optimality	Exchange and genetic algorithms	Assembly of an hydraulic gear pump and analysis of sound output
Kovach and Cho (2008c)	*D*-optimality	Robust design	The consideration of uncontrollable factors
Kang et al. (2009)	*I*-optimality	Process optimization	Etching experiments
Kovach and Cho (2009a)	*D*-optimality	Nonlinear goal programming	Multiple responses
Chen et al. (2010)	*D*-optimality	Orthogonal forward regression	Sparse kernel density estimations
He (2010)	*D*-optimality	Laplacian regularized	Image retrievals
Chen et al. (2011)	*D*-optimality	Response surface methodology	Micro-cutting tests
Corthals et al. (2011)	*D*-optimality	*D*-optimality vs. full factorial design	Dry reforming catalysts
Fang and Perera (2011)	*D*-optimality	Response surface methodology	Damage identifications
Robinson and Anderson-Cook (2010)	*D*-optimality	Multiple objective	Screening designs
Spaggiari et al. (2011)	*D*-optimality	Critical distance approach	Multiscale modelling of porous polymers
Gupta and Dhingra (2013)	*D*-optimality	Novel approach	Input load identification from optimally placed strain gages
Kuram et al. (2013)	*D*-optimality	Response surface methodology	Cutting fluids and cutting parameters during end milling

Rajmohan and Palanikumar (2013)	*D*-optimality	Response surface methodology	Drilling hybrid metal matrix composite examples
Abebe et al. (2014)	*D*-optimality	The logistic mixed model	Longitudinal data
Badawi and El-Khordagui (2014)	*D*-optimality	Quality by design approach	Emulsion composition
Coffey (2015)	*D*-optimality	Four-parameter logistic models	A bioassay case study
El-Gendy et al. (2015)	*D*-optimality	Response surface methodology	Produced biodiesel applications
Silvestrini (2015)	*D*-optimality	Sequential experiments	Examples of sequential optimal designs
L'Hocine and Pitre (2016)	*D*-optimality	Screening of optimal extraction conditions	Allergen extraction from peanuts and selected tree nuts
Dette et al. (2017)	*D*-optimality	Generalized linear models	Thermal spraying process
Saleh et al. (2017)	*D*-optimality	Greedy search strategy	Magnetic resonance imaging experiments
Smucker et al. (2017)	*D*- and *I*-optimality	Robustness of classical and optimal designs to missing observations	Missing observations in real-world experiments

CHAPTER THREE

A NONLINEAR INTEGER PROGRAMMING APPROACH TO SOLVING THE ROBUST PARAMETER DESIGN OPTIMIZATION PROBLEM

Introductory Remarks

Robust parameter design (RPD) has become well accepted by researchers as an effective engineering method for incorporating product quality into the design of processes. Originally conceptualized by Taguchi (1986), the primary goal of RPD methods is to determine the best factor level settings, or optimum operating conditions, that minimize the performance variability and the deviation from the target value of a product or process. Because of their practicality in reducing the inherent uncertainty associated with design factors and system performance across key process and product dimensions, the widespread application of RPD techniques has resulted in significant improvements in product quality.

Research Motivations

As shown in the literature studies, a vast majority of response surface methodology (RSM) based RPD models assume real-valued variables on a continuous scale. Despite their practical importance, however, there has been little research attempt to develop an RSM-based RPD model with integer-valued constraints. The main reason for a lack of research effort in developing the integer-constrained RPD models is attributed to the fact the design space for experimental purposes and the solution space for optimization purposes are different; consequently, it is believed that there are three major research components which have not been explored in the literature. First, the central composite design (CCD), the commonly used RSM-based RPD tool, may not be capable of assessing integer-valued design points due to the axial points inherent in the CCD. Accordingly, an alternative design tool needs to be implemented. Second, the rotatability property for maintaining predicted responses more consistently within the integer-valued design space also needs to be investigated. Finally, optimization schemes with the integer-valued solution space within the real number based design space need to be developed.

To address the aforementioned three problems, this chapter proposes the Box-Behnken design (BBD) as an alternative to the CCD and other three-level designs, which generates integer design points within its design space and also satisfies the rotatability property. This chapter then develops nonlinear integer programming models, followed by analytical and numerical solution methods, such as the Karush-Khun-Tucker conditions and sequential quadratic programming. This chapter is organized as follows. The model development is presented with a detailed description of each phase. A numerical example is conducted with a comparison study of the proposed models and traditional counterparts. Finally, the conclusion and further studies are discussed. The proposed procedure consists of four main phases: the design, modeling, optimization, and verification phases, which are summarized in Table 3.1.

Table 3.1: Research Phases

Phase I	The design phase
	Decide a response variable
	Decide input variables and their level settings (integer, continuous, or mixed)
	Explain why a BBD-based experiment is most appropriate
	Study the design space
	Study the design rotatability
Phase II	The modeling phase
	Check the normality, randomization, and constant variance assumptions
	Obtain estimated regression functions for the parameter of interest
	Define an objective function and constraints
	Develop optimization models
	Study the solution space
Phase III	The optimization phase
	Develop the sequential quadratic programming method
	Develop the Karush-Kuhn-Tucker (KKT) conditions and check the constraint qualifications
	Obtain the optimal robust parameter design solutions
Phase IV	The verification phase
	Compare the proposed models with existing models

Model Development

Abbreviations and Notation

The abbreviations and notation used in this chapter are summarized in Table 3.2.

Table 3.2: Abbreviations and Notation

Abbreviations/Notation	Description
y	Response variable
$\bar{y}_j$	Mean of the j^{th} experimental run where j = 1, …, m
x_i	The i^{th} input variable where i = 1, …, n
$\mathbf{x}$	The vector of input variables
$f(\mathbf{x})$	Objective function

$g_k(\mathbf{x})$	The k^{th} inequality constraint function
$\hat{\mu}(\mathbf{x})$	Fitted response function of mean
$\hat{\sigma}(\mathbf{x})$	Fitted response function of standard deviation
$\widehat{\sigma^2}(\mathbf{x})$	Fitted response function of variance
σ_{UB}^2	Upper bound of the desired variance
μ_τ	Target value
$\hat{\mu}(\mathbf{x})-\mu_\tau$	Estimated bias function
τ_b	Upper bound of the desired bias
s_i	Estimated standard deviation of the i^{th} run where $i = 1, \ldots, m$
s_i^2	Estimated variance of the i^{th} run where $i = 1, \ldots, m$
$\mathbb{R}^i$	Real valued space of the i^{th} continuous input variable
$\mathbb{Z}^i$	Integer valued space of the i^{th} integer input variable
RO	Randomization order
SO	Standard order
LB	Lower bound of an input variable
UB	Upper bound of an input variable
VM	Vining and Myers's model (1990)
LT	Lin and Tu's model (1995)

The Selection of the Response Surface Design

Unlike the traditional CCD which requires all input variables to be real valued on a continuous scale, the proposed integer-valued RPD models require the investigation of two major issues associated with the design space: the selection of response surface design method and the issue of the rotatability. As shown in Figures 3.1 and 3.2, the design spaces of the traditional CCDs, including the rotatable, inscribed, and face-centered CCDs, are real valued for two and three input variables, respectively, while the design space of the Box-Behnken design (BBD) forms integer cutting planes. The design matrices **D** for the BBD with three and four input variables, and the experimental format of the BBD for *m* runs and *r* replications are shown in Tables 3.3 and 3.4, respectively. The BBD may be preferred over the traditional CCD and other three-level designs for integer-valued RPD models. First, the three-level factorial design, which has -1, 0, and 1 coded levels, is a popular second-order design. However, this particular design is not rotatable and it can be excessively large (Khuri and Mukhopadhyay, 2010). Another popular three-level design is the face-centered CCD which is known to be not rotatable (Khuri and Cornell, 1996; Myers et al., 2009; Khuri and Mukhopadhyay, 2010). The property of rotatability affects the precision of a second-order model's parameters, especially pure quadratic coefficients; therefore, the face-centered CCD may give poor quadratic coefficients. Three-level optimal designs, such as *D*- or *I*-optimal design, may not be appropriate to address constant or nearly-constant prediction variance when integer design points with -1, 0, and 1 coded levels are under study, since $[iiii] \neq 3[iijj]\ (i \neq j)$ where $[iiii]$ and $[iijj]$ are the fourth pure and mixed moments, respectively (Khuri and Cornell, 1996). For example, suppose that we need 16 design-point runs for three input variables in the context of the *I*-optimal design with -1, 0, and 1 coded levels in order to obtain second-order model estimation coefficients. Thus, this particular optimal design is not rotatable, because the ratio moments become $[iiii] = 1.5[iijj]\ (i \neq j)$. On the other hand, the BBD using the three-coded levels with four or seven input variables is exactly rotatable (Myers et al., 2009), while other BBDs are near rotatable. Hence, the BBD may be preferred over the traditional CCD and other three-level designs when maintaining consistent prediction variance is crucial in the context of integer-valued RPD problems.

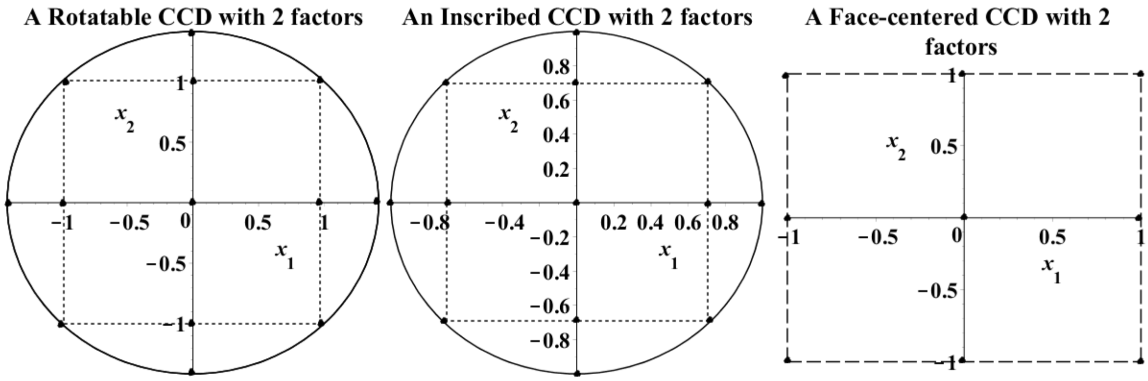


Figure 3.1: The RSM Approaches with Two Input Variables in the Real-valued Space

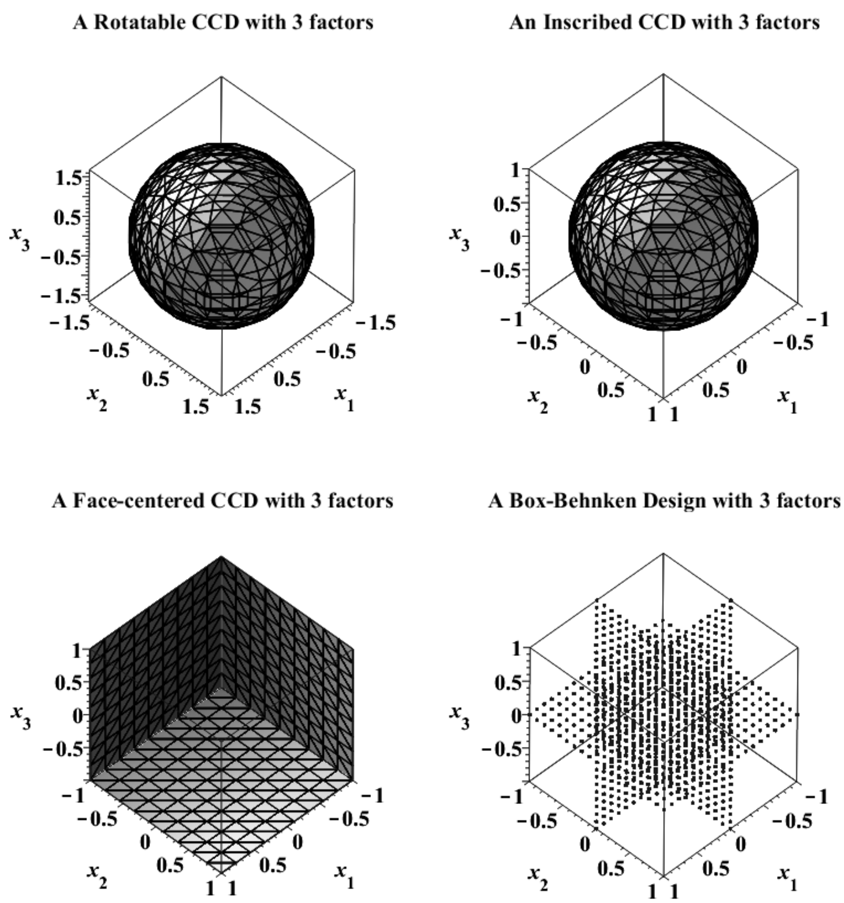


Figure 3.2: The Design Spaces of CCDs and BBD

Table 3.3: Design Matrices for the BBD

x_1	x_2	x_3
-1	-1	0
-1	1	0
1	-1	0
1	1	0
0	-1	-1
0	-1	1
0	1	-1
0	1	1
-1	0	-1
1	0	-1
-1	0	1
1	0	1
0	0	0
0	0	0
0	0	0

x_1	x_2	x_3	x_4
-1	-1	0	0
-1	1	0	0
1	-1	0	0
1	1	0	0
0	0	-1	-1
0	0	-1	1
0	0	1	-1
0	0	1	1
-1	0	0	-1
-1	0	0	1
1	0	0	-1
1	0	0	1
0	-1	-1	0
0	-1	1	0
0	1	-1	0
0	1	1	0
-1	0	-1	0
-1	0	1	0
1	0	-1	0
1	0	1	0
0	-1	0	-1
0	-1	0	1
0	1	0	-1
0	1	0	1
0	0	0	0
0	0	0	0
0	0	0	0

Table 3.4: Experimental Format for the BBD

RO Run	*SO* Run	Input variables (**x**)	Replications	y	s	s^2
m	1		y_{11} ... y_{1r}	$\bar{y}_1$	s_1	s_1^2
4	2		y_{21} ... y_{2r}	$\bar{y}_2$	s_2	s_2^2
1	3		y_{31} ... y_{3r}	$\bar{y}_3$	s_3	s_3^2
.	.	Design matrix of BBD	…	.	.	.
.	.		…	.	.	.
.	.		…	.	.	.
2	m		y_{m1} ... y_{mr}	$\bar{y}_m$	s_m	s_m^2

Once the BBD has been determined as the most appropriate experimental design method for integer-valued input variables, the next step is the check its rotatability. Rotatability is an important design property with constant prediction variance at all points that are equidistant from the design center at (0, ⋯, 0). The prediction variance at any point **x** in the design space is denoted as $Var[\hat{y}(\mathbf{x})] = \sigma^2 \mathbf{x}^{(m)\prime}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}^{(m)}$ where $\mathbf{x}^{(m)\prime}$ is denoted as $[1, x_1, x_2, ..., x_n, x_1^2, x_2^2, ..., x_n^2, x_1x_2, ..., x_{n-1}x_n]$ for the second-order model and $\mathbf{X} = [\mathbf{1}, \mathbf{D}]$. In addition, the scaled prediction variance function is given by $\dfrac{Var[\hat{y}(\mathbf{x})]}{\sigma^2} = N\mathbf{x}^{(m)\prime}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}^{(m)}$ where N denotes the number of runs in the experiment. Intuitively, the prediction variance provides an estimate of the variability of the response surface prediction at different points within the design space of interest. Obviously these predicted variances at different points need to be approximately constant to maintain the predication stability. Let x_i be an input variable of the BBD where $x_i \in \pm 1\ (i = 1,\ 2,\ ...,\ n)$. The distance from the center, ρ_i, is then $\sqrt{(x_i - 0)^2}$ for all i which results in

$\rho_1 = \rho_2 = ... = \rho_n$. Thus, the BBD maintains the rotatability or near rotatability. A detailed discussion of rotatability can be found in Box and Hunter (1957) and Khuri (1988).

In addition, the second-order model matrix is denoted by

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{21} & \cdots & x_{i1} & x_{11}^2 & \cdots & x_{i1}^2 & x_{11}x_{21} & \cdots & x_{i-11}x_{i1} \\ 1 & x_{12} & x_{22} & \cdots & x_{i2} & x_{12}^2 & \cdots & x_{i2}^2 & x_{12}x_{22} & \cdots & x_{i-22}x_{i2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & \cdots & x_{iN} & x_{1N}^2 & \cdots & x_{iN}^2 & x_{1N}x_{2N} & \cdots & x_{i-1N}x_{iN} \end{pmatrix} \tag{3.1}$$

where $i = 1, 2, ..., n$. The design moment matrix is also defined by $\mathbf{M} = \frac{(\mathbf{X}'\mathbf{X})}{N}$ where **M** is the design moment matrix and *N* is the number of total design points. The design moment matrix should have the following form for the rotatable second-order design with *n*-variables.

$$\mathbf{M} = \frac{(\mathbf{X}'\mathbf{X})}{N} = \begin{pmatrix} 1 & 0 & \lambda_2 j_n' & 0 \\ 0 & \lambda_2 I_n & 0 & 0 \\ \lambda_2 j_n' & 0 & \lambda_4(2I_n + j_n' j_n) & 0 \\ 0 & 0 & 0 & \lambda_2 I_t \end{pmatrix} \tag{3.2}$$

where $t = \frac{1}{2}n(n-1)$ and I_n, j_k, and λ_i $(i = 2 \text{ and } 4)$ represent the *n* by *n* unit matrix, the *n*th column vector, and the quantity of the scaling design variables, respectively. In addition, the design is called a precise rotatable design if and only if

1. All odd moments are zero. The odd moments are denoted by

$$[i] = \sum_{a=1}^{N} x_{ia} / N \quad i = 1, 2, ..., n \tag{3.3}$$

$$[ij] = \sum_{a=1}^{N} x_{ia} x_{ja} / N \quad i = 1, 2, ..., n \tag{3.4}$$

$$[iii] = \sum_{a=1}^{N} x_{ia}^3 / N \quad i = 1,\ 2,\ ...,\ n \tag{3.5}$$

$$[iij] = \sum_{a=1}^{N} x_{ia}^2 x_{ja} / N \quad i, j = 1,\ 2,\ ...,\ n \text{ and } i \neq j \tag{3.6}$$

$$[ijk] = \sum_{a=1}^{N} x_{ia} x_{ja} x_{ka} / N \quad i,\ j,\ k = 1,\ 2,\ ...,\ n \text{ and } i \neq j \neq k \tag{3.7}$$

$$[iiij] = \sum_{a=1}^{N} x_{ia}^3 x_{ja} / N \quad i,\ j = 1,\ 2,\ ...,\ n \text{ and } i \neq j \tag{3.8}$$

$$[iijk] = \sum_{a=1}^{N} x_{ia}^2 x_{ja} x_{ka} / N \quad i,\ j,\ k = 1,\ 2,\ ...,\ n \text{ and } i \neq j \neq k \tag{3.9}$$

2. The second pure moments, [*ii*], are denoted by

$$\begin{aligned} &[ii] = \lambda_2 \Rightarrow [ii] = \sum_{a=1}^{N} x_{ia}^2 / N \quad i = 1,\ 2, ..., n \\ &\text{where } \lambda_2 \neq 0 \end{aligned} \tag{3.10}$$

3. The fourth pure moments, [*iiii*], are denoted by

$$[iiii] = 3\lambda_4 \Rightarrow [iiii] = \sum_{a=1}^{N} x_{ia}^4 / N \quad i = 1, 2, ..., n \tag{3.11}$$

4. The fourth mixed moments, [*iijj*], are denoted by

$$[iijj] = \lambda_4 \Rightarrow [iijj] = \sum_{a=1}^{N} x_{ia}^2 x_{ja}^2 / N \quad i, j = 1, 2, ..., n \quad i \neq j \tag{3.12}$$

Note that Equations (3.11) and (3.12) may be combined as a condition, which is $[iiii]/[iijj] = 3$ for $i \neq j$. We investigate the rotatability conditions for the n=4 and 7 BBDs as follows:

$n=4$: All odd moments are zero and $\lambda_2 \neq 0$.

$$N = 24 + n_c \Rightarrow [iiii]/[iijj] = \frac{[12/(24+n_c)]}{[4/(24+n_c)]} = 3 \tag{3.13}$$

$n=7$: All odd moments are zero and $\lambda_2 \neq 0$.

$$N = 56 + n_c \Rightarrow [iiii]/[iijj] = \frac{[24/(56+n_c)]}{[8/(56+n_c)]} = 3 \tag{3.14}$$

where n_c is the number of the center points. Thus, we prove that the BBD is precise rotatable for n=4 and 7.

The Proposed Nonlinear Mixed and Pure Integer Programming Models

It is well known that many engineering problems are well approximated by second-order polynomial models (see Montgomery, 2012) which are given by

$$y = \phi_0 + \sum_{i=1}^{n} \phi_i x_i + \sum_{i=1}^{n} \phi_{ii} x_i^2 + \sum_{i<j=2} \sum_{i=1}^{n} \phi_{ij} x_i x_j + \varepsilon \tag{3.15}$$

where ϕ_i and ε represent regression coefficients and an observed experimental error, respectively. The estimated response of the process mean is then given by

$$\hat{\mu}(\mathbf{x}) = \hat{\alpha}_0 + \mathbf{x}'\mathbf{a} + \mathbf{x}'\mathbf{A}\mathbf{x}$$
$$\text{where } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \ \mathbf{a} = \begin{bmatrix} \hat{\alpha}_1 \\ \hat{\alpha}_2 \\ \vdots \\ \hat{\alpha}_n \end{bmatrix}, \text{ and } \mathbf{A} = \begin{pmatrix} \hat{\alpha}_{11} & \hat{\alpha}_{12}/2 & \dots & \hat{\alpha}_{1n}/2 \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\alpha}_{n1}/2 & \hat{\alpha}_{n2}/2 & \cdots & \hat{\alpha}_{nn} \end{pmatrix} \tag{3.16}$$

where α_i is the regression coefficients associated with estimated process mean, and **a** and **A** represent the vector of the estimated regression coefficients and the matrix of the estimated regression coefficients associated with the process mean, respectively. Similarly, the estimated response of the process standard deviation is expressed by

$$\hat{\sigma}(\mathbf{x}) = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x}$$
$$\text{where } \mathbf{x}=\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix},\ \mathbf{b}=\begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_n \end{bmatrix},\ \text{and } \mathbf{B}=\begin{pmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \dots & \hat{\beta}_{1n}/2 \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\beta}_{n1}/2 & \hat{\beta}_{n2}/2 & \cdots & \hat{\beta}_{nn} \end{pmatrix} \tag{3.17}$$

where β_i is the regression coefficients associated with estimated standard deviation, and **b** and **B** are the vector of the estimated regression coefficients and the matrix of the estimated regression coefficients associated with the process standard deviation, respectively. In addition, the estimated response of the process variance is shown as follows.

$$\widehat{\sigma^2}(\mathbf{x}) = \hat{\gamma}_0 + \mathbf{x}'\mathbf{c} + \mathbf{x}'\mathbf{C}\mathbf{x}$$
$$\text{where } \mathbf{x}=\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix},\ \mathbf{c}=\begin{bmatrix} \hat{\gamma}_1 \\ \hat{\gamma}_2 \\ \vdots \\ \hat{\gamma}_n \end{bmatrix},\ \text{and } \mathbf{C}=\begin{pmatrix} \hat{\gamma}_{11} & \hat{\gamma}_{12}/2 & \dots & \hat{\gamma}_{1n}/2 \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\gamma}_{n1}/2 & \hat{\gamma}_{n2}/2 & \cdots & \hat{\gamma}_{nn} \end{pmatrix} \tag{3.18}$$

where γ_i is the regression coefficients associated with estimated process variance, and **c** and **C** represent the vector of the estimated regression coefficients and the matrix of the estimated regression coefficients associated with the process variance, respectively.

There are two dominant traditional optimization models for solving RSM-based RPD optimization problems: the dual response model developed by Vining and Myers (1990), referred to as the *VM* model, and the mean squared error model developed by Lin and Tu (1995), referred to as the *LT* model. Note that these two models assume that input variables are real valued. The *VM* model is given by

$$\begin{aligned} &\text{Minimize } f(\mathbf{x}) = \hat{\sigma}(\mathbf{x}) \\ &\text{subject to } h_1(\mathbf{x}) = 0 \\ &\qquad\qquad \mathbf{x} \in X \end{aligned} \tag{3.19}$$

where $h_1(\mathbf{x}) = \hat{\mu}(\mathbf{x}) - \mu_\tau$ and $\mathbb{R}^n \supseteq X = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}^{'}\mathbf{x} \le \rho\}$. The goal of this optimization model is to reduce standard deviation while the mean should be located at the target value (i.e., the zero bias) in the bounded convex set. Along those lines, Goethals et al. (2009) investigated the different variability measurements to find optimum RPD solutions.

We propose the nonlinear mixed integer programming (NLMIP) and nonlinear pure integer programming (NLPIP) models which incorporate the variance estimator while relaxing the zero-bias assumption (i.e., allowing some distance between mean and the target value) based on the following mean squared error model:

$$\begin{aligned} &\text{Minimize } f(\mathbf{x}) = \left[\hat{\mu}(\mathbf{x}) - \mu_\tau\right]^2 + \left[\widehat{\sigma^2}(\mathbf{x})\right] \\ &\text{subject to } \mathbf{x} \in \mathrm{X} \\ &\qquad\qquad x_i \in \mathbb{Z},\ \forall_i \in I \end{aligned} \tag{3.20}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}^m$ are twice continuously differentiable functions, $\mathbb{R}^n \supseteq X$ is a bounded convex set, and $I \subseteq \{c+1, \ldots, n\}$ is the index set of integer-valued input variables in the model. Also, it would be more practical to impose an upper bound with the following constraint:

$$g_1(\mathbf{x}) \le 0 \Rightarrow g_1(\mathbf{x}) = \mid \hat{\mu}(\mathbf{x}) - \mu_\tau \mid - \tau_b \tag{3.21}$$

In addition, by imposing an upper bound on the process variance, we have the additional constraint as follows:

$$g_2(\mathbf{x}) \leq 0 \Rightarrow g_2(\mathbf{x}) = \widehat{\sigma^2}(\mathbf{x}) - \sigma_{UB}^2 \tag{3.22}$$

The constraint associated with the design space should also be included as follows:

$$g_3(\mathbf{x}) \leq 0 \Rightarrow g_3(\mathbf{x}) = \sum_{i=1}^{n} x_i^2 - n \tag{3.23}$$

Finally, the proposed NLMIP and NLPIP models are shown in Table 3.5, where $\hat{\mu}(\mathbf{x})$ and $\widehat{\sigma^2}(\mathbf{x})$ are given in Equations (3.16) and (3.18).

Table 3.5: The Proposed BB-Embedded NLMIP and NLPIP Robust Parameter Design Models

The objective Function	Minimize $f(\mathbf{x}) = \left[\hat{\mu}(\mathbf{x}) - \mu_\tau\right]^2 + \widehat{\sigma^2}(\mathbf{x})$
	subject to
Constraint associated with the bias	$g_1(\mathbf{x}) \leq 0 \Rightarrow \lvert \mu(\mathbf{x}) - \mu_\tau \rvert \leq \tau_b$
Constraint associated with the variance	$g_2(\mathbf{x}) \leq 0 \Rightarrow \widehat{\sigma^2}(\mathbf{x}) \leq \sigma_{UB}^2$
Constraint associated with the design space	$g_3(\mathbf{x}) \leq 0 \Rightarrow \sum_{i=1}^{n} x_i^2 \leq n$
Constraints associated with the boundaries of input variables	$LB \leq x_i \leq UB \Rightarrow -1 \leq x_i \leq 1 \ (i = 1,\ 2,\ \ldots,\ n)$
Other constraints associated with input variables	$NLMIP = \begin{cases} x_i \in \mathbb{R} \ (i = 1,\ \ldots,\ c) \\ x_i \in \mathbb{Z} \ (i = c+1,\ \ldots,\ n) \end{cases}$ or $NLPIP = \{\forall x_i \in \mathbb{Z} \ \ (i = 1,\ 2,\ \ldots,\ n)$

Notice that the convex hull of the solution space *S*, defined by $conv(S) = \{\sum_{i=1}^{n} \lambda_i x_i \mid \sum_{i=1}^{n} \lambda_i = 1,\ 0 \leq \lambda_i \leq 1,\ -1 \leq x_i \leq 1 \text{ and } \forall x_i \in S\}$, is a hypercube, while

$f(\mathbf{x})$ and $g_k(\mathbf{x})$ are convex combinations in the bounded convex set. In the next two sections, the analytical and numerical optimization methods are discussed as solution methods.

Solution Methods

In this section, two solution methods are discussed for solving the proposed BBD-embedded, RSM-based nonlinear integer programming model. They are the Karush-Khun-Tucker (KKT) conditions and the sequential quadratic programming method.

The Karush-Khun-Tucker Conditions

The constraint associated with process bias in the proposed model can be separated as follows:

$$\begin{aligned} &\hat{\mu}(\mathbf{x}) - \mu_\tau \le \tau_b \\ -&\hat{\mu}(\mathbf{x}) + \mu_\tau \ge \tau_b \end{aligned} \tag{3.24}$$

Intuitively, the separated constraints improve the running time of the proposed optimization model. The Lagrangian function of the relaxed model is associated with the function $L : S * \mathbb{R}^{n+k} \to \mathbb{R}$, which is expressed as

$$\begin{aligned} L(\mathbf{x}, \boldsymbol{\lambda}) = {} & f(\mathbf{x}) + \lambda^k g_k(\mathbf{x}) \\ & = [\hat{\alpha}_0 + \mathbf{x}'\mathbf{a} + \mathbf{x}'\mathbf{A}\mathbf{x} - \mu_\tau]^2 + \hat{\gamma}_0 + \mathbf{x}'\mathbf{c} + \mathbf{x}'\mathbf{C}\mathbf{x} \\ & \quad + \lambda_1(\hat{\alpha}_0 + \mathbf{x}'\mathbf{a} + \mathbf{x}'\mathbf{A}\mathbf{x} - \mu_\tau - \tau_b) + \lambda_2(-\hat{\alpha}_0 - \mathbf{x}'\mathbf{a} - \mathbf{x}'\mathbf{A}\mathbf{x} + \mu_\tau - \tau_b) \\ & \quad + \lambda_3(\hat{\gamma}_0 + \mathbf{x}'\mathbf{c} + \mathbf{x}'\mathbf{C}\mathbf{x} - \sigma_{UB}^2) + \lambda_4(\sum_{i=1}^{n} x_i^2 - n) \\ & \quad + \lambda_5(-x_1 - 1) + \ldots + \lambda_{k-n}(-x_n - 1) + \lambda_{k-n+1}(x_1 - 1) + \ldots + \lambda_k(x_n - 1) \end{aligned} \tag{3.25}$$

The set of active constraints is then expressed as follows: $I_{active}(\mathbf{x}) = \{i \in \{1, \ ..., \ k\} \mid g_k(\mathbf{x}) = 0, \mathbf{x} \in \mathbb{R}\}$, where $I_{active}(\mathbf{x})$ are referred as active constraints set. In addition, inactive constraints are denoted as $I_{inactive}(\mathbf{x}) = \{1, \ ..., \ k\} / I_{active}(\mathbf{x})$. The strict complementary slackness is then defined by

$$\begin{aligned} & g_i(\mathbf{x}^*)\lambda_i^* = 0, \ 1 \le i \le k \\ & \lambda_i^* \ge 0, \ i \in I_{active}(\mathbf{x}^*) \ when \ \mathbf{x} \in \mathbb{R} \end{aligned} \tag{3.26}$$

Let $\mathbf{x}^* \in \mathbb{R}$ denote a local minimum of the model, and also let $\boldsymbol{\lambda}^* \in \mathbb{R}$ denote the Lagrange multipliers. The Karush-Kuhn-Tucker (KKT) conditions can be defined by

$$\nabla L(\mathbf{x}^*, \boldsymbol{\lambda}^*) = \nabla f(\mathbf{x}^*) + \nabla g(\mathbf{x}^*)\boldsymbol{\lambda}^* = 0 \tag{3.27}$$

The three second-order sufficient optimality conditions can also be expressed. First, $G(\mathbf{x}^*)$ are linearly independent where $G(\mathbf{x}) = (\nabla g(\mathbf{x}^1), \ ..., \ \nabla g(\mathbf{x}^k))$. Second, the complementary slackness holds at $\mathbf{x}^*$. Third, $d'\mathbf{H}L^* d > 0$ for all $d \neq 0$ as $G(\mathbf{x}^*)^k d = 0$. It is noted that the Hessian matrix of the Lagrangian function, **H**, is positive definite on the null space of $G(\mathbf{x}^*)^k$. In addition, the second-order optimality conditions assure that $\mathbf{x}^*$ is the local minimum of the model and Lagrange multipliers ($\boldsymbol{\lambda}^*$) are unique.

The Sequential Quadratic Programming Method

Sequential quadratic programming (SQP) methods have proved highly effective for solving constrained optimization problems with smooth nonlinear functions in the objective function and the constraints (Gill et al., 2002). The essential notion of the SQP method is to formulate the model, such as the NLP at a given solution $\mathbf{x}^k$, by using it as a quadratic sub-problem model, and applying the solution to this sub-problem to build an improved approximation $\mathbf{x}^{k+1}$. The SQP process, which is also well-suited to inequality forms, is a strong and iterative solution procedure for the NLP models. This procedure makes a sequence of approximations that will merge to a solution for $\mathbf{x}^*$. Note that the SQP method is not a feasible-point optimization technique; that is, the SQP method allows the initial points which are not necessary to be feasible. Hence, the SQP method is a great choice as an optimization method for solving the proposed NLP problems since their design and solution spaces are not necessarily the same.

The objective function of the model $f(\mathbf{x})$ is defined by its local quadratic approximation by

$$f(\mathbf{x}) \approx f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)(\mathbf{x}-\mathbf{x}^k) + \frac{1}{2}(\mathbf{x}-\mathbf{x}^k)' H_{f(\mathbf{x}^k)}(\mathbf{x}-\mathbf{x}^k) \tag{3.28}$$

where $\nabla f(\mathbf{x})$ is the gradient of $f(\mathbf{x})$, and $H_{f(\mathbf{x})}$ is the Hessian of $f(\mathbf{x})$. Note that $g : S \to \mathbb{R}^n$ is the vector-valued form of each inequality constraint in the proposed model. Using local affine approximations, the constraints of g are then defined as

$$g(\mathbf{x}) \approx g(\mathbf{x}^k) + \nabla g(\mathbf{x}^k)(\mathbf{x}-\mathbf{x}^k) \tag{3.29}$$

where $\nabla g(\mathbf{x})$ is the gradient of $g(\mathbf{x})$, and $\Delta\mathbf{x} = \mathbf{x}^{k+1} - \mathbf{x}^k$.

The sub-problem of the proposed model is expressed as follows:

$$
\begin{aligned}
&\text{Minimize } \nabla f(\mathbf{x}^k)'\Delta\mathbf{x} + \tfrac{1}{2}(\Delta\mathbf{x})' H_{f(\mathbf{x}^k)}\Delta\mathbf{x} \\
&\text{subject to } g(\mathbf{x}^k) + \nabla g(\mathbf{x}^k)'\Delta\mathbf{x} \le 0 \Rightarrow g(\mathbf{x}^k) + J_g(\mathbf{x}^k)\Delta\mathbf{x} \le 0 \\
&\text{where } \nabla f(\mathbf{x}^k) = \left[\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}\right] = \left[2(\hat{\alpha}_0 + \mathbf{x}'\mathbf{a} + \mathbf{x}'\mathbf{A}\mathbf{x} - \mu_\tau)(\mathbf{a} + \mathbf{A}\mathbf{x}) + (\mathbf{c} + \mathbf{C}\mathbf{x})\right], \\
&\qquad H_{f(\mathbf{x}^k)} = \left[\frac{\partial f^2(\mathbf{x})}{\partial \mathbf{x}\partial \mathbf{x}}\right] = \left[2((\mathbf{a} + \mathbf{x}\mathbf{A})^2 + (\hat{\alpha}_0 + \mathbf{x}^T\mathbf{a} + \mathbf{x}^T\mathbf{A}\mathbf{x} - \tau)\mathbf{A}) + \mathbf{C}\right], \\
&\qquad J_g(\mathbf{x}^k) = \begin{bmatrix} \dfrac{\partial g_1(\mathbf{x})}{\partial \mathbf{x}} \\ \dfrac{\partial g_2(\mathbf{x})}{\partial \mathbf{x}} \\ \dfrac{\partial g_3(\mathbf{x})}{\partial \mathbf{x}} \end{bmatrix} = \begin{bmatrix} \dfrac{(\hat{\alpha}_0 + \mathbf{x}'\mathbf{a} + \mathbf{x}'\mathbf{A}\mathbf{x} - \mu_\tau)(\mathbf{a} + \mathbf{A}\mathbf{x})}{|\hat{\alpha}_0 + \mathbf{x}'\mathbf{a} + \mathbf{x}'\mathbf{A}\mathbf{x} - \mu_\tau|} \\ \mathbf{c} + \mathbf{C}\mathbf{x} \\ 2\mathbf{x} \end{bmatrix}, \\
&\qquad -1 \le \mathbf{x} \le 1 \text{ and } \Delta\mathbf{x} \in \mathbb{R}^n
\end{aligned}
\tag{3.30}
$$

where $J_g(\mathbf{x}^k)$ is the Jacobian function of g. This procedure is terminated when $\mathbf{x}^{k+1} - \mathbf{x}^k$ is smaller than the specified tolerance.

Note that the nonlinear branch-and-bound method may be performed based on lower and upper bounds in the integer-constrained solution space for the BBD to obtain integer-valued input variables and update continuous-valued input variables if the solutions of integer-valued variables are not integral. The nonlinear branch-and-bound method selects the branching input variables and branching nodes based on the iterative procedure. In addition, this procedure is repeated until all integer-valued variables obtained in the solution space. We also perform the sequential quadratic programming technique for the NLP optimization phase and we also use the Maple software. On the other hand, the idea of rounding is not a good notion because the optimum solution can change or be infeasible, and the continuous variables are also needed to update for optimal operating conditions.

Otherwise, one or more constraints can be violated finding the optimal solution for the optimization model if the rounding is just used to obtain integer variables.

Numerical Example

In this section, we consider a BBD with three input variables and four replications at each design point. The BBD is analyzed as the four-phased model development which has been explained in the proposed procedure flow map. Note that the computer codes are shown in Appendix A for this numerical example.

The Design Phase

In this study, the first and second input variables are assumed to be integer-valued variables, and the third input variable is assumed to be a continuous-valued variable. The experimental results are found using the four replications for the response. The coded variables and their levels for the BBD experiment are shown in Table 3.6.

Table 3.6: Coded Variables and Levels for the BBD Experiment

		Coded Levels		
	Coded	-1	0	1
The first input variable	x_1	1	2	3
The second input variable	x_2	1	2	3
The third input variable	x_3	4	5	6

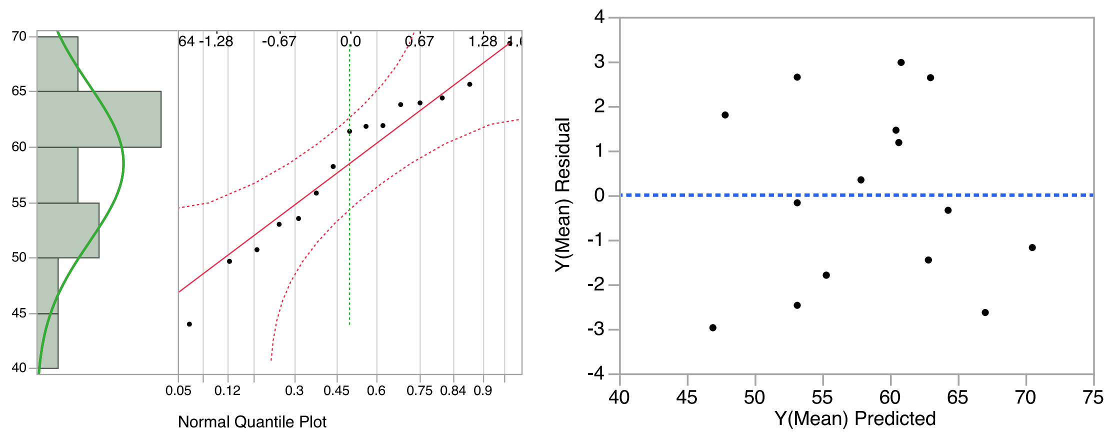
The Modeling Phase

The experimental results with four replications at each design point are shown in Table 3.7.

Table 3.7: The BBD Experiment

SO	x_1	x_2	x_3	y_1	y_2	y_3	y_4	$\bar{y}$	s	s^2
1	-1	-1	0	49.2	43.1	43.0	40.5	43.95	3.70	13.70
2	-1	1	0	62.6	52.7	68.0	62.2	61.38	6.36	40.44
3	1	-1	0	68.2	69.3	59.9	50.2	61.90	8.86	78.45
4	1	1	0	60.5	79.0	62.5	53.2	63.80	10.89	118.66
5	0	-1	-1	55.9	50.9	52.5	73.5	58.20	10.41	108.39
6	0	-1	1	70.0	58.4	71.5	47.4	61.83	11.26	126.75
7	0	1	-1	81.2	62.0	60.3	73.8	69.33	9.94	98.72
8	0	1	1	69.7	66.2	54.7	65.2	63.95	6.46	41.75
9	-1	0	-1	80.9	67.8	58.8	55.0	65.63	11.51	132.51
10	1	0	-1	43.3	40.8	72.3	57.6	53.50	14.56	211.86
11	-1	0	1	54.3	55.2	52.3	36.7	49.63	8.70	75.72
12	1	0	1	61.6	63.7	72.5	59.8	64.40	5.63	31.70
13	0	0	0	39.7	49.6	69.6	43.8	50.68	13.25	175.68
14	0	0	0	54.8	46.4	57.3	64.7	55.80	7.55	56.94
15	0	0	0	53.0	62.2	55.1	41.6	52.98	8.54	73.00

The normality and constant variance assumptions are checked using the normal probability and residual plots, shown in Figure 3.3 (a), and Figure 3.3 (b), respectively.



(a) (b)

Figure 3.3: (a) Normal Quantile Plot of the Process Mean; (b) Residual Plot of the Process Mean

The Shapiro-Wilk test was used to check the normality assumption, and the p-value is 0.565; therefore, it is concluded that the normality assumption is supported with alpha value = 0.05. In addition, the residual plot shows that the constant variance assumption is met. Using JMP software, the second-order response surface models of the mean, standard deviation, and variance are obtained as follows:

$$\begin{aligned}\hat{\mu}(\mathbf{x}) = {} & 53.15 + 2.88x_1 + 4.07x_2 - 0.86x_3 - 0.22x_1^2 + 4.82x_2^2 + 5.35x_3^2 \\ & - 3.88x_1x_2 + 6.73x_1x_3 - 2.25x_2x_3\end{aligned} \tag{3.31}$$

$$\begin{aligned}\hat{\sigma}(\mathbf{x}) = {} & 9.78 + 1.21x_1 - 0.07x_2 - 1.80x_3 - 0.87x_1^2 - 1.46x_2^2 + 1.19x_3^2 \\ & - 0.16x_1x_2 - 1.53x_1x_3 - 1.08x_2x_3\end{aligned} \tag{3.32}$$

$$\begin{aligned}\widehat{\sigma^2}(\mathbf{x}) = {} & 101.87 + 22.29x_1 - 3.47x_2 - 34.45x_3 - 10.01x_1^2 - 29.05x_2^2 + 21.08x_3^2 \\ & + 33.7x_1x_2 - 30.84x_1x_3 - 18.83x_2x_3\end{aligned} \tag{3.33}$$

The Optimization Phase

Using the Sequential Quadratic Programming Approach

The proposed optimization model is given in Table 3.8. The sequential quadratic programming in the Maple NLP solver uses a BBD to obtain the optimal RPD solutions, which are shown in Table 3.9; in addition, the optimal values of process mean and standard deviation, along with the objective functional value, are also shown in Table 3.9. The SQP provides a global minimum at the 11th iteration.

Table 3.8: The Optimization Model

Minimize	$[53.15+2.88x_1+4.07x_2-0.86x_3-0.22x_1^2+4.82x_2^2+5.35x_3^2-3.88x_1x_2$ $+6.73x_1x_3-2.25x_2x_3-60]^2+101.87+22.29x_1-3.47x_2-34.45x_3$ $-10.01x_1^2-29.05x_2^2+21.08x_3^2+3.37x_1x_2-30.84x_1x_3-18.83x_2x_3$
Subject to	$\lvert 53.15+2.88x_1+4.07x_2-0.86x_3-0.22x_1^2+4.82x_2^2+5.35x_3^2$ $-3.88x_1x_2+6.73x_1x_3-2.25x_2x_3-\mu_\tau \rvert \le \tau_b$
	$101.87+22.29x_1-3.47x_2-34.45x_3-10.01x_1^2-29.05x_2^2$ $+21.08x_3^2+3.37x_1x_2-30.84x_1x_3-18.83x_2x_3 \le \sigma_{UB}^2$
	$x_1^2+x_2^2+x_3^2 \le n$
Given	$\mu_\tau=60,\ \tau_b=0.6,\ \sigma_{UB}^2=144,$ and $n=3$
	$-1 \le x_i \le 1\ (i=1,2,3)$
	x_1 and $x_2 \in \mathbb{Z}; x_3 \in \mathbb{R}$
Find	Factor settings $\mathbf{x}^*=(x_1^*,\ x_2^*,\ x_3^*)^T$ and objective function value of the model

Table 3.9: The Result of the Optimization Problem by Using the SQP

Iteration Number	x_1^*	x_2^*	x_3^*	$\hat{\mu}(\mathbf{x}^*)$	$\hat{\sigma}(\mathbf{x}^*)$	$f(\mathbf{x}^*)$
11	-1.000	1.000	0.429	59.584	5.285	28.106

Using the Karush-Kuhn-Tucker Conditions

The proposed model is converted using the Lagrangian functions as follows:

$$
\begin{aligned}
\text{Minimize } L(\mathbf{x},\ \boldsymbol{\lambda}) = {} & (-6.85 + 2.88x_1 + 4.07x_2 - 0.86x_3 - 0.22x_1^2 + 4.82x_2^2 \\
& + 5.35x_2^3 - 3.88x_1x_2 + 6.73x_1x_3 - 2.25x_2x_3)^2 + 101.87 \\
& + 22.29x_1 - 3.47x_2 - 34.45x_3 - 10.01x_1^2 - 29.05x_2^2 \\
& + 21.08x_3^2 + 3.37x_1x_2 - 30.84x_1x_3 - 18.83x_2x_3 \\
& + \lambda_1(-6.85 + 2.88x_1 + 4.07x_2 - 0.86x_3 - 0.22x_1^2 \\
& + 4.82x_2^2 + 5.35x_3^2 - 3.88x_1x_2 + 6.73x_1x_3 - 2.25x_2x_3 \\
& - 0.6) + \lambda_2(+6.85 - 2.88x_1 - 4.07x_2 + 0.86x_3 + 0.22x_1^2 \\
& - 4.82x_2^2 - 5.35x_3^2 + 3.88x_1x_2 - 6.73x_1x_3 + 2.25x_2x_3 \\
& - 0.6) + \lambda_3(101.87 + 22.29x_1 - 3.47x_2 - 34.45x_3 \\
& - 10.01x_1^2 - 29.05x_2^2 + 21.08x_3^2 + 3.37x_1x_2 \\
& - 30.84x_1x_3 - 18.83x_2x_3 - 144) + \lambda_4(x_1^2 + x_2^2 + x_3^2 - 3) \\
& + \lambda_5(-1 - x_1) + \lambda_6(-1 + x_1) + \lambda_7(-1 - x_2) + \lambda_8(-1 + x_2) \\
& + \lambda_9(-1 - x_3) + \lambda_{10}(-1 + x_3)
\end{aligned}
\tag{3.31}
$$

The constraint qualifications are met. As such, the Lagrangian method and the KKT conditions are computed using the Maple software, which are shown in Table 3.10.

Table 3.10: The KKT Points and Multipliers for the Proposed Model

Model	Settings ($\mathbf{x}^*$)	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8	λ_9	λ_{10}
The proposed model	(-1.000, 1.000, 0.429)	0	0	0	0	30.525	0	0	86.826	0	0

Running times for completing this example using the SQP method and the KKT conditions took 0.15 and 4.71 seconds, respectively, on the computer, which has 2.6 GHz Intel Core i5 with 8 GB 1600 MHz DDR3 memory. It was observed that the SQP required 20.18 M (megabyte) for this numerical example, while the KKT conditions required 74.19 M. For this particular example, the SQP technique solved the problem more quickly and also required less memory. It is noted that the KKT conditions do not always guarantee the optimal solutions. It is also experimentally proved that the separation of the constraints may be a useful approach to reduce the computational time and increase the efficiency.

The Verification Phase

This section provides comparisons between the proposed model and traditional models (*VM* and *LT*), which are shown in Tables 3.11 and 3.12.

Table 3.11: Comparison Study between the Proposed Model and the *VM* and *LT* Models

Model	Settings ($\mathbf{x}^*$)	$\hat{\mu}(\mathbf{x}^*)$	$\hat{\sigma}(\mathbf{x}^*)$
VM	(1.000, 0, 0.493)	60.000	8.768
LT	(1.000, 1.000, 0.392)	56.938	6.884
Proposed	(-1.000, 1.000, 0.429)	59.584	5.285

Table 3.12: Six Different Cases with Results

Case Number	Variables Types	Model	Coded Settings ($\mathbf{x}^*$)	$\hat{\mu}(\mathbf{x}^*)$	$\hat{\sigma}(\mathbf{x}^*)$
Case 1	$x_1 \in \mathbb{Z}$	*VM*	(1.000, 0.668, 0.316)	60.000	8.154
	$x_2, x_3 \in \mathbb{R}$	*LT*	(1.000, 0.953, 0.418)	58.870	6.961
		Proposed	(-1.000, 1.000, 0.429)	59.584	5.285
Case 2	$x_2 \in \mathbb{Z}$	*VM*	(1.000, 0, 0.493)	60.000	8.768
	$x_1, x_3 \in \mathbb{R}$	*LT*	(-1.000, 1.000, 0.355)	59.999	6.001
		Proposed	(-1.000, 1.000, 0.429)	59.584	5.285
Case 3	$x_3 \in \mathbb{Z}$	*VM*	(-0.726, 1.000, 1.000)	60.000	6.450
	$x_1, x_2 \in \mathbb{R}$	*LT*	(-0.913, 1.000, 1.000)	58.865	6.273
		Proposed	(-0.825, 1.000, 1.000)	59.403	5.883
Case 4	$x_1, x_3 \in \mathbb{Z}$	*VM*	(1.000, 0.913, 0)	60.000	8.693
	$x_2 \in \mathbb{R}$	*LT*	(1.000, 1.000, 0)	60.82	8.430
		Proposed	(-1.000, 0.869, 0)	60.598	6.457
Case 5	$x_2, x_3 \in \mathbb{Z}$	*VM*	(0.247, 0, 1.000)	60.000	9.038
	$x_1 \in \mathbb{R}$	*LT*	(-0.913, 1.000, 1.000)	58.865	6.273
		Proposed	(-0.825, 1.000, 1.000)	59.403	5.883
Case 6	$x_1, x_2, x_3 \in \mathbb{Z}$	*VM*	-	-	-
		LT	(1.000, 1.000, 0)	60.820	8.430
		Proposed	(1.000, -1.000, 0)	60.440	9.230

It is observed that the proposed model gives a smaller standard deviation than the *VM* and *LT* models, but generates a larger process bias compared to the *VM* and *LT* models. This particular example shows that if variance reduction is more important than meeting the target value, perhaps the proposed model is more useful. Note that Case 6 represents the NLPIP model in Table 3.12.

Conclusions

In this chapter, a four-phased procedure was proposed to obtain the BBD-based RPD solutions with minimum process bias and variability. This chapter also discussed the conceptual and technical frameworks supporting the BBD as a preferred experimental design method over the CCD and other three-level designs with integer-valued variables. Nonlinear mixed and pure integer models were then proposed with two suggested solution methods: the sequential quadratic method and the Karush-Khun-Tucker conditions. A numerical example was illustrated to compare the proposed nonlinear mixed and pure integer programming models with the existing models. It was observed that the proposed models generally provide a better solution in terms of process variance. It was also found that both solution procedures we suggested, particularly the sequential quadratic programming method, were efficient in finding robust parameter solutions. As an extension, incorporating multiple quality characteristics could be a fruitful future research area. Another extension would be the consideration of binary input variables in the context of the nonlinear mixed or binary integer programming framework.

CHAPTER FOUR

A 0-1 MIXED INTEGER NONLINEAR PROGRAMMING MODEL TO SOLVE THE RESPONSE SURFACE-BASED ROBUST PARAMETER DESIGN PROBLEM WITH QUALITATIVE AND QUANTITATIVE VARIABLES

Introductory Remarks

The robust parameter design (RPD) methodology, originally proposed by Taguchi, is an efficient tool for building quality into the design of processes and products by determining optimal operating conditions for input variables. The main concept of the RPD is to minimize variability in the output response of a product around the target value. A number of RPD models have been proposed and reported a significant improvement in product and process quality.

Research Motivations

The main purpose of this chapter is to establish the modeling and optimization framework when both quantitative and 0-1 based qualitative input variables are integrated into the response surface based RPD. To this end, we propose three phases: a statistical design phase, an optimization modeling phase, and a comparison phase. In the statistical design phase, we lay out the foundation of a special factorial design by embedding those input variables into a factorial design with pseudo-center points. In the optimization modeling phase, we formulate the proposed RPD problem with the binary-valued constraints which can efficiently provide solutions for both quantitative and qualitative input variables in the 0-1 mixed integer nonlinear programming (MINLP) framework. Finally, we compare the solutions using three optimization tools, such as the outer approximation (OA) method, the branch-and-bound (BB) technique, and the hybrid branch-and-cut (HNBC) algorithm, with traditional counterparts.

This chapter is organized as follows. First, the model development is presented. The proposed model is then shown. Next, the numerical example is conducted. Finally, conclusions and further study are drawn.

Model Development

Abbreviations and Notation

The abbreviations and notation used in this chapter are described in Table 4.1.

Table 4.1: Abbreviations and Notation

Abbreviations/Notation	**Description**
y	Response variable
$\bar{y}_j$	Mean value of the j^{th} experimental run where j = 1, …, n
x_i	The i^{th} quantitative input variable where i = 1, …, l
$\mathbf{x}$	The vector of input variables
z_j	The j^{th} qualitative input variable where j= 1, …, m
$f(\mathbf{x})$	The objective function of the model
$g_k(\mathbf{x})$	The kth inequality constraint of the model
$\hat{\mu}(\mathbf{x})$	The fitted response function of process mean
$\hat{\sigma}(\mathbf{x})$	The fitted response function of process standard deviation
$\widehat{\sigma^2}(\mathbf{x})$	The fitted response function of process variance
τ	The target value of a quality characteristic
Δ_{σ^2}	A desired upper bound of process variance
s_i	The estimated standard deviation of the i^{th} run
s_i^2	The estimated variance of the i^{th} run

n_f	Number of factorial points
n_c	Number of center points
n_{pc}	Number of pseudo-center points
$\mathbb{R}^i$	Real space of the i^{th} continuous input variable
$\mathbb{Z}^j$	Integer valued space of the j^{th} integer input variables
NLP	Nonlinear programming
VM	Model of Vining and Myers (1990)
LT	Model of Lin and Tu (1995)

The Selection of Coded Levels for Qualitative and Quantitative Input Variables

In this chapter, the coded levels of input variables, denoted by -1, 0, and 1, represent low, intermediate, and high levels, respectively. Qualitative variables are classified as binary and trinary and their coded levels are denoted as

$$\left.\begin{array}{l} z_j = -1 \text{ if the level is low} \\ \text{Binary}\begin{cases} z_j = \ \ 0 \text{ if the level is low/intermediate} \\ z_j = \ \ 1 \text{ if the level is high} \end{cases} \end{array}\right\} \text{Trinary and } j = 1,\ 2,\ \ldots.,\ m \quad (4.1)$$

In addition, quantitative variables are classified as continuous or integer valued variables whose coded levels are denoted as

$$\left.\begin{array}{l} x_i = -1 \text{ if the level is low} \\ x_i = \ \ 0 \text{ if the level is intermediate} \\ x_i = \ \ 1 \text{ if the level is high} \end{array}\right\} x_i \in R \text{ or } Z \ (i = 1,\ 2,\ \ldots.,\ l) \qquad (4.2)$$

The Inclusion of Center and Pseudo-Center Points

Draper (1982) reviewed the existing approaches for selecting the number of center points in certain types of second-order response surface designs and discussed an integrated variance criterion for fewer center points. The proper choice of the number of center points is important and it should be accurately set for a good design (see Box and Draper, 1987; Draper and Lin, 1996). Furthermore, Myers et al. (2009) conducted the most recent study for choosing the number of center points. They suggested that one or two and three to five center points are sufficient to provide a reasonable stability of the scaled prediction variance in the cuboidal and spherical design spaces, respectively.

The number of center points influences the prediction variance,

$$Var[\hat{y}(\mathbf{x})] = \mathbf{x}^{(m)\prime}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}^{(m)}\sigma^2, \tag{4.3}$$

where $Var[\hat{y}(\mathbf{x})]$, $\mathbf{x}^{(m)}$, $\mathbf{X}$, and σ^2 represent the variance of a predicted value (or the prediction variance), a vector corresponding to the model terms, the model matrix, and a variance, respectively. It is known that the prediction variance, $Var[\hat{y}(\mathbf{x})]$, is based on the location of **x** which is dependent on the inverse matrix of information matrix ($\mathbf{X}'\mathbf{X}$). In this chapter, we include center point runs to obtain an independent estimate of pure error for a lack-of-fit test and we then verify the adequacy of the fitted model. It is needed to run at least one center point for fitting a quadratic model; otherwise, the information matrix will be singular and cannot be inverted to obtain a least square fit. Checking the adequacy of a fitted model is also crucial to avoid misleading conclusions. In addition, the inclusion of center points also provides the variance stability and check for curvature for second-order models.

Table 4.2 shows values of $Var[\hat{y}(\mathbf{x})]$ at design points and the degrees of freedom (*df*) for pure error for two, three and four quantitative input variables in factorial designs with center points. In Table 4.2, we consider the center points for quantitative input variables in the design; however, a proper selection of actual center points does not exist in the literature when both qualitative and quantitative input variables are under study.

Table 4.2: Selected Numbers of Center Points in Factorial Designs

Input variables	n_c	Var$[\hat{y}(\mathbf{x})]$ at design points			df for pure error
		(0, 0)	(-1, -1) or (1, 1)	(-0.5, -0.5) or (0.5, 0.5)	
x_1 and x_2	1	$0.200\sigma^2$	$0.950\sigma^2$	$0.341\sigma^2$	-
	2	$0.167\sigma^2$	$0.917\sigma^2$	$0.307\sigma^2$	1
	3	$0.143\sigma^2$	$0.893\sigma^2$	$0.283\sigma^2$	2
	4	$0.125\sigma^2$	$0.875\sigma^2$	$0.266\sigma^2$	3
	5	$0.111\sigma^2$	$0.861\sigma^2$	$0.252\sigma^2$	4
	6	$0.100\sigma^2$	$0.850\sigma^2$	$0.241\sigma^2$	5
		(0, 0, 0)	(-1, -1, -1) or (1, 1, 1)	(-0,5, -0.5, -0.5) or (0.5, 0.5, 0.5)	
x_1, x_2 and x_3	1	$0.111\sigma^2$	$0.861\sigma^2$	$0.228\sigma^2$	-
	2	$0.100\sigma^2$	$0.850\sigma^2$	$0.217\sigma^2$	1
	3	$0.091\sigma^2$	$0.841\sigma^2$	$0.208\sigma^2$	2
	4	$0.083\sigma^2$	$0.833\sigma^2$	$0.201\sigma^2$	3
	5	$0.077\sigma^2$	$0.827\sigma^2$	$0.194\sigma^2$	4
	6	$0.071\sigma^2$	$0.821\sigma^2$	$0.189\sigma^2$	5
		(0, 0, 0, 0)	(-1, -1, -1, -1) or (1, 1, 1, 1)	(-0.5, -0.5, -0.5, -0.5) or (0.5, 0.5, 0.5, 0.5)	
x_1, x_2, x_3 and x_4	1	$0.059\sigma^2$	$0.684\sigma^2$	$0.145\sigma^2$	-
	2	$0.056\sigma^2$	$0.681\sigma^2$	$0.141\sigma^2$	1
	3	$0.053\sigma^2$	$0.678\sigma^2$	$0.139\sigma^2$	2
	4	$0.500\sigma^2$	$0.675\sigma^2$	$0.136\sigma^2$	3
	5	$0.048\sigma^2$	$0.673\sigma^2$	$0.134\sigma^2$	4
	6	$0.045\sigma^2$	$0.670\sigma^2$	$0.131\sigma^2$	5

The inclusion of pseudo-center points for the qualitative input variables is recommended in such a way that the pseudo-center points are added to the low- and high-level treatment combinations of the qualitative input variables. In other words, we can assign pseudo-center points to the centers of the left and right surface of the factorial design space. For example, consider a 2^2 full factorial design with one qualitative input variable and three center points. In this case, six pseudo-center points are added, three at each of the 2 combinations of the quantitative input variables.

Table 4.3 examines the prediction variance at different design points and the degrees of freedom for pure error for quantitative and qualitative input variables in a factorial design with pseudo-center points (FDPCP) where $\mathbf{x}^{(m)\prime} = [1\ z_1\ x_1\ z_1x_1\ x_1^2]$. This table shows that the stability of the prediction variance, detection of curvature, and the degrees of freedom for pure error increase, as the number of pseudo-center points increases.

Table 4.3: Pseudo-Center Points in Factorial Designs

n_{pc}	Var$[\hat{y}(\mathbf{x})]$ at design points		*df* for pure error
	(0, 0) or (1,0)	(0, -1), (0, 1), (-1, 1) or (1, 1)	
2	$0.667\sigma^2$	$0.917\sigma^2$	-
4	$0.375\sigma^2$	$0.875\sigma^2$	2
6	$0.267\sigma^2$	$0.850\sigma^2$	4
8	$0.208\sigma^2$	$0.833\sigma^2$	6
10	$0.171\sigma^2$	$0.821\sigma^2$	8
12	$0.146\sigma^2$	$0.813\sigma^2$	10

The Design Rotatability Issue

A rotatable design should have the same variance of a predicted response, $Var[\hat{y}(\mathbf{x})]$, when the design is rotated around its center point. The rationale of the design rotatability indicates that the prediction variance has the same value at any two points, which are equidistant from the design center. In an FDPCP, the inclusion of pseudo-center points changes the prediction variance with any rotation in the Cartesian coordinate space because the distances from the pseudo-center points, ρ_{i0} and ρ_{i1}, are $\rho_{i0} = \sqrt{(x_i - 0)^2}$ and

$\rho_{i1} = \sqrt{(x_i - 1)^2}$ for $i = 1, 2, \ldots, l$ which does not result in $\rho_{10} = \ldots = \rho_{l0} = \rho_{11} = \ldots = \rho_{l1}$. Thus, the point **x** does not maintain the equidistance from the pseudo-center points of an FDPCP. This observation is proved through the following proposed lemma:

Lemma: An FDPCP with coded $x_i = \pm 1$ and $z_j = 0$ and 1 for i = 1, 2, …, l and j = 1, 2, …, m is not a rotatable design.

Proof: As a counter argument, assume that an FDPCP is a rotatable design. Suppose there are two input variables, z_1 and x_1, in a 2^2 design with six pseudo-center points. A model matrix is given below.

$$\mathbf{X} = \begin{array}{c} \begin{array}{ccccc} 1 & z_1 & x_1 & x_1x_1 & z_1x_1 \end{array} \\ \begin{pmatrix} 1 & 0 & -1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix} \end{array} \tag{4.4}$$

Then, we have the information matrix as follows:

$$\mathbf{X'X} = \begin{pmatrix} 10 & 5 & 0 & 4 & 0 \\ 5 & 5 & 0 & 2 & 0 \\ 0 & 0 & 4 & 0 & 2 \\ 4 & 2 & 0 & 4 & 0 \\ 0 & 0 & 2 & 0 & 2 \end{pmatrix} \tag{4.5}$$

The design moment matrix (**M**) is then found as follows:

$$\mathbf{M} = \frac{\mathbf{X'X}}{N} = \frac{\mathbf{X'X}}{10} = \begin{pmatrix} 1 & 0.5 & 0 & 0.4 & 0 \\ 0.5 & 0.5 & 0 & 0.2 & 0 \\ 0 & 0 & 0.4 & 0 & 0.2 \\ 0.4 & 0.2 & 0 & 0.4 & 0 \\ 0 & 0 & 0.2 & 0 & 0.2 \end{pmatrix} \tag{4.6}$$

where $N = n_f + n_{pc}$. This design is not rotatable because the design moment matrix in Equation (4.6) does not have the following form (see Box and Draper, 1963; Khuri, 1988):

$$\mathbf{M} = \frac{\mathbf{X'X}}{N} = \frac{\mathbf{X'X}}{10} = \begin{pmatrix} 1 & 0 & 0 & \lambda_2 & 0 \\ 0 & \lambda_2 I & 0 & 0 & 0 \\ 0 & 0 & \lambda_2 & 0 & 0 \\ \lambda_2 & 0 & 0 & 3\lambda_4 & 0 \\ 0 & 0 & 0 & 0 & \lambda_4 I \end{pmatrix} \tag{4.7}$$

where λ_2 and λ_4 represent the quantities determined by the scaling of the input variables. Thus, an FDPCP is not a rotatable design. Further, we also observe that rotatability or near-rotatability is not a significant priority due to cuboidal design regions (see Myers et al., 2009). It is also clear that we do not have the advantage of the rotatable design for the variance stability. However, pseudo-center point runs may be sufficient to produce a reasonable stability of the scaled prediction variance ($SPV(\mathbf{x})$) where $SPV(\mathbf{x}) = NVar[\hat{y}(\mathbf{x})]/\sigma^2 = \mathbf{x}^{(m)'}\left(\frac{\mathbf{X'X}}{N}\right)^{-1}\mathbf{x}^{(m)} = N\mathbf{x}^{(m)'}\left(\mathbf{X'X}\right)^{-1}\mathbf{x}^{(m)}$.

The Experimental Format

The experimental format is shown in Table 4.4, where SDP stands for standard design points. Design matrix (DM) examples for two, three and four input variables are illustrated in Table 4.5 where the numbers in the parentheses represent the numbers of quantitative and qualitative input variables, respectively.

Table 4.4: Experimental Format

SDP	Input variables (**x**)	Observations (Replications)	$\bar{y}$	s	s^2
1	**D** (design matrix) with factorial points + pseudo-center points	$y_{11} \cdots y_{1u}$	$\bar{y}_1$	s_1	s_1^2
2		$y_{21} \cdots y_{2u}$	$\bar{y}_2$	s_2	s_2^2
3		$y_{31} \cdots y_{3u}$	$\bar{y}_3$	s_3	s_3^2
.		$\cdots$	.	.	.
.		$\cdots$	.	.	.
.		$\cdots$	.	.	.
n		$y_{n1} \cdots y_{nu}$	$\bar{y}_u$	s_u	s_u^2

Table 4.5: (a) DM for Two Input Variables (1, 1); (b) DM for Three Input Variables (1, 2); (c) DM for Four Input Variables (1, 3)

(a)

	z_1	x_1
n_f	0	-1
	0	1
	1	-1
	1	1
n_{pc}	0	0
	1	0
	0	0
	1	0
	0	0
	1	0

(b)

	z_1	x_1	x_2
n_f	0	-1	-1
	0	-1	1
	0	1	-1
	0	1	1
	1	-1	-1
	1	-1	1
	1	1	-1
	1	1	1
n_{pc}	0	0	0
	1	0	0

(c)

	z_1	x_1	x_2	x_3
n_f	0	-1	-1	-1
	0	-1	-1	1
	0	-1	1	-1
	0	-1	1	1
	0	1	-1	-1
	0	1	-1	1
	0	1	1	-1
	0	1	1	1
	1	-1	-1	-1
	1	-1	-1	1

	0	0	0
	1	0	0
	0	0	0
	1	0	0

	1	-1	1	-1
	1	-1	1	1
	1	1	-1	-1
	1	1	-1	1
	1	1	1	-1
	1	1	1	1
	0	0	0	0
	1	0	0	0
	0	0	0	0
n_{pc}	1	0	0	0
	0	0	0	0
	1	0	0	0

Linking the Experimental Design Space of the FDPCP to the Solution Space for Optimization

The solution space of the FDPCP problem, defined as a set of all feasible points satisfying inequality constraints, including boundary, continuous, integer and binary constraints, is a bounded convex set (BCS) due to a bounded square or *n*-cube design space involving both qualitative and quantitative input variables with pseudo-center points. The design and solution spaces associated with the FDPCP are summarized in Table 4.6.

Table 4.6: Design and Solution Spaces for an FDPCP

Number of input variables (*n*)	FDPCP	
	Design space	Solution space
2	Square region	BCS
3	Cube region	BCS
4 or more	*n*-cube region	BCS

The feasible solution spaces of two- and three-dimensional FDPCPs are given in Figure 4.1, where $z_1 \in \{0,\ 1\}$ and $x_1,\ x_2 \in \mathbb{R}$.

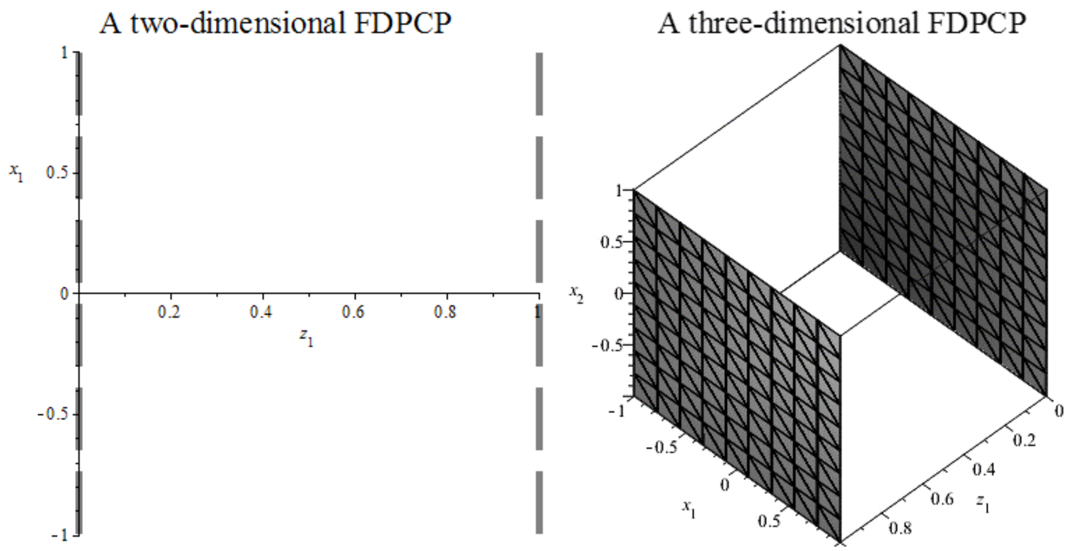


Figure 4.1: Two- and Three-Dimensional FDPCPs

Model Selection and Formulation Phase

When both quantitative and qualitative input variables are used in response surface designs, a traditional response surface design, such as the central composite design, may not be applicable to fit a second-order model. This is because the central composite design requires five coded levels which the binary qualitative input variables cannot have. The true response surface function is denoted as follows:

$$y = f(\mathbf{x}) + \varepsilon \tag{4.8}$$

where f is an unknown function of $\mathbf{x}$, $\mathbf{x} = [x_1,\ ...,\ x_l,\ z_1,\ ...,\ z_m]'$ and ε is an observed error. Our goal is to approximate the functional relationship between y and $\mathbf{x}$. A Taylor series expansion of $f(\mathbf{x})$ about $\mathbf{x}_0 = [x_{01},\ ...,\ x_{0l},\ z_{01},\ ...,\ z_{0m}]'$ is

$$f(\mathbf{x}) \cong \alpha_0 + \alpha_{x_1}(x_1 - x_{01}) + \ldots + \alpha_{x_l}(x_l - x_{0l}) + \frac{1}{2}\alpha_{x_1x_1}(x_1 - x_{01})^2$$
$$+ \ldots + \frac{1}{2}\alpha_{x_lx_l}(x_l - x_{0l})^2 + \alpha_{x_1x_2}(x_1 - x_{01})(x_2 - x_{02}) \tag{4.9}$$
$$+ \ldots + \alpha_{x_{l-1}x_l}(x_{l-1} - x_{0l-1})(x_l - x_{0l}) + \upsilon_{z_1}(z_1 - z_{01}) + \ldots + \upsilon_{z_m}(z_m - z_{0m})$$
$$+ \pi_{x_1z_1}(x_1 - x_{01})(z_1 - z_{01}) + \ldots + \pi_{x_lz_m}(x_l - x_{0l})(z_m - z_{0m})$$

where $\alpha_0 = \mathbf{x}_0$, $\alpha_{x_i} = \frac{\partial f(\mathbf{x})}{\partial x_i}\Big|_{\mathbf{x}_o}$, $\alpha_{x_ix_i} = \frac{\partial f(\mathbf{x})}{\partial x_i^2}\Big|_{\mathbf{x}_o}$, $\alpha_{x_{i-1}x_i} = \frac{\partial f(\mathbf{x})}{\partial x_{i-1}\partial x_i}\Big|_{\mathbf{x}_o}$, $\alpha_{z_j} = \frac{\partial f(\mathbf{x})}{\partial z_j}\Big|_{\mathbf{x}_o}$,

$\alpha_{x_iz_j} = \frac{\partial f(\mathbf{x})}{\partial x_i \partial z_j}\Big|_{\mathbf{x}_0}$, i=1, 2, …, l and j=1, 2, …, m. The above expression can be written as

$$y = \beta_0 + \sum_{i=1}^{l}\beta_i x_i + \sum_{i=1}^{l}\beta_{ii}x_i^2 + \sum_{i<j=2}\sum_{i=1}^{l}\beta_{ij}x_ix_j + \sum_{j=1}^{m}\phi_j z_j + \sum_{i=1}^{l}\sum_{j=1}^{m}\gamma_{ij}x_iz_j + \varepsilon \tag{4.10}$$

where β_i, ϕ_j and γ_i represent regression coefficients, and ε is an observed error. Then, the second-order fitted function of the process mean is expressed as:

$$\hat{\mu}(\mathbf{x}) = \mathbf{X}\hat{a} \text{ where } \hat{a} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}},$$
$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{i1} & x_{11}^2 & \cdots & x_{i1}^2 & x_{11}x_{21} & \cdots & x_{i-11}x_{i1} & z_{11} & \ldots & z_{i1} & x_{11}z_{11} & \ldots & x_{i1}z_{i1} \\ 1 & x_{12} & \cdots & x_{i2} & x_{12}^2 & \cdots & x_{i2}^2 & x_{12}x_{22} & \cdots & x_{i-12}x_{i2} & z_{12} & \ldots & z_{i2} & x_{12}z_{12} & \ldots & x_{i2}z_{i2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1l} & \cdots & x_{il} & x_{1l}^2 & \cdots & x_{il}^2 & x_{1l}x_{2l} & \cdots & x_{i-1l}x_{il} & z_{1m} & \ldots & z_{im} & x_{1l}z_{1m} & \ldots & x_{il}z_{im} \end{pmatrix} \tag{4.11}$$
and $\bar{\mathbf{y}} = [\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_n]'$

Similarly, the fitted function of process standard deviation and variance are:

$$\hat{\sigma}(\mathbf{x}) = \mathbf{X}\hat{b} \text{ where } \hat{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s},\ \mathbf{s} = [s_1, s_2, \ldots, s_n]' \tag{4.12}$$

$$\widehat{\sigma^2}(\mathbf{x}) = \mathbf{X}\hat{c} \text{ where } \hat{c} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2,\ \mathbf{s}^2 = [s_1^2, s_1^2, \ldots, s_n^2]' \tag{4.13}$$

In addition, the inclusion of all quadratic effects in the second-order model may not be possible for all quantitative input variables in the FDPCP because the quadratic effect vectors may not be linearly independent due to $col_1\mathbf{x_1^2}+col_2\mathbf{x_2^2}+...+col_l\mathbf{x_l^2}=0$ where $col_1,\ col_2,\ ...,\ col_l$ are real numbers and $col_i \neq 0$ (i = 1, 2, …, l). It means that **X** will not have full rank; therefore, $\mathbf{X}'\mathbf{X}$ is rank-deficient and singular. The rank deficiency and singularity indicate that there are no unique estimators of the regression coefficients. However, we desire to have unbiased estimators with minimum variance (see Montgomery, 2013). Therefore, it is proposed that some quadratic effects indicator columns from **X** be dropped until a finite set of vectors is linearly independent to avoid linear dependent vectors for this particular situation.

Proposed Model

Review of *VM* and *LT* models

The *VM* and *LT* models assume that input variables are real valued. First, *VM* proposed the dual response model that the process variation is minimized while adjusting the process mean to the target value. The model is shown below:

$$\begin{aligned}&\text{Minimize } \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s} \text{ (The fitted variability function)}\\&\text{subject to } \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}}=\tau \text{ (The mean constraint)}\\&\mathbf{x}\in[LB,\ UB] \text{ (Boundary constraints)}\end{aligned} \tag{4.14}$$

where *LB* and *UB* denote lower and upper bounds, respectively. However, this zero-bias assumption associated with the mean constraint can sometimes cause infeasible solutions, when integer and binary valued input variables are used. Further, the mean squared error (MSE) model, proposed by *LT*, may not achieve a desired upper bound of the process bias. Notice that we consider these models as a 0-1 MINLP problem in order to obtain integer-valued and binary-valued input variables.

The Proposed 0-1 MINLP Model

The objective of the proposed model is to minimize the estimated fitted variance function while allowing a process bias. The proposed model may result in a further reduction of the variance than traditional models proposed by *VM* and *LT*. Therefore, the objective function of the proposed model is written as follows:

$$\text{Minimize } [\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s^2}] + [\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\overline{\mathbf{y}} - \tau]^2 \tag{4.15}$$

Three constraints due to the boundary requirements associated with process mean and variability and the boundary requirements associated with the design space of the FDPCP are explained below.

1. *Constraints due to boundary requirements associated with process mean*: Taguchi's main idea is that the process mean is at the desired target value while the process variation is as small as possible (Taguchi, 1986). However, the mean may not be achieved at the target value in many real-life engineering situations. These lower and upper limits of a process mean are often specified by the customer, and incorporating the customer's voice is an important part of continuous quality improvement program. The two bounds are the values within which products should operate. Therefore, it can be more practical that these requirements need to be characterized by the lower and upper limits on the process mean. The constraints are then written as follows:

$$\left.\begin{array}{l}\hat{\mu}(\mathbf{x}) \leq UB_{\mu} \Rightarrow \mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\bar{\mathbf{y}} \leq UB_{\mu} \\ \hat{\mu}(\mathbf{x}) \geq LB_{\mu} \Rightarrow \mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\bar{\mathbf{y}} \geq LB_{\mu}\end{array}\right\} \Rightarrow LB_{\mu} \leq \mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\bar{\mathbf{y}} \leq UB_{\mu} \tag{4.16}$$

where LB_{μ} and UB_{μ} represent the lower and upper bounds for the process mean, respectively.

2. *Constraints due to boundary requirements associated with process variability*: A process variance should always be minimized, and this can be done by imposing the upper bound, often specified by the customer, on the process variance. In an optimization sense, the epsilon-constraint method is closely associated with the bounds of constraints imposed on process mean and variance. In fact, the epsilon-constraint method is one of the most popular optimization methods in the literature, and many authors have reported advantages of the method. As outlined in Steuer (1986) and Mavrotas (2009), the epsilon-constraint method, unlike other methods such as the weighting method, is capable of generating non-extreme efficient solutions and the user can control the number of the generated efficient solutions by adjusting the number of grid points in the range of an objective function. It is also noted that $[\hat{\sigma}(\mathbf{x})]^2 \neq \widehat{\sigma^2}(\mathbf{x})$ (see Goethals et al., 2009). This implies that the selection of variability measures affects optimal RPD solutions. Therefore, the variance estimator may produce a better point estimation than the standard deviation counterpart. Finally, the variance must be non-negative. As a result, the constraints are written as follows:

$$0 \le \widehat{\sigma^2}(\mathbf{x}) \le \Delta_{\sigma^2} \Rightarrow 0 \le \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2 \le \Delta_{\sigma^2} \tag{4.17}$$

3. *Boundary requirements associated with the design space of the FDPCP*: The FDPCP contains the coded design points at -1, 0, and 1. The associated design boundary constraints are shown as:

$$\begin{aligned} &-1 \le x_i \le 1 \text{ for } x_i \in \mathbb{R} \;\; i = 1,\ 2,\ ...,\ l-c \\ &-1 \le x_i \le 1 \text{ for } x_i \in \mathbb{Z} \;\; i = l-c+1,\ ...,\ l \\ &z_j \in \{0,\ 1\} \text{ for } j = 1,\ 2,\ ...,\ m \\ &\text{Number of design points: } n_f + n_{pc} \end{aligned} \tag{4.18}$$

The proposed 0-1 MINLP optimization model is summarized in Table 4.7.

Table 4.7: The Proposed Model

Given	Response (y)
	Fitted response models ($\hat{\mu}(\mathbf{x})$) and $\sigma^2(\mathbf{x})$)
	Desired target value (τ)
	Lower and upper bounds of the mean (LB_μ and UB_μ)
	Desired upper bound for the variance (Δ_{σ^2})
	Design region (An *n*-cuboidal design region due to an FDPCP where $n_f + n_{pc}$)
Goal	Minimize $[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2] + [\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\overline{\mathbf{y}} - \tau]^2$
Subject to	Constraints:
	(1) $LB_\mu \le \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\overline{\mathbf{y}} \le UB_\mu$
	(2) $0 \le \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2 \le \Delta_{\sigma^2}$
	$-1 \le x_i \le 1$ for $x_i \in \mathbb{R}$ $i = 1,\ 2,\ ...,\ l-c$
	(3) $-1 \le x_i \le 1$ for $x_i \in \mathbb{Z}$ $i = l-c+1,\ ...,\ l$
	$z_j \in \{0,\ 1\}$ for $j = 1,\ 2,\ ...,\ m$
Method	MINLP optimization methods
Find	Robust parameter design solutions (x_i^* and z_j^* where i = 1, …, l and j = 1, …, m)

Investigation of convexity and quality of solutions

(1) Convexity: A close look at the proposed model for the RPD optimization problem defined in Table 4.7 reveals that $[\mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\overline{\mathbf{y}}-\tau]^{2}$ is of a fourth-order function because $\mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\overline{\mathbf{y}}-\tau$ is a quadratic function which is a strictly convex function. Denoting $\mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\overline{\mathbf{y}}-\tau$ as u, it is noted that u^2 is also a convex function since u: $\mathbb{R}\rightarrow[0,\infty)$ is a convex function and u is twice-differentiable. The term u, also referred to as a product bias, represents the deviation of the expected value of a process mean from the customer-specified target value τ. It is noted that the objective function is a convex function and the constraints form a bounded feasible region, which now satisfies the convexity assumption.

(2) Quality of solutions: One of the most effective methods to determine the quality of the solutions is done by checking the optimality gap which is a measure for how close the solutions are to the optimal solution. The proposed model in Table 4.7 guarantees the objective value of the solution within the optimality gap of the optimal solution. The first step in checking the optimality gap is done by examining the local and global minima for the proposed model. It is noted that a feasible solution $\mathbf{X}^{*}$ and u^{*} for $[\mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\mathbf{s}^{2}]+u^{2}$ is the global minimum solution for the model if $[\mathbf{X}^{*}((\mathbf{X}^{*})^{'}\mathbf{X}^{*})^{-1}(\mathbf{X}^{*})^{'}\mathbf{s}^{2}]+(u^{*})^{2}\leq[\mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\mathbf{s}^{2}]+u^{2}$. It is also noted that the value of the allowable gap is zero for the global minimum solution, while a feasible solution $\mathbf{X}^{*}$ and u^{*} for $[\mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-1}\mathbf{X}^{'}\mathbf{s}^{2}]+u^{2}$ becomes the local minimum

solution if $[\mathbf{X}^*((\mathbf{X}^*)'\mathbf{X}^*)^{-1}(\mathbf{X}^*)'\mathbf{s}^2] + (u^*)^2 \le [\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2] + u^2$ and $\left\|\mathbf{X} - \mathbf{X}^*\right\| \le e$ for $e > 0$ where e is a quite small value. The solution does not violate the constraints defined in Table 4.7.

The Solution Procedures of the Proposed Model

In the literature, Borchers and Mitchell (1997) reported that both the branch-and-bound (BB) and outer approximation (OA) methods for a 0-1 MINLP resulted in optimal solutions with less computational times. In particular, the OA method is known to be quite effective in solving convex problems (see Duran and Grossmann, 1986; Fletcher and Leyffer, 1994). On the other hand, the BB method can be used for both convex and nonconvex problems (see Gupta and Ravindran, 1985; Borchers and Mitchell, 1997). Also, Bonami et al. (2008) concluded that the hybrid nonlinear based branch-and-cut (HNBC) algorithm was effective for a large number of design points. In this chapter, we perform the OA, BB, and HNBC algorithms for solving the proposed 0-1 MINLP models. Although no specific theoretical efficiency results are available for solving RPD problems in the literature, the three methods have been successful for solving practical problems. Computational results are then compared. The outline of the optimization phases is shown in Table 4.8.

In Figure 4.2, a better approximation of the objective function and constraints can be found from the outside. In addition, the linearization provides valid over estimators of the feasible solution space because the objective function and constraints are convex.

Figure 4.3 also shows the feasible solution spaces of the BB and hybrid based BC methods using the integrality relaxations.

Table 4.8: Optimization Phases for the Proposed Model

Phase I	Relaxation type
	The polyhedral relaxation for the OA method
	The integrality relaxation for the BB and hybrid based BC methods
Phase II	Deterministic method
	The OA algorithm for a convex MINLP
	The BB and HNBC algorithms for a convex or nonconvex MINLP
Phase III	Comparisons
	Compare the solutions
Phase IV	Model verification
	Compare the proposed model with the *VM* and *LT* models

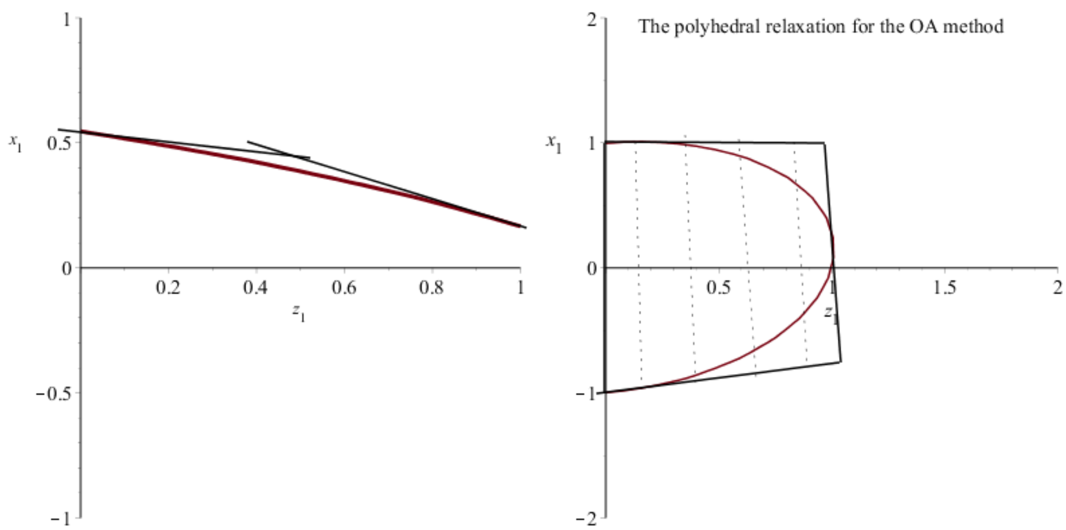


Figure 4.2: Geometric Interpretation of the OA Method

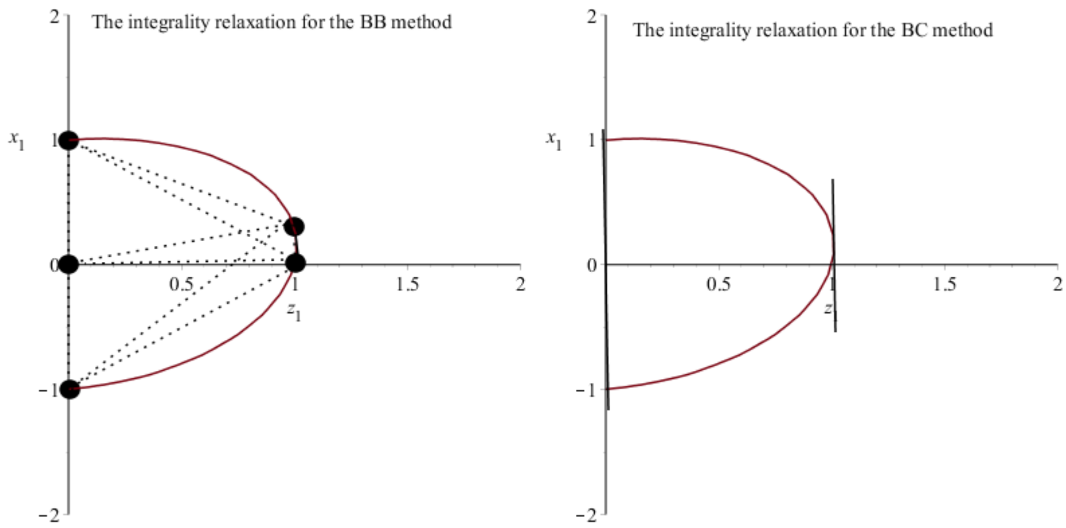


Figure 4.3: Geometric Interpretation of the BB and BC Methods

Note that the proposed FDPCP has a convex region (see Figure 4.1). With a convex objective function, convex constraint functions, and a convex feasible region, an optimization problem is convex. Hence, there will be only one optimal solution which is global optimal. Geometrically, a function, $f(\mathbf{x})$, is called convex if a line segment drawn any point $(\mathbf{x}_1, f(\mathbf{x}_1))$ to another point $(\mathbf{x}_2, f(\mathbf{x}_2))$ lies on or above the graph of $f(\mathbf{x})$. Algebraically, $f(\mathbf{x})$ is called convex if $f[\lambda\mathbf{x}_1 + (1-\lambda)\mathbf{x}_2] \le \lambda f(\mathbf{x}_1) + (1-\lambda) f(\mathbf{x}_2)$ where $\mathbf{x}_1$ and $\mathbf{x}_2$ are any two points on an interval with any λ where $0 \le \lambda \le 1$. If $f(\mathbf{x})$ has a second derivative on an interval, then the function is convex on that interval where $f''(\mathbf{x}) \ge 0$ for all $\mathbf{x}$ on an interval.

Some Insights

Two observations are made.

1. The set of feasible solution is a bounded polyhedral set due to the solution space. Therefore, the convexity becomes an important aspect to obtain a feasible solution for the proposed model for the following reasons. First, nonconvex functions may cause concerns and therefore the BB method should have an accurate lower bound for a global solution. Second, if a nonconvex function exists in any constraint, it may end up with an overestimation or underestimation of the function. For example, assuming *f(***x***)* is a nonconvex function for a response, and a quadratic function, which is an inequality form, may be underestimated over a design region. It is also denoted below:

$$L(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{l} \lambda_i (-1 - x_i)(1 - x_i) + \sum_{j=1}^{m} \pi_j (0 - z_j)(1 - z_j) \tag{4.19}$$

where $\mathbf{x} = [x_1,\ ...,\ x_l,\ z_1,\ ...,\ z_m]'$

2. The functions $f(\mathbf{x})$ and $g_k(\mathbf{x})$ are twice continuously differentiable convex functions. Since the proposed model satisfies a constraint qualification for all points in the convex hull of the feasible set *S* of the proposed model, the convex hull of *S*, *conv(S),* is then expressed as follows:

$$\begin{aligned} conv(S) = \{ & \sum_{i=1}^{l} \lambda_i x_i + \sum_{j=1}^{m} \pi_j z_j \mid \sum_{i=1}^{l} \lambda_i + \sum_{j=1}^{m} \pi_j = 1,\ \forall 0 \le \lambda_i \le 1, \\ & \forall 0 \le \pi_j \le 1,\ \forall x_i \in S \text{ and } \forall z_j \in S \} \\ \text{where } X_1 = & \{x_i \in \mathbb{R} \mid -1 \le x_i \le 1,\ i = 1,\ 2,\ ...,\ l - c\} \\ X_2 = & \{x_i \in \mathbb{Z} \mid -1 \le x_i \le 1,\ i = l - c + 1,\ ...,\ l\} \\ X_3 = & \{z_j \in \{0,\ 1\} \mid j = 1,\ 2,\ ...,\ m\} \end{aligned} \tag{4.20}$$

and X_i represents a set of feasible solution and *i* = 1, 2, 3.

The Outer Approximation (OA) Method for the Proposed Model

The solution of the continuous relaxation of the proposed model is not an extreme point of the feasible set. As a one-unit distance extends beyond the design space, the prediction variance increases, thereby decreasing the precision of the solution. As a result, the feasible set lies in the strict interior of the solution space associated with the proposed model. We can reformulate in Table 4.7 by defining the objective function η and the constraint $[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2]+u^2 \leq \eta$ because the optimal solution of the equivalent MINLP defined in Equation (4.21) always lies on the boundary of the convex hull of the feasible set. The equivalent proposed MINLP is then as follows:

$$
\begin{aligned}
&\underset{\eta,\, x}{\text{Minimize}} \;\; \eta \\
&\text{subject to } [\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2]+u^2 \leq \eta \\
&\qquad\qquad \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\overline{\mathbf{y}}-\tau \leq u \\
&\qquad\qquad \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\overline{\mathbf{y}}-\tau \geq u \\
&\qquad\qquad LB_{\mu}-\tau \leq u \leq UB_{\mu}-\tau \\
&\qquad\qquad 0 \leq \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s}^2 \leq \Delta_{\sigma^2} \\
&\qquad\qquad -1 \leq x_i \leq 1 \text{ for } x_i \in \mathbb{R} \;\; i=1,\ 2,\ \ldots,\ l-c \\
&\qquad\qquad -1 \leq x_i \leq 1 \text{ for } x_i \in \mathbb{Z} \;\; i=l-c+1,\ \ldots,\ l \\
&\qquad\qquad z_j \in \{0,\ 1\} \text{ for } j=1,\ 2,\ \ldots,\ m
\end{aligned}
\tag{4.21}
$$

The constraint qualification test is necessary to ensure the existence of multipliers and the convergence of the NLP solvers. As a result, Slater's constraint qualification is valid due to the existence of an interior feasible point for the proposed model (see Griva et al., 2009). Note that the objective function and constraints of the proposed model can be relaxed with a set of hyperplanes acquiring from the first-order Taylor Series approximation as follows:

$$
\begin{aligned}
&\eta \geq f^{v}(\mathbf{x}) + \nabla f^{v}(\mathbf{x})' \Delta\mathbf{x} \\
&0 \geq g^{v}(\mathbf{x}) + \nabla g^{v}(\mathbf{x})' \Delta\mathbf{x} \\
&\text{where } \mathbf{x} = [x_1,\ ...,\ x_l,\ z_1,\ ...,\ z_m,\ u]' \text{ and } \Delta\mathbf{x} = \mathbf{x}^{v} - \mathbf{x}^{v-1}, \\
&\nabla f(\mathbf{x})' = \left[\frac{\partial f(\mathbf{x})}{\mathbf{x}}\right] = \left[\mathbf{c} + \mathbf{C}\mathbf{X}\ \ 2u\right]_{1*(m+l+1)}, \\
&\nabla g(\mathbf{x})' = \left[\frac{\partial g_1(\mathbf{x})}{\mathbf{x}}\ \cdots\ \frac{\partial g_6(\mathbf{x})}{\mathbf{x}}\right] \\
&\qquad = \begin{bmatrix} \mathbf{a}_{11} + \mathbf{A}_{12}\mathbf{X} & -\mathbf{a}_{12} - \mathbf{A}_{12}\mathbf{X} & 0 & 0 & -\mathbf{c}_{15} - \mathbf{C}_{15}\mathbf{X} & \mathbf{c}_{16} + \mathbf{C}_{16}\mathbf{X} \\ \mathbf{a}_{21} + \mathbf{A}_{21}\mathbf{X} & -\mathbf{a}_{22} - \mathbf{A}_{22}\mathbf{X} & 0 & 0 & -\mathbf{c}_{25} - \mathbf{C}_{25}\mathbf{X} & \mathbf{c}_{26} + \mathbf{C}_{26}\mathbf{X} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & 1 & -1 & 1 & 0 & 0 \end{bmatrix}_{(m+l+1)*6}
\end{aligned}
\tag{4.22}
$$

where **a** and **c** represent the vectors of the estimated coefficients for the process mean and variance, respectively, and **A** and **C** denote the matrices of the estimated coefficients associated with the process mean and variance, respectively. This type of relaxation is called a polyhedral relaxation and it will be used in the outer approximation algorithm in a later section of this chapter. We initially solve an NLP, given initial point $\mathbf{x}^{(v-1)} = \mathbf{x}^{(0)}$ and a subset $X^k \subset X$ with $X^k = \{0\}$, by including an upper bound on η as follows:

$$\eta \leq UB^k \text{ where } UB^k = \min\{f(\mathbf{x}^{(v)}):\ \text{NLP}(\mathbf{x}_I^{(v)}) \text{ is feasible}\} \tag{4.23}$$

where $\mathbf{x}_I^{(v)}$ is the fixed integer variables for the NLP sub-problem and $\mathbf{x}_I = \mathbf{x}_I^{(v)}$. We can then replace the constraint in Equation (4.23) with $\eta \leq UB^k - e$ for computational efficiency where $e > 0$ is a small tolerance. The master problem solved at iteration *k* is then shown as

$$
\begin{aligned}
&\underset{\eta,\, x}{\text{Minimize}}\ \ \eta \\
&\text{subject to } \eta \le UB^k \text{ - } e \\
&\qquad\qquad \eta \ge f^v(\mathbf{x}) + \nabla f^v(\mathbf{x})' \Delta\mathbf{x} \\
&\qquad\qquad 0 \ge g^v(\mathbf{x}) + \nabla g^v(\mathbf{x})' \Delta\mathbf{x} \\
&\qquad\qquad -1 \le x_i \le 1 \text{ for } x_i \in \mathbb{R}\ i = 1,\ 2,\ \ldots,\ l-c \\
&\qquad\qquad -1 \le x_i \le 1 \text{ for } x_i \in \mathbb{Z}\ i = l-c+1,\ \ldots,\ l \\
&\qquad\qquad z_j \in \{0,\ 1\} \text{ for } j = 1,\ 2,\ \ldots,\ m
\end{aligned}
\tag{4.24}
$$

The detailed description of the outer approximation (OA) algorithm is given in Table 4.9.

Table 4.9: The Outer Approximation for 0-1 MINLP Problems

Given an initial point, choose a tolerance, set $U^{-1} = \infty$, set k=0 and initialize $X^{-1} = \{\}$
do
Solve NLP $(\mathbf{x}_I^{(v)})$ and let the solution be $\mathbf{x}^{(v)}$
If NLP $(\mathbf{x}_I^{(v)})$ is feasible and $f^v(\mathbf{x}) < U^{k-1}$ **then**
Update current point: $\mathbf{x}^* = \mathbf{x}^v$ and $U^k = f^v(\mathbf{x})$
Else
Set $U^k = U^{k-1}$
Linearize objective and constraint $f(\mathbf{x})$ and $g(\mathbf{x})$ and set $X^k = X^{k-1} \cup \{v\}$.
Solve the master problem and let $\mathbf{x}^{k+1}$ and set $k = k+1$
until the model in Equation (4.24) is not feasible at iteration k

The Branch-and-Bound Method for the Proposed Model

A branch-and-bound (BB) method implements a top-down recursive search by updating solutions through a decision tree. The BB method starts by solving the continuous NLP relaxation. If all quantitative input variables take integer values, the search is stopped. Otherwise, a tree search is performed in the space of the integer variables (see Gupta and Ravindran, 1985). The BB method is particularly effective in solving the proposed RPD model because of the low dimensionality of the qualitative variables, as a typical number of qualitative and quantitative input variables is three or four in RPD programs. The algorithm of the BB method for the proposed model is shown in Table 4.10.

Table 4.10: Branch-and-Bound Algorithm for the Proposed 0-1 MINLP Problems

Given choose a tolerance, set $U = \infty$, set k=0 and initialize the heap $H = \{\}$.
Add NLP to the heap where $H = H \cup \{\text{NLP}(-\infty, \infty)$.
do
Remove an NLP problem from the heap: $H = H \setminus \{\text{NLP}(LB,\ UB)\}$
Solve NLP $(LB,\ UB)$ and let the solution be $\mathbf{x}^{(LB,\ UB)}$
If $\mathbf{x}_I^{(LB,\ UB)}$ is integral then
Update solution: $U = f(\mathbf{x}^{(LB,\ UB)})$ and $\mathbf{x}^* = \mathbf{x}^{(LB,\ UB)}$
else if $f(\mathbf{x}^{(LB,\ UB)}) > U$ **then**
Node can be pruned
else if NLP(LB, UB) is not feasible **then**
Node can be pruned
else branch on a fractional input variable ($\mathbf{x}_i^{(LB,\ UB)}$ for $i \in I$) and set
$UB_i^- = \left\lfloor \mathbf{x}_i^{(LB,\ UB)} \right\rfloor$, $LB^- = LB$ and $LB_i^+ = \left\lceil \mathbf{x}_i^{(LB,\ UB)} \right\rceil$, $UB^+ = UB$. The heap is updated and $H = H \cup \{\text{NLP}(LB^-,\ UB^-),\ \text{NLP}(LB^+,\ UB^+)\}$.
until $H \neq \{\}$

The Hybrid Nonlinear Based Branch-and-Cut Method for the Proposed Model

A hybrid nonlinear based branch-and-cut (HNBC) algorithm, like the OA algorithm, uses linear relaxation concepts in solving MINLP problems. However, instead of successive approximations, the HNBC algorithm performs a branch-and-cut procedure, where the linear outer approximation is updated at selected nodes of the search tree (see Bonami et al., 2008). This particular method may be useful, especially when there is a large number of design points. The description of the algorithm for the proposed model is defined in Table 4.11.

Table 4.11: Hybrid Nonlinear Based Branch-and-Cut Algorithm for 0-1 MINLP Problems

Given choose a tolerance, set $U = \infty$, set *k*=0 and initialize the heap $H = \{\}$.
Add NLP to the heap where $H = H \cup \{\text{NLP}(-\infty, \infty)$.
do
Remove an NLP problem from the heap: $H = H \setminus \{\text{NLP}(LB,\ UB)\}$
repeat
Solve NLP $(LB,\ UB)$ and let the solution be $\mathbf{x}^{(LB,\ UB)}$
If $\mathbf{x}_I^{(LB,\ UB)}$ is integral then
Update solution: $U = f(\mathbf{x}^{(LB,\ UB)})$ and $\mathbf{x}^* = \mathbf{x}^{(LB,\ UB)}$
else if $f(\mathbf{x}^{(LB,\ UB)}) > U$ **then**
Node can be pruned
else if NLP(*LB*, *UB*) is not feasible **then**
Node can be pruned
else if more cuts would be generated **then**
Generate cuts ($\mathbf{x}^{(LB,\ UB)}$, *j*) where generate a valid inequality that cuts off $\mathbf{x}_j^{(LB,\ UB)} \notin \{0,\ 1\}$. Solve a problem in $\mathbf{x}^{(LB,\ UB)}$ in order to obtain an inequality that cuts off $\mathbf{x}_j^{(LB,\ UB)} \notin \{0,\ 1\}$ from the feasible set of NLP (*LB*, *UB*). And then, this inequality is added to NLP (*LB*, *UB*).
until new cuts are not generated
if NLP (*LB*, *UB*) is not pruned **then** branch on a fractional input variable ($\mathbf{x}_i^{(LB,\ UB)}$ for $i \in I$) and set $UB_i^- = \left\lfloor \mathbf{x}_i^{(LB,\ UB)} \right\rfloor$, $LB^- = LB$ and $LB_i^+ = \left\lceil \mathbf{x}_i^{(LB,\ UB)} \right\rceil$, $UB^+ = UB$. The heap is updated and
$H = H \cup \{\text{NLP}(LB^-,\ UB^-),\ \text{NLP}(LB^+,\ UB^+)\}$.
until $H \neq \{\}$

Numerical Example

Consider the problem of optimizing the amount of extraction which is a function of solvent (z_1) in addition to temperature (x_1), pressure (x_2) and time (x_3), where z_1 is a 0-1 input variable and others are continuous variables. This optimization model becomes a 0-1 MINLP model. The desired target value for the amount of extraction is 20 grams, where the allowable lower and upper bounds are 19.5 and 20.5 grams, respectively. Additionally, the maximum process variation we want to allow is 0.02. The goal is to determine the optimal operating conditions while the process bias and variance are minimized at the same time. Note that the computer codes are shown in Appendix B for this numerical example.

To estimate a quadratic model of the response, a 2^4 factorial design with six pseudo-center design points is decided for this experiment. In addition, the experiment is replicated four times and data are collected. The experimental design and the data are shown in Table 4.12.

Table 4.12: Experimental Design and Observations

SDP	Coded units				Observations				$\bar{y}_u$	s_u	s_u^2
	z_1	x_1	x_2	x_3	y_{u1}	y_{u2}	y_{u3}	y_{u4}			
1	0	-1	-1	-1	20.934	20.009	19.967	19.527	20.109	0.592	0.350
2	0	-1	-1	1	20.008	20.515	20.095	19.827	20.111	0.292	0.085
3	0	-1	1	-1	20.503	19.865	20.590	20.899	20.464	0.434	0.188
4	0	-1	1	1	20.311	20.107	19.838	20.419	20.169	0.256	0.065
5	0	1	-1	-1	20.237	20.053	20.247	18.766	19.826	0.712	0.507
6	0	1	-1	1	19.491	19.408	19.870	20.514	19.821	0.504	0.254
7	0	1	1	-1	19.740	20.165	19.967	20.545	20.104	0.341	0.116
8	0	1	1	1	20.242	19.528	19.740	20.049	19.890	0.318	0.101
9	1	-1	-1	-1	20.140	19.757	19.821	20.241	19.990	0.237	0.056
10	1	-1	-1	1	19.615	19.767	20.425	20.157	19.991	0.368	0.136
11	1	-1	1	-1	20.337	20.084	19.351	19.772	19.886	0.425	0.181
12	1	-1	1	1	20.062	20.039	20.290	19.661	20.013	0.260	0.068
13	1	1	-1	-1	19.849	20.842	19.914	19.536	20.035	0.563	0.316
14	1	1	-1	1	19.796	20.063	20.761	19.621	20.060	0.501	0.251
15	1	1	1	-1	19.944	19.711	19.844	20.212	19.928	0.212	0.045
16	1	1	1	1	19.188	20.428	19.723	20.087	19.856	0.531	0.282
17	0	0	0	0	19.875	19.934	20.154	19.701	19.916	0.187	0.035
18	1	0	0	0	20.272	19.774	19.928	20.057	20.008	0.210	0.044
19	0	0	0	0	19.687	19.822	19.984	20.009	19.876	0.151	0.023
20	1	0	0	0	19.912	19.688	19.730	19.712	19.760	0.102	0.010
21	0	0	0	0	19.725	19.460	19.714	20.551	19.863	0.475	0.226
22	1	0	0	0	19.883	19.519	19.525	20.884	19.953	0.644	0.415

We run a full second-order model with x_1, x_2, x_3, and z_1. Notice that the full second-order model with all quadratic effects has the singular $\mathbf{X}'\mathbf{X}$ matrix. The response surface polynomial model is then expressed as follows:

$$\begin{aligned} y = {} & \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 \\ & + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \phi_1 z_1 + \gamma_{11} x_1 z_1 + \gamma_{22} x_2 z_1 + \gamma_{33} x_3 z_1 + \varepsilon \end{aligned} \tag{4.25}$$

where $\beta_{22} = 0$ and $\beta_{33} = 0$ because the quadratic effect vectors are linearly dependent. In addition, β_{11} is a biased estimator. Therefore, we drop x_2^2 and x_3^2 indicator columns from the $\mathbf{X}$ model matrix. In addition, the updated $\mathbf{X}'\mathbf{X}$ matrix is not singular and therefore all estimators are unbiased. Then, the response surface polynomial model is shown below:

$$\begin{aligned} y = {} & \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \phi_1 z_1 \\ & + \gamma_{11} x_1 z_1 + \gamma_{22} x_2 z_1 + \gamma_{33} x_3 z_1 + \varepsilon \end{aligned} \tag{4.26}$$

Using JMP software (2013), the fitted response surface functions for the process mean, process standard deviation, and process variance are obtained as follows:

$$\begin{aligned} \hat{\mu}(\mathbf{x}) = {} & 19.986 - 0.076 x_1 + 0.023 x_2 - 0.027 x_3 + 0.12 x_1^2 - 0.018 x_1 x_2 \\ & - 0.006 x_1 x_3 - 0.03 x_2 x_3 + 0.03 z_1 - 0.076 z_1 x_1 + 0.072 z_1 x_2 - 0.037 z_1 x_3 \end{aligned} \tag{4.27}$$

$$\begin{aligned} \hat{\sigma}(\mathbf{x}) = {} & 0.295 + 0.051 x_1 - 0.062 x_2 - 0.03 x_3 + 0.114 x_1^2 - 0.048 x_1 x_2 \\ & + 0.037 x_1 x_3 + 0.024 x_2 x_3 + 0.01 z_1 - 0.014 z_1 x_1 - 0.032 z_1 x_2 - 0.058 z_1 x_3 \end{aligned} \tag{4.28}$$

$$\begin{aligned} \widehat{\sigma^2}(\mathbf{x}) = {} & 0.126 + 0.046 x_1 - 0.057 x_2 - 0.032 x_3 + 0.062 x_1^2 - 0.041 x_1 x_2 \\ & + 0.02 x_1 x_3 + 0.031 x_2 x_3 + 0.006 z_1 - 0.01 z_1 x_1 - 0.034 z_1 x_2 - 0.05 z_1 x_3 \end{aligned} \tag{4.29}$$

These fitted functions are now incorporated into the BB and HNBC algorithms, as shown in Table 4.13.

Table 4.13: Proposed Model Using the BB and HNBC Methods

Given	$\tau = 20,\ \Delta_{\sigma^2} = 0.02,\ LB_\mu = 19.5,\ UB_\mu = 20.5,\ n_f = 16$ and $n_{pc} = 6$
Objective	Minimize $0.126 + 0.046x_1 - 0.057x_2 - 0.032x_3 + 0.062x_1^2 - 0.041x_1x_2$ $+0.02x_1x_3 + 0.031x_2x_3 + 0.006z_1 - 0.01z_1x_1 - 0.034z_1x_2 - 0.05z_1x_3$ $+(19.986 - 0.076x_1 + 0.023x_2 - 0.027x_3 + 0.12x_1^2 - 0.018x_1x_2$ $-0.006x_1x_3 - 0.03x_2x_3 + 0.03z_1 - 0.076z_1x_1 + 0.072z_1x_2 - 0.037z_1x_3 - 20)^2$
Subject to	C(1) $19.986 - 0.076x_1 + 0.023x_2 - 0.027x_3 + 0.12x_1^2 - 0.018x_1x_2$ $-0.006x_1x_3 - 0.03x_2x_3 + 0.03z_1 - 0.076z_1x_1 + 0.072z_1x_2 - 0.037z_1x_3 \geq 19.5$ C(2) $19.986 - 0.076x_1 + 0.023x_2 - 0.027x_3 + 0.12x_1^2 - 0.018x_1x_2$ $-0.006x_1x_3 - 0.03x_2x_3 + 0.03z_1 - 0.076z_1x_1 + 0.072z_1x_2 - 0.037z_1x_3 \leq 20.5$ C(3) $0.126 + 0.046x_1 - 0.057x_2 - 0.032x_3 + 0.062x_1^2 - 0.041x_1x_2$ $+0.02x_1x_3 + 0.031x_2x_3 + 0.006z_1 - 0.01z_1x_1 - 0.034z_1x_2 - 0.05z_1x_3 \geq 0$ C(4) $0.126 + 0.046x_1 - 0.057x_2 - 0.032x_3 + 0.062x_1^2 - 0.041x_1x_2$ $+0.02x_1x_3 + 0.031x_2x_3 + 0.006z_1 - 0.01z_1x_1 - 0.034z_1x_2 - 0.05z_1x_3 \leq 0.02$ Boundary constraints: $-1 \leq x_i \leq 1$ and $x_i \in \mathbb{R}$ $(i = 1, 2, 3)$; $z_1 \in \{0,\ 1\}$
Method	The branch-and-bound and hybrid nonlinear based branch-and-cut methods
Find	Factor settings $\mathbf{x}^* = (z_1^*,\ x_1^*,\ x_2^*,\ x_3^*)'$ and an objective function value of the model

In addition, we propose another optimization model for the outer approximation using the extraction process, as shown in Table 4.14. Notice that the model in Table 4.13 is reformulated based on Equation (4.21) due to the boundary of the convex hull of the feasible set.

Table 4.14: Proposed Model Using the OA Method

Given	$\tau = 20,\ \Delta_{\sigma^2} = 0.02,\ LB_{\mu} = 19.5,\ UB_{\mu} = 20.5,\ n_f = 16$ and $n_{pc} = 6$
Objective	Minimize η
Subject to	C(1) $0.126 + 0.046x_1 - 0.057x_2 - 0.032x_3 + 0.062x_1^2 - 0.041x_1x_2$ $+0.02x_1x_3 + 0.031x_2x_3 + 0.006z_1 - 0.01z_1x_1 - 0.034z_1x_2 - 0.05z_1x_3 + u^2 \le \eta$ C(2) $19.986 - 0.076x_1 + 0.023x_2 - 0.027x_3 + 0.12x_1^2 - 0.018x_1x_2$ $-0.006x_1x_3 - 0.03x_2x_3 + 0.03z_1 - 0.076z_1x_1 + 0.072z_1x_2 - 0.037z_1x_3 - 20 \le u$ C(3) $19.986 - 0.076x_1 + 0.023x_2 - 0.027x_3 + 0.12x_1^2 - 0.018x_1x_2$ $-0.006x_1x_3 - 0.03x_2x_3 + 0.03z_1 - 0.076z_1x_1 + 0.072z_1x_2 - 0.037z_1x_3 - 20 \ge u$ C(4) $u \ge -0.5$ C(5) $u \le 0.5$ C(6) $0.126 + 0.046x_1 - 0.057x_2 - 0.032x_3 + 0.062x_1^2 - 0.041x_1x_2$ $+0.02x_1x_3 + 0.031x_2x_3 + 0.006z_1 - 0.01z_1x_1 - 0.034z_1x_2 - 0.05z_1x_3 \ge 0$ C(7) $0.126 + 0.046x_1 - 0.057x_2 - 0.032x_3 + 0.062x_1^2 - 0.041x_1x_2$ $+0.02x_1x_3 + 0.031x_2x_3 + 0.006z_1 - 0.01z_1x_1 - 0.034z_1x_2 - 0.05z_1x_3 \le 0.02$ Boundary constraints: $-1 \le x_i \le 1$ and $x_i \in \mathbb{R}$ $(i = 1,2,3);\ z_1 \in \{0,\ 1\}$
Method	The outer approximation method
Find	Factor settings $\mathbf{x}^* = (z_1^*,\ x_1^*,\ x_2^*,\ x_3^*)'$ and an objective function value of the model

The results of the proposed models with the three different method using BONMIN (basic open-source nonlinear mixed integer programming) are summarized in Table 4.15.

Table 4.15: Results of the Proposed Model Using the BB, HNBC, and OA Methods

Method	Input variables				$f(\mathbf{x}^*)$	Total running time (seconds)	Total memory
	z_1^*	x_1^*	x_2^*	x_3^*			
BB	1	0.106	0.924	0.945	9.91E-09	0.103	330736
HNBC	1	0.109	0.928	0.942	9.65E-09	0.257	330736
OA	1	0.107	0.925	0.944	9.98E-09	0.078	328704

It is observed that the three methods basically provide almost identical solutions. For this particular problem, however, the OA method seems a bit more effective than the other two methods in terms of the required total memory and total running time. Response surface plots and optimal solutions are depicted in Figure 4.4.

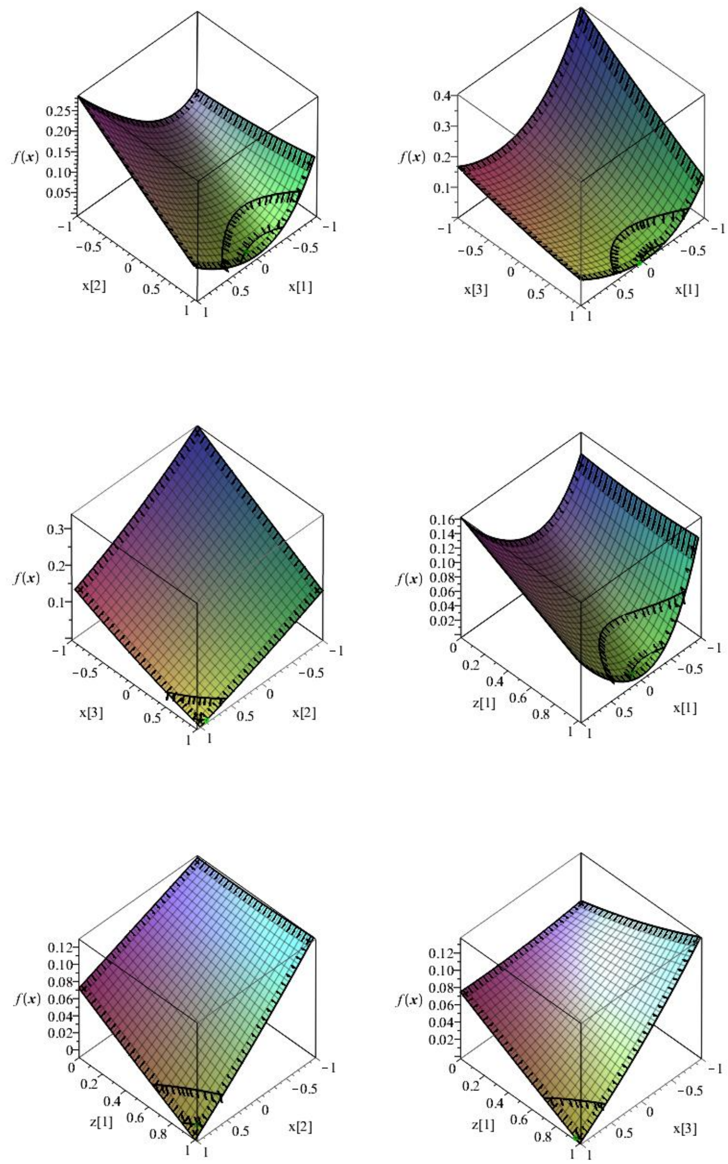


Figure 4.4: Response Surface Plots of the Proposed Model

We now provide the comparisons of solutions using the proposed model with the OA method and traditional models (*VM* and *LT*) in the 0-1 MINLP framework, which are summarized in Table 4.16.

Table 4.16: Comparison Study between the Proposed Model Using the OA Method and Traditional Models

Model	Input variables				$\hat{\mu}(\mathbf{x}^*)$	$\sigma^2(\mathbf{x}^*)$
	z_1^*	x_1^*	x_2^*	x_3^*		
VM	1	0.104	1	1	20.000	0.023
LT	1	-0.012	1	1	19.981	0.022
Proposed	1	0.107	0.925	0.944	20.000	0.001

Note that the *VM* model is convex, while The *LT* model is nonconvex due to a fourth-order objective function. We also observe that both the *VM* and proposed models achieve the desired target value. In this particular example, the proposed model using the OA method outperforms the traditional *VM* and *LT* models for three reasons. One, the *VM* and *LT* models provide larger variances. Two, the *VM* and *LT* models do not satisfy the desired upper bound for the process variance. Three, the proposed model gives the smallest optimum objective value, the smallest optimum standard deviation, and the smallest bias value. The particular numerical example supports the merit of the proposed models in finding better solutions.

Conclusions

Following the pioneering work of Taguchi (1986) and Vining and Myers (1990), a number of research attempts have been made to strive for better RPD solutions. Common denominators of those attempts include central composite designs and convex RPD problems with quantitative input variables on a continuous scale. In this chapter, we have developed special 0-1 mixed integer nonlinear programming models using a response surface based factorial design with pseudo center points by incorporating both qualitative and quantitative input variables. Compared to the existing RPD models, such as the dual response and MSE models, the proposed models may significantly reduce process variation, thereby obtaining better RPD solutions, as shown in the numerical example. Three different solution methods, which are the outer approximation method, the branch-and-bound method, and the hybrid nonlinear based branch-and-cut algorithm, were selected in order to measure computational efficiency and computing time to solve proposed convex and nonconvex RPD problems. The numerical example shows that the outer approximation method for the proposed models may be superior to the branch-and-bound method and the hybrid nonlinear based branch-and-cut algorithm for the particular numerical example illustrated in this chapter.

The proposed model may have limitations which can serve as fruitful future research areas. One, engineers may need to deal with more than one quality characteristic in real-life situations. Our proposed models allow only one quality characteristic. As such, models need to be expanded into a multi-response design of experiments and possibly multi-criteria integer programming models by balancing trade-offs between conflicting objectives. Two, there are situations in which a design space where the model is fitted may not be the same as a solution space where the optimal solution is to be determined. Incorporating such ideas into optimal designs may be worth some attention. Finally, the proposed model allows only three levels mainly because factorial designs with center points consists of -1, 0, and +1. If main factors are of primary interest, Taguchi's orthogonal designs may be effective with more than three levels.

CHAPTER FIVE

ROBUST PARAMETER DESIGN OPTIMIZATION WITH A NONLINEARLY-CONSTRAINED IRREGULAR EXPERIMENTAL DESIGN SPACE

Introductory Remarks

Continuous process improvement is a critical concept in maintaining a competitive advantage in the marketplace. It is also recognized that process improvement activities are most efficient and cost-effective when implemented during the early design stage. Based on this awareness, robust parameter design (RPD) was introduced as a systematic method for applying experimental design and optimization tools. The primary goal of RPD is to determine the best design factor settings, or optimum operating conditions, that minimize performance variability and deviations from the target value of a product. Because of their practicability in reducing the inherent uncertainty associated with system performance, the widespread application of RPD techniques has resulted in significant improvements in product quality, manufacturability, and reliability at low cost.

Research Motivations

When designing an experiment, there are numerous situations in which standard multi-level, multi-factor experimental designs, such as full factorial designs, fractional factorial designs, Box-Behnken designs, and central composite designs, are no longer effective. The situations include that the experimental design space of interest may be constrained, or already-performed experiments many have to be included. The experiment may involve qualitative factors with more than two levels, mixture and process factors in the same design, or the experimenter may specify a certain set of design points. In addition, the situation may call for reducing the number of experimental runs or using a reduced regression model in fitting the data. Optimal designs, also referred to as computer-generated designs, are an effective experimental design platform for handling these special situations. In loose terms, the optimality of a design is defined with respect to two main characteristics. One is the ability to estimate accurately the coefficients of the regression model and the other is to estimate accurately the response function. The first approach is very useful when the experimenter knows the exact form of a response function. The latter case corresponds to a situation in which the underlying model is not known and therefore the experimenter wants to approximate a functional relationship within a given region of interest defined by the intersection of the ranges for several critical parameters. Among the optimal designs available in the literature, *D*-optimal designs are perhaps one of the most popular designs.

This chapter focuses on *D*-optimal designs when the experimental region of interest, or an experimental design space, is irregular due to non-linear process constraints. Several algorithms for linearly-constrained *D*-optimal designs are available. They are the Fedorov exchange algorithm (Fedorov, 1972), the search algorithm (Dykstra, 1971), the exchange algorithm (Mitchell and Miller, 1970), and the DETMAX algorithm (Mitchell, 1974); however, there has been little research work on nonlinearly-constrained *D*-optimal designs. Also, standard statistical software packages, including SAS, JMP, MATLAB, Minitab, and Design-Expert, do not support nonlinearly-constrained *D*-optimal designs.

This chapter uses a linearization scheme for nonlinear constraints on the design space. By implementing the linearization process, two challenges are observed. First, some of generated optimal design points may be infeasible since they can be located in between the approximate linear constraints and the original nonlinear constraints. This can be overcome by imposing additional piecewise linear functions until the feasibility condition is met. Another challenge is to establish a mechanism for the optimality condition, noting that the *D*-efficiency decreases as additional piecewise linear functions are imposed on the design space. This chapter proposes an algorithm for generating optimal design points based on the *D*-efficiency concept that satisfy both feasibility and optimality conditions for the nonlinearly-constrained design space. Once the *D*-optimal design points with both conditions met are obtained in the experimentation phase, the next task is to obtain a fitted response function and develop nonlinear programming RPD models, referred to as *D*-optimality-embedded RPD models in this chapter, to obtain the optimum operating conditions for process factors on the nonlinearly-constrained design space.

Review of the *D*-Optimality Criterion

The abbreviations and notation used in this chapter are described below.

y	: A scalar-valued response
N	: The total number of design points
x_i	: Input variables where $i = 1, 2, \ldots, m$
$\mathbf{X}$	: An $m \times k$ matrix consisting of the levels of the input variables
s_i	: The estimated standard deviation of the i^{th} run

s_i^2 : The estimated variance of the i^{th} run

$f(\mathbf{x})$: A function where $f(\mathbf{x}) = [f_1(\mathbf{x}_1),\ f_2(\mathbf{x}_2),\ ...,\ f_N(\mathbf{x}_N)]'$

$\mathbf{M}(\boldsymbol{\xi})$: The design moment matrix

$\Psi[\mathbf{M}(\boldsymbol{\xi})]$: A function of the design moment matrix

D^L : The minimum desired *D*-efficiency defined by the user

$\mathcal{X}$: Design space

k : The number of parameters in the model

N_a : The number of additional design points

LB : Lower bound of $\mathbf{x}$

UB : Upper bound of $\mathbf{x}$

$\hat{\mu}(\mathbf{x})$: The fitted response function for process mean

μ_τ : A desired target value of process mean

$|\hat{\mu}(\mathbf{x}) - \mu_\tau|$: A process bias

$\hat{\sigma}(\mathbf{x})$: The fitted response function for process standard deviation

$\widehat{\sigma^2}(\mathbf{x})$: The fitted response function for process variance

LSL : Lower specification limit for process output

USL : Upper specification limit for process output

Traditional experimental designs, such as full factorial designs, fractional factorial designs, Box-Behnken designs, and response surface designs, are appropriate for the experiment where all factor settings are feasible in the design space. In some engineering situations, however, certain combinations of factor levels are infeasible or too expensive to measure, and as a result, its design space becomes asymmetric and irregular. *D*-optimal designs, one of the classes of computer-generated optimal designs, seek optimal design points that minimize the covariance of the parameter estimates by a computer-aided iterative exchange algorithm. Unlike the aforementioned traditional experimental designs, *D*-optimal designs are not typically orthogonal and as a result, parameter estimates may be often correlated. Since *D*-optimality is essentially a parameter estimation criterion, the quality of the parameter estimates is determined by their covariance structure. Minimizing the covariance of the parameter estimates is equivalent to maximizing the determinant of the information matrix $\mathbf{X}'\mathbf{X}$, or $|\mathbf{X}'\mathbf{X}|$, where $\mathbf{X}$ is the design matrix. It can be shown that for fixed diagonal terms in $\mathbf{X}$, $|\mathbf{X}'\mathbf{X}|$ becomes the largest when all off-diagonal terms are zero. Note that the determinant is the product of the eigenvalues, which is inversely proportional to the product of the axes of the confidence ellipsoid around the parameter estimates. Accordingly, maximizing the determinant of the information matrix is also equivalent to minimizing the volume of the confidence ellipsoid on the vector of regression coefficients. Thus, maximizing the determinant of the information matrix leads to minimizing the covariance of the parameter estimates and minimizing the volume of the confidence ellipsoid.

The design moment matrix is found using the information matrix ($\mathbf{X}'\mathbf{X}$) as follows:

$$\mathbf{M}(\xi) = \frac{\mathbf{X}'\mathbf{X}}{N} \tag{5.1}$$

where ξ is a matrix of design points for a set of *N* experimental runs. The *D*-optimality criterion focuses on good estimation of model parameters and it is defined as follows:

$$\Psi[\mathbf{M}(\xi)] = |\mathbf{M}(\xi)| \text{ and } \psi(\mathbf{x}, \xi) = k - d(\mathbf{x}, \xi) \tag{5.2}$$

where $d(\mathbf{x}, \xi) = f'(\mathbf{x})\mathbf{M}^{-1}(\xi) f(\mathbf{x})$ for an *D*-optimal experimental design. Then, we have the following equations, which are equivalent to

$$\xi^* = \arg \max_{\xi} |\mathbf{M}(\xi)| \tag{5.3}$$

$$\Rightarrow \xi^* = \arg \min_{\xi} \max_{\mathbf{x}} d(\mathbf{x}, \xi) \tag{5.4}$$

$$\Rightarrow \max_{\mathbf{x}\in X} d(\mathbf{x}, \xi^*) = k \tag{5.5}$$

The design ξ^* is *D*-optimal if and only if $f'(\mathbf{x})\mathbf{M}^{-1}(\xi) f(\mathbf{x}) \leq k$ for $\forall \mathbf{x} \in \mathcal{X}$. Note that the *D*-optimality criterion satisfies all the assumptions below (Kiefer, 1959; Cook and Federov, 1995):

- $\mathcal{X}$ is a compact design space.
- $f(\mathbf{x})$ is a continuous function and $f: \mathbb{R} \to \mathbb{R}$.
- $\Psi[\mathbf{M}(\xi)]$ is a convex function.
- $\{\xi: \Psi[\mathbf{M}(\xi)] \leq q < \infty\}$ for a real number *q*.
- $\Psi[(1-\alpha)\mathbf{M}(\xi) + \alpha\mathbf{M}(\bar{\xi})] \leq (1-\alpha)\Psi[\mathbf{M}(\xi)] + \alpha\mathbf{M}(\bar{\xi})$

  where $\bar{\xi} \in (-\infty, \infty]$ and $\forall \alpha \in [0,1]$.

Proposed Cutting-Plane Outer Linearization Scheme for Nonlinear Constraints within an Irregular Design Shape

Let nonlinear constraints consist of nonlinear functions $g_i(\mathbf{x})$. We assume that all constraints are active, which means that constraints will influence finding design points and that the set of $\mathbf{x}$ satisfying Equation (5.6) is not empty. Then, we consider a *D*-optimal experimental design problem with a nonlinearly-constrained design space in order to maximize the determinant of the $\mathbf{M}(\xi)$ while satisfying the nonlinear constraints in the convex design space. The conceptual optimization model is then written as:

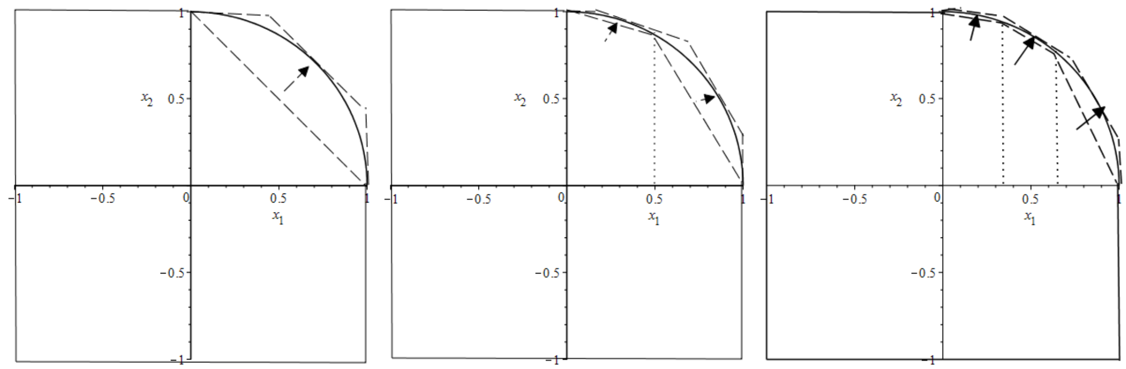
$$
\begin{aligned}
&\Psi\left(\xi^*\right) = \arg \max_{\xi} \left|\mathbf{M}(\xi)\right| \text{ or } \Psi\left(\xi^*\right) = \arg \min_{\xi} \left|\mathbf{M}(\xi)^{-1}\right| \\
&\text{subject to } g_i(\mathbf{x}) \le 0 \text{ for } i = 1, 2, \ldots, l \ (\text{Nonlinear constraints}) \\
&\qquad h_j(\mathbf{x}) \le 0 \text{ for } j = 1, 2, \ldots, p \ (\text{Linear constraints}) \\
&\qquad LB \le \mathbf{x} \le UB \ (\text{Boundary constraints for input variables}) \\
&\qquad N \ (\text{The total number of design points}) \\
&\qquad \mathbf{M}(\xi) = \frac{\mathbf{X}'\mathbf{X}}{N}
\end{aligned}
\tag{5.6}
$$

where $g_i(\mathbf{x})$ are convex and twice continuously differentiable functions. Given the total number of runs for an experiment, the computer-generated candidate sets of design points are updated until $\Psi\left(\xi^*\right)$ is achieved.

We apply the outer approximation concept to convert a nonlinearly-constrained experimental design into a linearized experimental design space for obtaining optimal interior design points. For the nonlinear functions $g_i(\mathbf{x})$ associated with the nonlinear constraints in Equation (5.6) on the design space, linearization of the nonlinear constraints is used in this chapter. Linearization is a linear approximation of a nonlinear function in a small region around anchor points. As shown in Figure 5.1a, inner linearization of $g_i\left(\mathbf{x}\right)$ is done first and the inner linear function would move parallel towards the nonlinear function until it touches any point on the nonlinear function. In this chapter, the touching point will be referred to as an anchor point. Around the anchor point at *a*=(0.707, 0.707), three outer linear functions are created on the design space. Due to the nature of outer linear functions, infeasible design spaces are often created and computer-generated optimal design points may fall in those regions. In order to reduce the infeasible space, imposing additional outer linear functions on the design space is recommended. As shown in Figure 5.1b and 5.1c, the nonlinear function is well approximated by imposing additional outer linear functions on the design space. The potential question is how many piecewise outer linear functions are needed. This is an issue of feasibility conditions, and the proposed exchange algorithm outlined in the proposed exchange algorithm section defines the required number of outer linear functions. Outer linear functions can be obtained as follows:

$$\begin{aligned}&\frac{\partial g_i}{\mathbf{x}}\left(\mathbf{a}^{(r)}\right)\left(\mathbf{x}-\mathbf{a}^{(r)}\right)+g_i\left(\mathbf{a}^{(r)}\right)\le 0,\ \forall i\in\left\{1,\ 2,\ \ldots,\ l\right\},\\&\mathbf{a}^{(r)}\in P \text{ and } P=\left\{\mathbf{a}^{(1)},\ \mathbf{a}^{(2)},\ \ldots,\ \mathbf{a}^{(r)}\right\}.\end{aligned} \tag{5.7}$$

where $\mathbf{a}^{(r)}$ is the r^{th} anchor point which touches the nonlinear function.



(a) (b) (c)

Figure 5.1: (a) Three Outer Linear Constraints with One Anchor Point; (b) Four Outer Linear Constraints with Two Anchor Points; (c) Five Outer Linear Outer Constraints with Three Anchor Points

The corresponding design problem in Equation (5.6) can be stated for each iteration in the following way:

$$
\begin{aligned}
&\Psi(\boldsymbol{\xi}^*) = \arg \max_{\xi} |\mathbf{M}(\boldsymbol{\xi})| \text{ or } \Psi(\boldsymbol{\xi}^*) = \arg \min_{\xi} |\mathbf{M}(\boldsymbol{\xi})^{-1}| \\
&\text{subject to } L_i(\mathbf{x}) \le 0 \ \forall i \in \{1,\ 2,\ ...,\ l\} \text{ (Outer linear constraints)} \\
&\qquad\qquad h_j(\mathbf{x}) \le 0 \ \forall j \in \{1,\ 2,\ ...,\ p\} \ (\text{Linear constraints}) \\
&\qquad\qquad LB \le \mathbf{x} \le UB \\
&\qquad\qquad N \ (\text{The total number of design points}) \\
&\text{where } \mathbf{M}(\boldsymbol{\xi}) = \frac{\mathbf{X}'\mathbf{X}}{N}.
\end{aligned}
\tag{5.8}
$$

where $L_i(\mathbf{x}) \approx \frac{\partial g_i}{\mathbf{x}}\left(\mathbf{a}^{(r)}\right)\left(\mathbf{x}-\mathbf{a}^{(r)}\right)+g_i\left(\mathbf{a}^{(r)}\right)$. We can reformulate the design problem in Equation (5.8) with the Lagrangian function to verify a solution of optimal design points for piecewise linear functions on an experimental design space as follows:

$$\max_{\mathbf{x}} \; q(\mathbf{x}, \mathbf{u}, \mathbf{v}, \boldsymbol{\xi}) = \psi(\mathbf{x}, \; \boldsymbol{\xi}) - \sum_{i=1}^{l} u_i L_i(\mathbf{x}) - \sum_{j=1}^{p} v_j h_j(\mathbf{x}) \tag{5.9}$$

where u_i and v_j are the Lagrange multipliers for $\forall i \in \{1, \; 2, \; ..., \; l\}$ and $\forall j \in \{1, \; 2, \; ..., \; p\}$. For each iteration, a D-optimal experimental design ($\boldsymbol{\xi}^*$) is optimal with the existence of $\mathbf{u}^*$, $\mathbf{v}^*$ and $\boldsymbol{\xi}^*$ if Equation (5.10) holds true.

$$\begin{aligned}
&\max_{x} \; q\left(\mathbf{x}, \mathbf{u}^*, \mathbf{v}^*, \boldsymbol{\xi}^*\right) = \psi(\mathbf{x}, \; \boldsymbol{\xi}^*) - \sum_{i=1}^{l} u_i^* L_i(\mathbf{x}) - \sum_{j=1}^{p} v_j^* h_j(\mathbf{x}) \\
&\text{where } \psi\left(\mathbf{x}, \; \boldsymbol{\xi}^*\right) - \sum_{i=1}^{l} u_i^* L_i(\mathbf{x}) - \sum_{j=1}^{p} v_j^* \left[h_j(\mathbf{x}) - R_j\right] = 0 \\
&\qquad u_i^* L_i(\mathbf{x}) = 0 \\
&\qquad v_j^* h_j(\mathbf{x}) = 0 \\
&\qquad u_i^* \geq 0, \; u_i \in \mathbb{R}^l \text{ and } i = 1, \; 2, \; ..., \; l \\
&\qquad v_j^* \geq 0, \; v_j \in \mathbb{R}^p \text{ and } j = 1, \; 2, \; ..., \; p \\
&\qquad LB \leq \mathbf{x} \leq UB \text{ and } N.
\end{aligned} \tag{5.10}$$

Note that $q\left(\mathbf{x}, \mathbf{u}^*, \mathbf{v}^*, \boldsymbol{\xi}^*\right) = 0$ due to the Lagrangian stationarity where $q\left(\mathbf{x}, \mathbf{u}^*, \mathbf{v}^*, \boldsymbol{\xi}^*\right)$ is zero.

Simulation Study on the Effect of Number of Runs and Number of Piecewise Outer Linear Functions on *D*-Efficiency

In this section, we study the effect of number of runs and number of outer linear functions on D-efficiency. The findings are then incorporated into the proposed algorithm outlined in the proposed exchange algorithm section. Recall that a design is said to be D-optimal if $|\mathbf{X}'\mathbf{X}|$ is maximized or $\left|(\mathbf{X}'\mathbf{X})^{-1}\right|$ is minimized. Note that the D-efficiency can be found as follows:

$$D-\text{efficiency} = \frac{\left|\left(\mathbf{X}'\mathbf{X}\right)^{-1}\right|^{1/k}}{N} \tag{5.11}$$

where $\left|\left(\mathbf{X}'\mathbf{X}\right)^{-1}\right|$ is the product of the eigenvalues of $\left(\mathbf{X}'\mathbf{X}\right)^{-1}$ and the k^{th} root of the determinant is the geometric mean. Lucas (1976) further developed a measure of the relative *D*-efficiency, D_e, of design 1 to design 2 based on the *D*-criterion, which is defined as

$$D_e = \left(\frac{\left|\left(\mathbf{X}_2'\mathbf{X}_2\right)^{-1}\right|}{\left|\left(\mathbf{X}_1'\mathbf{X}_1\right)^{-1}\right|} \right)$$

where $\mathbf{X}_1$ and $\mathbf{X}_2$ are the design matrices for the two designs and k is the number of model parameters. A Relative *D*-efficiency ranges from 0% to 100%. When designs are balanced and the factor levels appear an equal number of times (i.e., orthogonal) within the design, the *D*-efficiency of those designs will be 100%. As such, full factorial designs have a 100% *D*-efficiency measure.

Consider the nonlinear constraint $x_1^2 + x_2^2 \le 1$ for $x_i \in [0,1]\ \forall i$ and the linear constraint $x_1 + x_2 \ge -1.5$ for $x_i \in [-1,0]\ \forall i \in \{1,2\}$ over the design space $\mathcal{X}$ = $\{x_i \,|\, x_i \in [-1,1] \forall i \in \{1,2\}\}$. Table 5.1 shows the results of *D*-efficiencies with different numbers of runs, piecewise outer linear constraints (POLCs) and linear constraints (LCs). Two observations are made. First, as the number of runs increases, *D*-efficiency increases and reaches a state of little change when the number of runs is very large. Second, for a fixed number of runs, *D*-efficiency decreases for a large number of runs, as more POLCs are added. This is because the design space becomes smaller by imposing additional POLCs. However, for a relatively small number of runs, *D*-efficiency does not always decrease as more POLCs are added to the design space. This pattern is observed when the numbers of runs are 1, 10, and 100. This pilot study indicates that for the small number of POLCs, 1,000 runs seem to provide the nearly highest *D*-efficiency. However, when POLCs are added due to the existence of infeasible design points in any iteration, it is recommended to significantly increase the number of runs. These observations are of a particular importance in developing the exchange algorithm in the proposed exchange algorithm section.

Table 5.1: Simulation Study

D –efficiency (D_e) with (POLCs, LC)	Number of runs					
	1	10	100	1,000	10,000	100,000
D_e with (3, 1)	38.719↑	38.911↑	38.912↑	38.913↑	38.913↑	38.914
	↓	↓	↓	↓	↓	↓
D_e with (4, 1)	36.662↑	37.926↑	37.933↑	37.935↑	37.936↑	37.937
	↑	↓	↓	↓	↓	↓
D_e with (6, 1)	**36.895**↑	37.116↑	37.117↑	37.121↑	37.125↑	37.127
	↓	↓	↓	↓	↓	↓
D_e with (10, 1)	34.974↑	36.870↑	36.904↑	36.967↑	36.970↑	36.971
	↑	↑	↑	↓	↓	↓
D_e with (14, 1)	**35.281**↑	**36.919**↑	**36.923**↑	36.931↑	36.933↑	36.934

Proposed Exchange Algorithm for *D*-Optimal Design Points within an Irregular Design Space

D-optimal designs are model-specified designs. In this chapter, a second-order model is considered. Based on the results, we propose the iterative exchange algorithm to obtain the *D*-optimal design with the *D*-efficiency close to the highest, which satisfy the feasibility and optimality requirements, over a nonlinearly-constrained design space. As shown in Table 5.2, the purpose of the proposed exchange algorithm is to find *D*-optimal design points by maximizing the determinant of $\mathbf{M}(\boldsymbol{\xi})$ at each step by incrementally exchanging design points in the design matrix **X**.

The complexity of the algorithm is $O(N_d)+O(N_e)+O(N_{in})$, where $O(N_d)$, $O(N_e)$ and $O(N_{in})$ are the size of the desired design, the number of edge points, and the number of interior points, respectively. Compared to first-order models, second-order models will require significantly large number of runs to achieve very high *D*-efficiency. We recommend at least 1,000 random runs and the proposed exchange algorithm should be able to find nearly global optimal design points.

Decision makers should choose the number of design points based on cost considerations and resource limitations. Equation (5.7) implies that we have *k* design points in order to construct a *D*-optimal design. Imposing additional design points may be beneficial in maximizing the determinant of $\mathbf{M}(\boldsymbol{\xi})$ while retaining near orthogonality as much as possible (see de Auigar et al., 1995). Therefore, the total number of design points is $N = k + N_a$ for *D*-optimal designs.

Table 5.2: Proposed Exchange Algorithm for a Nonlinearly-Constrained Design Space

Phase	Explanation
I	Specify input variables where x_i , $LB \le x_i \le UB$ and $i = 1,\ 2,\ ...,\ m$.
II	Specify process parameters.
III	Find outer linear constraints using Equation (5.7).
IV	Determine a linearized-constrained irregular experimental design space.
V	Determine the number of design points for the *D*-optimal experimental design and the number of random runs.
VI	Construct a random design matrix where $f'(\mathbf{x})\mathbf{M}^{-1}(\xi) f(\mathbf{x}) \le k$ for $\forall \mathbf{x} \in \mathcal{X}$ and $\lvert \mathbf{M}(\xi) \rvert \neq 0$.
VII	Set j=0.
VIII	Calculate $\lvert \mathbf{M}(\xi) \rvert$ where $\mathbf{M}(\xi_j) = \dfrac{\mathbf{X}'\mathbf{X}}{N}$, $\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{m1} & x_{11}x_{21} & \cdots & x_{(m-1)1}x_{m1} & x_{11}^2 & \cdots & x_{m1}^2 \\ 1 & x_{12} & \cdots & x_{m2} & x_{12}x_{22} & \cdots & x_{(m-1)2}x_{m2} & x_{12}^2 & \cdots & x_{m2}^2 \\ \vdots & & \vdots & & & \vdots & & & \vdots & \\ 1 & x_{1m} & \cdots & x_{mN} & x_{1N}x_{2N} & \cdots & x_{(m-1)N}x_{mN} & x_{1N}^2 & \cdots & x_{mN}^2 \end{pmatrix}$ and ξ_j represents a design matrix with design points of the j^{th} run.
IX	Define the new design matrix as ξ_j using each coordinate for each input variable for each point by other coordinates and new points in the design.
X	Set j=j+1 and define the new design matrix (ξ_j).
XI	Repeat steps (VIII-X) until the number of runs improves the *D*-efficiency.
XII	Check the optimality and feasibility requirements for *D*-optimal design points. • The optimality requirement: $D_e \ge D^L$ where D^L is the desired lower bound of *D*-efficiency. • The feasibility requirement: All design points are feasible. If both requirements are met, then stop and ξ^* has been obtained. If the optimality requirement is not met but the feasibility requirement is met, then increase number of runs significantly and go to phase step (VIII). If the feasibility requirement is not met but the optimality requirement is met, then go to phase (XIII).
XIII	Find new outer approximation constraints using Equation (5.7) for each nonlinear function using new anchor points.
XIV	Modify the linearized design space from phase (XIII) and go to phase (V).

Some common design properties in the response surface methodology include orthogonality and rotatability. A design is orthogonal if the information matrix is diagonal (see Khuri and Mukhopadhyay, 2010). The aim is to minimize the variance of the estimated parameters while maximizing determinant of the diagonal matrix. The off-diagonal entries of the variance of the estimated parameters will be zero because the entries outside the diagonal are all zeros. Therefore, the effects of regression parameters can be independent while the design is orthogonal. In addition, all odd moments should be zero, such as $[i] = \sum_{a=1}^{N} x_{ia} / N$ and $i = 1,\ 2,\ \ldots,\ m$ if the design is orthogonal. As for rotatability, a design is rotatable if the prediction variance, $Var[\hat{y}(\mathbf{x})]$, is approximately constant at all the points in the design space that are equidistant from the center point. In general, however, *D*-optimal designs for a constrained design space are not rotatable because odd moments are not zero and $[iiii]/[iijj] = \sum_{a=1}^{N} x_{ia}^4 / \sum_{a=1}^{N} x_{ia}^2 x_{ja}^2 \neq 3$ and $i,\ j = 1,\ 2,\ \ldots,\ m\ (i \neq j)$ where $[iiii]$ and $[iijj]$ represent the fourth pure and mixed moments, respectively. In addition, the rotatability may not be a desirable priority in the constrained design space because the design space is not a hypercube, sphere, or hyper-sphere.

Proposed *D*-Optimal Design-Embedded Robust Parameter Design Models

The next task is to make transitions of the *D*-optimal points obtained in the proposed exchange algorithm section into the robust parameter design phase. Recall that the primary goal of robust parameter design (RPD) is to determine the best design factor settings, or optimum operating conditions, that minimize performance variability and deviations from the target value of a product. This is done by obtaining fitted response surface functions. Consider the following second-order response model:

$$y = \phi_0 + \sum_{i=1}^{m} \phi_i x_i + \sum_{i<j=2} \sum_{i=1}^{m} \phi_{ij} x_i x_j + \sum_{i=1}^{m} \phi_{ii} x_i + \varepsilon \tag{5.12}$$

where ϕ_i and ε are regression coefficients and an uncorrelated observed error, respectively. Using the *D*-optimal design points that have been generated using the proposed exchange algorithm, Respective fitted response functions for process mean, standard deviation, and variance are as follows.

$$\hat{\mu}(\mathbf{x}) = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}} = \mathbf{X}\left[\mathbf{M}(\xi)N\right]^{-1}\mathbf{X}'\bar{\mathbf{y}} \text{ and } \bar{\mathbf{y}}=\left[\bar{y}_1,\ \bar{y}_2,\ ...,\ \bar{y}_N\right] \tag{5.13}$$

$$\hat{\sigma}(\mathbf{x}) = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s} = \mathbf{X}\left[\mathbf{M}(\xi)N\right]^{-1}\mathbf{X}'\mathbf{s} \text{ and } \mathbf{s}=\left[s_1,\ s_2,\ ...,\ s_N\right] \tag{5.14}$$

$$\widehat{\sigma^2}(\mathbf{x}) = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{s^2} = \mathbf{X}\left[\mathbf{M}(\xi)N\right]^{-1}\mathbf{X}'\mathbf{s^2} \text{ and } \mathbf{s^2}=\left[s_1^2,\ s_2^2,\ ...,\ s_N^2\right] \tag{5.15}$$

where $\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{m1} & x_{11}x_{21} & \cdots & x_{(m-1)1}x_{m1} & x_{11}^2 & \cdots & x_{m1}^2 \\ 1 & x_{12} & \cdots & x_{m2} & x_{12}x_{22} & \cdots & x_{(m-1)2}x_{m2} & x_{12}^2 & \cdots & x_{m2}^2 \\ \vdots & \vdots & & & & \vdots & & & \vdots & \\ 1 & x_{1m} & \cdots & x_{mN} & x_{1N}x_{2N} & \cdots & x_{(m-1)N}x_{mN} & x_{1N}^2 & \cdots & x_{mN}^2 \end{pmatrix}$.

The system requirements are important in determining an effective RPD optimization model. For some situations, it is important that the mean response needs to be strictly equal to the desired target value. Then, the goal is to minimize the response standard deviation subject to the process mean equal to the target value of interest. Vining and Myers (1995) proposed the following dual response model:

$$\begin{aligned} &\text{Minimize } \hat{\sigma}(\mathbf{x}) \\ &\text{subject to } \hat{\mu}(\mathbf{x})=\mu_\tau \\ &\qquad LB \le \mathbf{x} \le UB \text{ and } \mathbf{x} \in \mathbb{R} \end{aligned} \tag{5.16}$$

It should be noted that the outer linear constraints in the design stage are now part of constraints in this optimization model. Under some other engineering situations, the mean-squared error (MSE) optimization model may be preferred over the dual response model. The MSE model, proposed by Cho (1994) and Lin and Tu (1995), incorporates the concept of the squared deviations of the process mean from the target value and the process variance. The optimum operating conditions are then obtained by minimizing the squared deviations from the target and the variance at the same time. The model is given as follows:

$$\begin{aligned}&\text{Minimize } \left[\hat{\mu}(\mathbf{x})-\mu_\tau\right]^2+\widehat{\sigma^2}(\mathbf{x})\\&\text{subject to } LB \le \mathbf{x} \le UB \text{ and } \mathbf{x}\in\mathbb{R}\end{aligned} \tag{5.17}$$

Three observations are made. First, both dual response and MSE RPD models were developed under the assumption that the design space of interest was either a cube for a full factorial design or a sphere for the central composite design. There has been little work on RPD models that incorporate *D*-optimality concepts. Second, the dual response model may create a relatively large amount of variability around the mean but the process bias would be essentially zero due to the equality constraint. Contrarily, the MSE model may provide less variability but may create some process bias. Finally, the variability measures may change optimum operating conditions for a response surface (see Goethals et al., 2009). The standard deviation estimator may produce a better point estimator than the variance counterpart. However, the variance estimator may result in smaller values of mean squared error than the one from the dual response model. While both RPD models are their own merits, in practice, however, the requirement for the process mean being at the target as a strict system constraint would result in large process variability. Also, large process bias would exhibit by minimizing the process variability. To address these potential weaknesses, the new RPD model, namely the *D*-optimal design embedded RPD model for nonlinearly constrained design space, is proposed, as shown in Table 5.3. The proposed model includes the proposed concepts of the outer linear constraints and the proposed exchange algorithm for *D*-optimal design points. In addition, the lower and upper bounds of process mean defined by users are included as a constraint. Finally, the proposed model allows users to choose either standard deviation or variance measure.

Table 5.3: Proposed *D*-Optimal-Design-Embedded RPD Optimization Model for Nonlinearly-Constrained Design Space

Minimize	$\mathbf{X}\left[\mathbf{M}\left(\boldsymbol{\xi}^*\right)N\right]^{-1}\mathbf{X}'\mathbf{s}$ or $\mathbf{X}\left[\mathbf{M}\left(\boldsymbol{\xi}^*\right)N\right]^{-1}\mathbf{X}'\mathbf{s}^2$; see Table 5.2
Subject to	$LSL \le \mathbf{X}\left[\mathbf{M}\left(\boldsymbol{\xi}^*\right)N\right]^{-1}\mathbf{X}'\overline{\mathbf{y}} \le USL$
	$\mathbf{X}\left[\mathbf{M}\left(\boldsymbol{\xi}^*\right)N\right]^{-1}\mathbf{X}'\mathbf{s} \ge 0$ or $\mathbf{X}\left[\mathbf{M}\left(\boldsymbol{\xi}^*\right)N\right]^{-1}\mathbf{X}'\mathbf{s}^2 \ge 0$
	$L_i\left(\mathbf{x}\right) \le 0 \ \forall i \in \{1,\ 2,\ ...,\ l\}$ (Outer linear constraints)
	$h_j\left(\mathbf{x}\right) \le 0 \ \forall j \in \{1,\ 2,\ ...,\ p\}$ (Linear constraints)
	$LB \le \mathbf{x} \le UB,\ \mathbf{x} \in \mathbb{R}$ and N
Given	$\mu_\tau,\ USL,\ LSL$ and a linearized-constrained design space
Find	Factor settings $\mathbf{x}^*$ and an objective function value of the model where $\mathbf{x}^* = [x_1, x_2, ..., x_m]'$

The optimum operating conditions, or the RPD solutions, to the proposed model provide the global minimum since the objective function and constraints are convex. These observations are proved through the following proposed lemma.

Lemma: Assume that $\mathbf{x}^*$ is the minimum of the problem in Table 5.3, the objective function, $f(\cdot)$, is continuous at a feasible point $\mathbf{x}^*$ and Slater's condition is satisfied. Then, there exists $\boldsymbol{\lambda}^* \in \mathbb{R}_+$ subject to

$$\begin{aligned} 0 \in \partial\hat{\sigma}(\mathbf{x}^*) &+ \lambda_1(-\hat{\mu}(\mathbf{x}) + LSL) + \lambda_2(\hat{\mu}(\mathbf{x}) - USL) \\ &+ \lambda_3(-\hat{\sigma}(\mathbf{x})) + \lambda_{3+m}(-\mathbf{x} + LB) + \lambda_{3+2m}(\mathbf{x} - UB) \\ &+ \lambda_{3+2m+l}(g_i(\mathbf{x})) \\ \lambda_1 * (-\hat{\mu}(\mathbf{x}) &+ LSL) = 0,\ \lambda_2 * (\hat{\mu}(\mathbf{x}) - USL) = 0, \\ &\lambda_3 * (-\hat{\sigma}(\mathbf{x})) = 0,\ \lambda_{3+m} * (-\mathbf{x} + LB) = 0, \\ &\lambda_{3+2m} * (\mathbf{x} - UB) = 0, \text{ and } \lambda_{3+2m+l} * (g_i(\mathbf{x})) = 0 \end{aligned} \tag{5.18}$$

Furthermore, if the objective function and constraints are convex and $\mathbf{x}^*$ and $\boldsymbol{\lambda}^* \in \mathbb{R}_+$ are satisfied, then $\mathbf{x}^*$ is the global minimum of the problem shown in Table 5.3.

Proof: There exists $s \in \partial\hat{\sigma}(\mathbf{x}^*)$ subject to $-s \in N_{X_0}(\mathbf{x}^*)$. In addition, the following equation is hold:

$$[T_X(\mathbf{x}_0)]^{\mathrm{o}} = [T_{X_0}(\mathbf{x}_0)]^{\mathrm{o}} + \sum_{i \in I^0(\mathbf{x}_0)} \text{cone}[\partial g_i(\mathbf{x}_0)] \tag{5.19}$$

where $T_X(\mathbf{x}_0)$ is the set of all tangent directions for X at $\mathbf{x}$ is a closed cone, $I^0(\mathbf{x}_0)$ is the set of $i = \{1,\ 2,\ 3,\ ...,\ 3 + 2m + l\}$, and $[T_{X_0}(\mathbf{x}^*)]^{\mathrm{o}} = N_{X_0}(\mathbf{x}^*)$. Equation (5.19) is valid because Slater's condition is satisfied. We then have

$$-s \in N_{X_0}(\mathbf{x}^*) + \sum_{i \in I^0(\mathbf{x}^*)} \text{cone}[\partial g_i(\mathbf{x}^*)] \tag{5.20}$$

Using Equation (5.20), there exists $\lambda_i^* \geq 0$ and $i \in I^0(\mathbf{x}^*)$. Thus, we have the following equation

$$-s \in N_{X_0}(\mathbf{x}^*) + \sum_{i \in I^0(\mathbf{x}^*)} \lambda_i^* \partial g_i(\mathbf{x}^*) \tag{5.21}$$

By setting $\lambda_i^* = 0$ for $i \notin I^0(\mathbf{x}^*)$ in Equation (5.18), there exist sub-gradients $s \in \partial\hat{\sigma}(\mathbf{x}^*),\ s_i \in \partial g_i(\mathbf{x}^*),\ i \in I^0(\mathbf{x}^*)$ and $v \in N_{X_0}(\mathbf{x}^*)$ subject to

$$0 = s + \sum_{i \in I^0(\mathbf{x}^*)} \lambda_i^* s_i + v \tag{5.22}$$

Suppose that $\mathbf{x}_f$ is a feasible point of the problem in Table 5.3. We obtain the following equation using the scalar product of $\mathbf{x}_f - \mathbf{x}^*$:

$$0 = \left\langle s,\ \mathbf{x}_f - \mathbf{x}^* \right\rangle + \sum_{i \in I^0(\mathbf{x}^*)} \lambda_i^* \left\langle s_i,\ \mathbf{x}_f - \mathbf{x}^* \right\rangle + \left\langle v,\ \mathbf{x}_f - \mathbf{x}^* \right\rangle \tag{5.23}$$

where $\mathbf{x}_f - \mathbf{x}^* \in N_{X_0}(\mathbf{x}^*)$ because $\mathbf{x}_f$ is feasible and $\left\langle v,\ \mathbf{x}_f - \mathbf{x}^* \right\rangle \le 0$ due to $v \in N_{X_0}(\mathbf{x}^*)$. In addition, we have

$$\left\langle s_i,\ \mathbf{x}_f - \mathbf{x}^* \right\rangle \le 0 \Rightarrow g_i(\mathbf{x}_f) - g_i(\mathbf{x}^*) \le 0 \tag{5.24}$$

$$\left\langle s,\ \mathbf{x}_f - \mathbf{x}^* \right\rangle \ge 0 \tag{5.25}$$

where $i \in I^0(\mathbf{x}^*)$ and $g_i(\mathbf{x}_f) \le 0$. Then, $\hat{\sigma}(\mathbf{x}_f) \ge \hat{\sigma}(\mathbf{x}^*)$. Therefore, $\mathbf{x}^*$ is the minimum of the problem. Since $\mathbf{x}^* \in X_0$, $\mathbf{x}^*$ is the global minimum of the optimization problem in Table 5.3 where X_0 is a convex polyhedron. ∎

<u>Numerical Example</u>

We consider the adhesive bonding experiment described in Myers *et al.* (2009). In the experiment, there are two input variables, which are the amount of adhesive (x_1) and cure temperature (x_2).The response of interest is the pull-off force and its desired target value is 195, and the allowable lower and upper bounds of the force are 190 and 200, respectively. The coded low and high levels of those input variables are denoted by -1 and +1, respectively; thus, the design space is jointly formed by_ $x_1 \in [-1,\ 1]$ and $x_2 \in [-1,\ 1]$. This leads to a regularly-shaped square design space. Consider the two constraints on the current design space are imposed as follows.

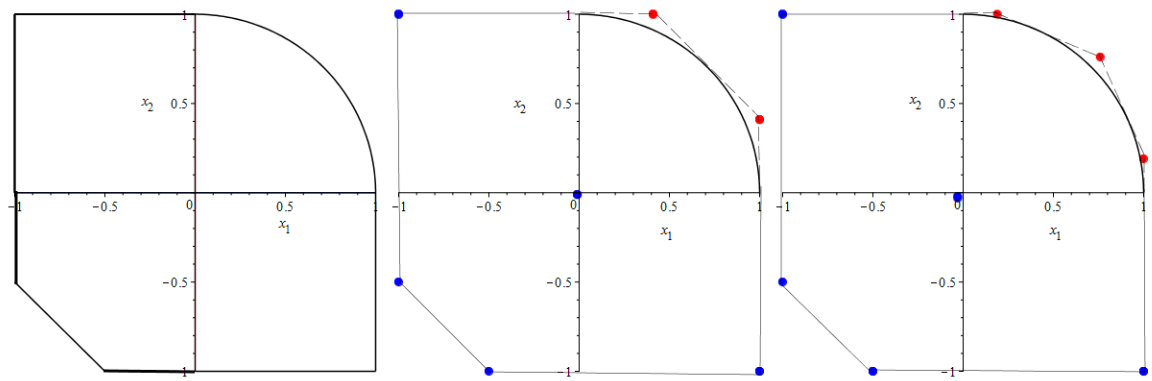
$$\text{Constraints on design space} = \begin{cases} x_1^2 + x_2^2 \le 1 \text{ for } x_1 \in [0,1] \text{ and } x_2 \in [0,1] \\ x_1 + x_2 \ge -1.5 \text{ for } x_1 \in [-1,0] \text{ and } x_2 \in [-1,0] \end{cases} \tag{5.26}$$

Figure 5.2a shows the irregular design space that results from applying these linear and nonlinear constraints. This section illustrates the application of the proposed exchange algorithm to generate the *D*-optimal design for *N* = 12 by linearizing the nonlinear constraint on the design space. This was executed using JMP and MATLAB software on the computer with 2.3 GHz Intel Core i5 and 8 GB DDR4 memory (see Appendix C for the computer code and procedure). Based on the *D*-optimal design points that are generated, several optimization models are developed and the optimum operating conditions are compared.

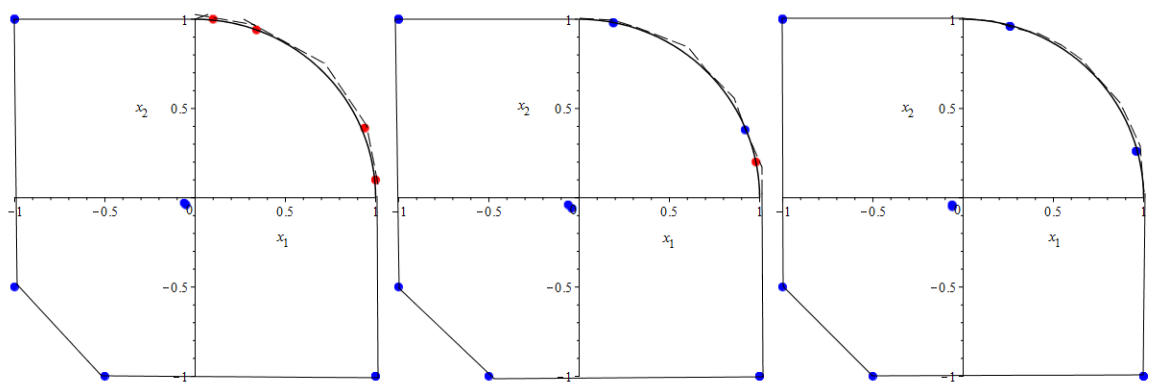
Generating *D*-Optimal Design Points for the Nonlinear Design Space

The proposed computer-aided coordinate-exchange algorithm requires multiple stages Using the outer approximation method described, $x_1^2 + x_2^2 \le 1$ for $x_1 \in [0,1]$ and $x_2 \in [0,1]$ is approximated by $0.707x_1 + 0.707x_2 \le 1, x_1 \le 1$ and $x_2 \le 1$. Figure

5.2 shows the nonlinear design space and linearized approximation of the design space for the i^{th} iteration $\forall i \in \{1,\ 2,\ ...,\ 5\}$.



(a) (b) (c)



(d) (e) (f)

Figure 5.2: (a) The Nonlinear Design Space; (b) The Linearized Design Space for the First Iteration; (c) The Linearized Design Space for the Second Iteration; (d) The Linearized Design Space for the Third Iteration; (e) The Linearized Design Space for the Fourth Iteration; (f) The Linearized Design Space for the Fifth Iteration

As shown in Figure 5.2, blue points are feasible design points and red points are infeasible design points for each iteration. Figures 5.2a-5.2f show that the nonlinearly-constrained design space is convex and the linearized design space is a convex polyhedron for each iteration. We start the first iteration of the proposed algorithm with points (0, 1), (0.707, 0.707) and (1, 0) to linearize the nonlinear function for the irregular experimental design. The outer linear functions are found as follows:

$$0.707x_1 + 0.707x_2 \le 1, x_1 \le 1 \text{ and } x_2 \le 1$$

The primary design problem can be expressed in the following models:

$$\begin{aligned}
&\text{Maximize } |\mathbf{M}(\xi)| \\
&\text{subject to } 0.707x_1 + 0.707x_2 \le 1 \\
&\qquad\qquad x_1 \le 1 \\
&\qquad\qquad x_2 \le 1 \\
&\qquad\qquad x_1 + x_2 \ge -1.5 \\
&\qquad\quad -1 \le x_i \le 1 \text{ and } i = 1,\ 2 \\
&\text{where } \mathbf{M}(\xi) = \frac{\mathbf{X}'\mathbf{X}}{N} \text{ and } \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{21} & x_{11}x_{21} & x_{11}^2 & x_{21}^2 \\ 1 & x_{12} & x_{22} & x_{12}x_{22} & x_{12}^2 & x_{22}^2 \\ \vdots & \vdots & & \vdots & \vdots & \\ 1 & x_{1N} & x_{2N} & x_{1N}x_{2N} & x_{1N}^2 & x_{2N}^2 \end{pmatrix}_{N\times 6}
\end{aligned} \tag{5.27}$$

Since the number of parameters is six, we need at least six design points to run the *D*-optimal design for this experiment. For *N*=12 design points, Tables 5.4 and 5.5 show the *D*-optimal design points for the i^{th} iteration and their associated piecewise linear constraints, respectively.

Table 5.4: Iterations 1-5

Iteration i	1		2		3		4		5	
Input variables	x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2
Design Matrix **(DM)**	1.00	-1.00	-0.50	-1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00
	-1.00	-0.50	1.00	-1.00	1.00	-1.00	0.92	0.38	0.96	0.26
	-1.00	1.00	-1.00	-0.50	-0.50	-1.00	0.19	0.98	0.96	0.26
	1.00	**0.41**	-1.00	1.00	-1.00	-0.50	-1.00	-0.50	0.26	0.96
	0.41	**1.00**	**0.76**	**0.76**	**0.94**	**0.39**	-0.06	-0.04	-1.00	-0.50
	1.00	**0.41**	-0.03	-0.02	**0.10**	**1.00**	1.00	-1.00	-0.50	-1.00
	-0.50	-1.00	**1.00**	**0.19**	-1.00	1.00	1.00	-1.00	1.00	-1.00
	-1.00	1.00	-0.03	-0.03	1.00	-1.00	0.19	0.98	0.26	0.96
	-0.01	-0.01	-1.00	1.00	**0.39**	**0.94**	-1.00	1.00	1.00	-1.00
	-0.01	-0.01	-0.50	-1.00	**1.00**	**0.10**	-0.50	-1.00	-0.06	-0.05
	0.41	**1.00**	**0.19**	**1.00**	-0.05	-0.04	**0.98**	**0.20**	-1.00	1.00
	1.00	-1.00	1.00	-1.00	-0.06	-0.03	-0.04	-0.06	-0.06	-0.04
Number of runs	100,000		100,000		100,000		100,000		100,000	
Relative D_e	38.914		37.937		37.127		36.971		36.934	
Feasibility condition	No		No		No		No		Yes	
Optimality condition	Yes		Yes		Yes		Yes		Yes	
Number of constraints	4		5		7		11		15	

The optimality requirement, $D_e \geq D^L = 36,$ is met in the fifth iteration. The feasibility requirement is met because all design points in the fifth iteration are feasible. Therefore, both feasibility and optimality conditions for this particular *D*-optimal design are satisfied in the fifth iteration. Note that the *D*-optimal design shown in the fifth iteration provides a near orthogonality because [1]=0.068 and [2]=0.070. As expected, however, this D-optimal design is not rotatable because the design space is asymmetric and irregular, or because $\frac{[1111]}{[1122]} = 1.425$ and $\frac{[2222]}{[2211]} = 1.425$.

Table 5.5: Piecewise Linear Constraints

Iteration i	Piecewise linear constraints
1	$0.707x_1 + 0.707x_2 \le 1, x_1 \le 1,\ x_2 \le 1,$ and $x_1 + x_2 \ge -1.5$
2	$0.414x_1 + x_2 \le 1.082,\ 2.414x_1 + x_2 \le 2.613$ $x_1 \le 1,\ x_2 \le 1,$ and $x_1 + x_2 \ge -1.5$
3	$0.198x_1 + x_2 \le 1.020,\ 0.667x_1 + x_2 \le 1.203$ $1.497x_1 + x_2 \le 1.801,\ 5.025x_1 + x_2 \le 5.128$ $x_1 \le 1,\ x_2 \le 1,$ and $x_1 + x_2 \ge -1.5$
4	$0.0974x_1 + x_2 \le 1.005,\ 0.303x_1 + x_2 \le 1.046,\ 0.534x_1 + x_2 \le 1.135,$ $0.820x_1 + x_2 \le 1.293,\ 1.217x_1 + x_2 \le 1.577,\ 1.870x_1 + x_2 \le 2.123,$ $3.296x_1 + x_2 \le 3.448,\ 10.153x_1 + x_2 \le 10.204,\ x_1 \le 1,$ $x_2 \le 1,$ and $x_1 + x_2 \ge -1.5$
5	$0.0651x_1 + x_2 \le 1.003,\ 0.198x_1 + x_2 \le 1.020,\ 0.339x_1 + x_2 \le 1.057,$ $0.493x_1 + x_2 \le 1.116,\ 0.667x_1 + x_2 \le 1.203,\ 0.877x_1 + x_2 \le 1.331,$ $1.139x_1 + x_2 \le 1.517,\ 1.497x_1 + x_2 \le 1.801,\ 2.027x_1 + x_2 \le 2.262,$ $2.947x_1 + x_2 \le 3.115,\ 5.025x_1 + x_2 \le 5.128,\ 15.338\ x_1 + x_2 \le 15.384,$ $x_1 \le 1,\ x_2 \le 1,$ and $x_1 + x_2 \ge -1.5$

RPD Optimization and Comparison Study

For the robust parameter design optimization, the experiment is replicated four times at each D-optimal design point and data are collected, as shown in Table 5.6.

Table 5.6: *D*-Optimal Design and Relevant Summary Statistics

Design point run	Input variables		Observations				$\bar{y}_u$	s_u	s_u^2
	x_1	x_2	y_{u1}	y_{u2}	y_{u3}	y_{u4}			
1	-1.00	1.00	184.2	170.1	174.2	181.4	177.5	6.5	41.9
2	0.96	0.26	202.6	184.0	177.8	193.2	189.4	11.0	11.8
3	0.96	0.26	193.1	199.6	177.2	192.9	190.7	9.5	90.7
4	0.26	0.96	191.2	210.9	195.4	202.9	200.1	8.7	75.3
5	-1.00	-0.50	179.7	164.7	180.2	181.4	176.5	7.9	62.4
6	-0.50	-1.00	186.2	182.4	185.0	204.0	189.4	9.9	97.3
7	1.00	-1.00	196.0	213.0	202.6	200.8	203.1	7.2	51.2
8	0.26	0.96	215.8	192.3	196.4	194.0	199.6	11.0	119.0
9	1.00	-1.00	190.5	200.1	201.8	193.6	196.5	5.3	28.5
10	-0.06	-0.05	203.0	204.4	202.6	196.1	201.5	3.7	13.7
11	-1.00	1.00	160.5	194.3	185.1	159.7	174.9	18.0	306.0
12	-0.06	-0.04	200.2	188.0	201.3	204.5	198.5	7.2	52.3

The fitted response functions for process mean, standard deviation, and variance are found as follows:

$$\hat{\mu}(\mathbf{x}) = 200.50 + 8.75x_1 - 2.25x_2 - 4.31x_1x_2 - 17.11x_1^2 + 0.29x_2^2 \qquad (5.28)$$

$$\hat{\sigma}(\mathbf{x}) = 5.51 - 0.36x_1 + 2.11x_2 + 2.09x_1x_2 + 3.23x_1^2 + 2.59x_2^2 \qquad (5.29)$$

$$\widehat{\sigma^2}(\mathbf{x}) = 33.94 - 14.90x_1 + 41.66x_2 + 18.08x_1x_2 + 53.88x_1^2 + 37.15x_2^2 \qquad (5.30)$$

The *D*-optimal-design-embedded RPD model and the optimum operating conditions are shown in Tables 5.7 and 5.8, respectively. For this particular example, the optimal operating conditions from the proposed RPD model with $\hat{\sigma}(\mathbf{x})$ provide the smallest objective function value. Therefore, **x*** = (-0.104, -0.317).

Table 5.7: Proposed RPD Model

Given	$\mu_\tau = 195,\ LSL = 190,\ USL = 200,$ and $N = 12$	
Objective	Minimize	
	$\hat{\sigma}(\mathbf{x}) = 5.51 - 0.36x_1 + 2.11x_2 + 2.09x_1x_2 + 3.23x_1^2 + 2.59x_2^2$	
	or	
	$\widehat{\sigma^2}(\mathbf{x}) = 33.94 - 14.90x_1 + 41.66x_2 + 18.08x_1x_2 + 53.88x_1^2 + 37.15x_2^2$	
Subject to	$190 \le 200.50 + 8.75x_1 - 2.25x_2 - 4.31x_1x_2 - 17.11x_1^2 + 0.29x_2^2$	
	$200.50 + 8.75x_1 - 2.25x_2 - 4.31x_1x_2 - 17.11x_1^2 + 0.29x_2^2 \le 200$	
	$5.51 - 0.36x_1 + 2.11x_2 + 2.09x_1x_2 + 3.23x_1^2 + 2.59x_2^2 \ge 0$ for $\hat{\sigma}(\mathbf{x}) \ge 0$	
	$33.94 - 14.90x_1 + 41.66x_2 + 18.08x_1x_2 + 53.88x_1^2 + 37.15x_2^2$ for $\widehat{\sigma^2}(\mathbf{x}) \ge 0$	
	$0.0651x_1 + x_2 \le 1.003,\ 0.198x_1 + x_2 \le 1.020,$ $0.339x_1 + x_2 \le 1.057,\ 0.493x_1 + x_2 \le 1.116,$ $0.667x_1 + x_2 \le 1.203,\ 0.877x_1 + x_2 \le 1.331,$ $1.139x_1 + x_2 \le 1.517,\ 1.497x_1 + x_2 \le 1.801,$ $2.027x_1 + x_2 \le 2.262,\ 2.947x_1 + x_2 \le 3.115,$ $5.025x_1 + x_2 \le 5.128,\ 15.338\,x_1 + x_2 \le 15.384$	Outer linear constraints
	$x_1 + x_2 \ge -1.5$	Linear constraint
	$-1 \le x_i \le 1$ and $x_i \in \mathbb{R}\ (i = 1,\ 2)$	Boundary constraints
Find	Input variables $\mathbf{x}^* = [x_1^*,\ x_2^*]'$ and an objective function value of the model	

Table 5.8: Results of Each Model

Model	The dual response model	The MSE model	Proposed model with $\hat{\sigma}(\mathbf{x})$	Proposed model with $\widehat{\sigma^2}(\mathbf{x})$
Objective function	5.927	34.420	5.243	26.349
Optimal setting $(\mathbf{x}^*)$	(-0.374, -0.223)	(-0.336, -0.245)	(-0.104, -0.317)	(-0.124, -0.465)
Standard deviation	5.927	5.806	5.243	5.133
Bias	0.000	0.842	5.000	5.000

Conclusions

Due to potential safety concerns, physical processing constraints, or the scarcity of resources, all factor combinations may not be implemented when conducting the experiment. In such situations, standard experimental designs are practically ineffective and as a result, the experimental design space forms an asymmetric and irregular space. While *D*-optimal designs for a linearly-constrained irregular design space are available in the literature, perhaps, to the best of our knowledge, this study on the development of *D*-optimal design models and their associated RPD models for a nonlinearly-constrained experimental region is the first research attempt in the literature. The contribution of this chapter to the body of knowledge is threefold. First, the selection scheme of *D*-optimal design points and the exchange algorithm is proposed by using the outer linear approximation concept. Second, the feasibility and optimality conditions were developed. In particular, the proposed exchange algorithm can determine how many piecewise linear functions are required to meet the optimality condition. Finally, new RPD models were developed by linking the proposed exchange algorithm. We also proved that the proposed RPD model provides the global solutions.

The proposed methodology may have some limitations, which can serve as fruitful further research areas. First, the *D*-optimality criterion does not address the prediction variance to generate a measure of prediction performance. In this particular situation, the *I*-optimality criterion would be a suitable alternative for constructing optimal design points. Second, we assumed that nonlinear constraints form a convex set. Optimal designs for non-convex design spaces could be another future study. Finally, we consider a single quality characteristic in this chapter; however, incorporating multiple quality characteristics could be another potential future research area.

CHAPTER SIX

CONCLUSIONS AND FURTHER STUDIES

In this chapter, conclusions are drawn for solving response surface-based robust parameter design optimization problems considering both qualitative and quantitative input variables using special experimental designs and further studies are also discussed.

Concluding Remarks

Many RPD models have focused on continuous valued input variables in the literature. In this dissertation, response surface-based robust parameter optimization models were proposed to obtain robust optimal solutions for both qualitative and quantitative input variables using special experimental design methods. In Chapter III, a four-phased methodology was developed for finding optimal operating conditions with striving minimum bias and variance. It was also discussed that the Box-Behnken design was preferred over the other second-order designs, such as the traditional central composite design and three-level designs. The Box-Behnken design provides some important design properties, such as orthogonality, rotatability or near rotatability in order to maintain a consistent prediction variance over the design space. In addition, Box-Behnken design incorporated nonlinear mixed and pure integer programming optimization models were developed with the sequential quadratic integer programming and the Karush-Kuhn-Tucker method. The numerical example showed that the proposed integer programming model provided a better optimal solution when considering more variance reduction.

In Chapter IV, a response surface-based factorial design with pseudo-center points was proposed to attain optimal operating conditions for both quantitative and qualitative input variables. Compared to the existing RPD methods, such as the dual response and MSE methods, the proposed model may significantly reduce the process variation when determining optimal solutions of 0-1 MINLP problems, where other methods may not be tailored to satisfy the process requirements for RPD optimization problems. The three different solution methods, such as the outer approximation, branch-and-bound and hybrid nonlinear based branch-and-cut algorithms, were performed in order to increase computational efficiency and reduce computing time for convex or nonconvex problems. Further, an application of the proposed model was illustrated and its computational results with the three different solution algorithms were found. The numerical example showed that the outer approximation method for the proposed model might be superior to the traditional methods, such as the branch-and-bound algorithm, in finding an optimal solution efficiently.

Traditional experimental designs are not suitable to conduct experiments for nonlinearly-constrained irregular experimental design spaces due to safety concerns, process requirements and the scarcity of resources. In Chapter V, a *D*-optimal design was used to generate optimal design points with the proposed exchange algorithm as an efficient, fast and reliable method. In addition, *D*-optimal design embedded robust parameter design models were proposed to obtain global robust parameter design solutions for continuous-valued input variables. The proposed models resulted in more variance reduction than the traditional counterparts.

Finally, the proposed RSM-based RPD models in this dissertation may significantly decrease process variation for a wide range of many quality engineering problems while considering both qualitative and quantitative input variables using special experimental designs.

Further Studies

While we bridge the research gap between experimental designs and optimization models in this dissertation, there are a number of situations that may be unexplored. Therefore, we may make some possible extensions of the entire work. First, we considered single quality characteristic in the entire dissertation. In such situations, multiple quality characteristics would be considered to conduct special experimental designs. In addition, multi-criteria nonlinear programming models would be incorporated in order to obtain optimal operating conditions for input variables. Second, response surface design models are polynomial in nature due to second-order models. Indeed, second-order models are used in the response surface methodology due to flexibility, easy estimations and working well in solving real-world quality engineering problems. However, non-polynomial response functions would be another fruitful research area for some situations. Third, the ordinary least square method was used to generate unbiased estimators and statistics in regression analysis for the modelling phase. However, the weighed least square regression method would be useful for estimating the values of parameters in the model when the estimators have different weights. Finally, we would like to prioritize several objective functions for products and processes. Therefore, we would incorporate a nonlinear integer goal programming model as another fruitful research area in order to obtain optimal operating conditions for both qualitative and quantitative input variables using special experimental designs.

APPENDICES

Appendix A

Maple Codes for the Numerical Example in Chapter Three

Sequential quadratic programming solution for the proposed RPD model (Maple)

```
restart; with(Optimization);
f := proc (x1, x2, x3) options operator, arrow; (53.15+2.88*x1+4.07*x2+(-1)*.86*x3+(-
1)*.22*x1^2+4.82*x2^2+5.35*x3^2+(-1)*3.88*x1*x2+6.73*x1*x3+(-1)*2.25*x2*x3-
60)^2+101.87+22.29*x1+(-1)*3.47*x2+(-1)*34.45*x3+(-1)*10.01*x1^2+(-
1)*29.05*x2^2+21.08*x3^2+3.37*x1*x2+(-1)*30.84*x1*x3+(-1)*18.83*x2*x3 end
proc;
g1 := proc (x1, x2, x3) options operator, arrow; abs(53.15+2.88*x1+4.07*x2+(-
1)*.86*x3+(-1)*.22*x1^2+4.82*x2^2+5.35*x3^2+(-1)*3.88*x1*x2+6.73*x1*x3+(-
1)*2.25*x2*x3-60)-.6 end proc;
g2 := proc (x1, x2, x3) options operator, arrow; 101.87+22.29*x1+(-1)*3.47*x2+(-
1)*34.45*x3+(-1)*10.01*x1^2+(-1)*29.05*x2^2+21.08*x3^2+3.37*x1*x2+(-
1)*30.84*x1*x3+(-1)*18.83*x2*x3-144 end proc;
g3 := proc (x1, x2, x3) options operator, arrow; x1^2+x2^2+x3^2-3 end proc;
g4 := proc (x1, x2, x3) options operator, arrow; -1-x1 end proc;
g5 := proc (x1, x2, x3) options operator, arrow; -1+x1 end proc;
g6 := proc (x1, x2, x3) options operator, arrow; -1-x2 end proc;
g7 := proc (x1, x2, x3) options operator, arrow; -1+x2 end proc;
g8 := proc (x1, x2, x3) options operator, arrow; -1-x3 end proc;
g9 := proc (x1, x2, x3) options operator, arrow; -1+x3 end proc;
m := NLPSolve(f(x1, x2, x3), [g1(x1, x2, x3) <= 0, g2(x1, x2, x3) <= 0, g3(x1, x2, x3)
<= 0, g4(x1, x2, x3) <= 0, g5(x1, x2, x3) <= 0, g6(x1, x2, x3) <= 0, g7(x1, x2, x3) <= 0,
g8(x1, x2, x3) <= 0, g9(x1, x2, x3) <= 0], method = sqp, output = solutionmodule);
m:-Results()
```

Karush-Kuhn-Tucker points for the proposed RPD model (Maple)

```
restart; with(VectorCalculus); with(LinearAlgebra); with(Optimization);
f := proc (x1, x2, x3) options operator, arrow; (53.15+2.88*x1+4.07*x2+(-1)*.86*x3+(-
1)*.22*x1^2+4.82*x2^2+5.35*x3^2+(-1)*3.88*x1*x2+6.73*x1*x3+(-1)*2.25*x2*x3-
60)^2+101.87+22.29*x1+(-1)*3.47*x2+(-1)*34.45*x3+(-1)*10.01*x1^2+(-
1)*29.05*x2^2+21.08*x3^2+3.37*x1*x2+(-1)*30.84*x1*x3+(-1)*18.83*x2*x3 end
proc;
NULL;
Delf := unapply(Gradient(f(x1, x2, x3), [x1, x2, x3]), [x1, x2, x3]);
NULL;
g1 := proc (x1, x2, x3) options operator, arrow; 53.15+2.88*x1+4.07*x2+(-1)*.86*x3+(-
1)*.22*x1^2+4.82*x2^2+5.35*x3^2+(-1)*3.88*x1*x2+6.73*x1*x3+(-1)*2.25*x2*x3-
60-.6 end proc;
```

```
g2 := proc (x1, x2, x3) options operator, arrow; -53.15+(-1)*2.88*x1+(-
1)*4.07*x2+.86*x3+.22*x1^2+(-1)*4.82*x2^2+(-1)*5.35*x3^2+3.88*x1*x2+(-
1)*6.73*x1*x3+2.25*x2*x3+60-.6 end proc;
g3 := proc (x1, x2, x3) options operator, arrow; 101.87+22.29*x1+(-1)*3.47*x2+(-
1)*34.45*x3+(-1)*10.01*x1^2+(-1)*29.05*x2^2+21.08*x3^2+3.37*x1*x2+(-
1)*30.84*x1*x3+(-1)*18.83*x2*x3-144 end proc;
g4 := proc (x1, x2, x3) options operator, arrow; x1^2+x2^2+x3^2-3 end proc;
g5 := proc (x1, x2, x3) options operator, arrow; -1-x1 end proc;
g6 := proc (x1, x2, x3) options operator, arrow; -1+x1 end proc;
g7 := proc (x1, x2, x3) options operator, arrow; -1-x2 end proc;
g8 := proc (x1, x2, x3) options operator, arrow; -1+x2 end proc;
g9 := proc (x1, x2, x3) options operator, arrow; -1-x3 end proc;
g10 := proc (x1, x2, x3) options operator, arrow; -1+x3 end proc;
g := proc (x1, x2, x3) options operator, arrow; `<,>`(g1(x1, x2, x3), g2(x1, x2, x3), g3(x1,
x2, x3), g4(x1, x2, x3), g5(x1, x2, x3), g6(x1, x2, x3), g7(x1, x2, x3), g8(x1, x2, x3),
g9(x1, x2, x3), g10(x1, x2, x3)) end proc; g(x1, x2, x3);
#Enter vector-valued constraint function.
lambda := `<,>`(lambda1, lambda2, lambda3, lambda4, lambda5, lambda6, lambda7,
lambda8, lambda9, lambda10);
L := unapply(f(x1, x2, x3)+Transpose(lambda) . g(x1, x2, x3), [x1, x2, x3, lambda1,
lambda2, lambda3, lambda4, lambda5, lambda6, lambda7, lambda8, lambda9,
lambda10]);
L(x1, x2, x3, lambda1, lambda2, lambda3, lambda4, lambda5, lambda6, lambda7,
lambda8, lambda9, lambda10);
LG := Gradient(L(x1, x2, x3, lambda1, lambda2, lambda3, lambda4, lambda5, lambda6,
lambda7, lambda8, lambda9, lambda10), [x1, x2, x3]);
CS := seq(g(x1, x2, x3)[i]*lambda[i] = 0, i = 1 .. 10);
solutions := evalf(solve({CS, LG[1] = 0, LG[2] = 0, LG[3] = 0}, {lambda1, lambda2,
lambda3, lambda4, lambda5, lambda6, lambda7, lambda8, lambda9, x1, x2, x3,
lambda10})); n := nops([solutions]);
NULL;
for i to n do print(i, subs(solutions[i], g(x1, x2, x3)), subs(solutions[i], [`l&lambda;1`,
lambda2, lambda3, lambda4, lambda5, lambda6, lambda7, lambda8, lambda9,
lambda10])) end do;
k := 16;
        #The sixteenth solution is both feasible and satisfies multiplier conditions.
solution := solutions[k]; #The KKT point for the RPD model.
```

Appendix B

BONMIN Codes for the Numerical Example in Chapter Four

Branch-and-Bound Method code for the proposed RPD model

```
reset;
var z binary;
var x{1..3} >=-1 <= 1;
minimize MSE: (19.986 - 0.076 * x[1] + 0.023 * x[2] - 0.027 * x[3] + 0.12 * x[1]^2 -
0.018 * x[1] * x[2] - 0.006 * x[1] * x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] +
0.072*z*x[2] - 0.037*z*x[3] -20)^2 + 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] +
0.062*x[1]^2 - 0.041*x[1]*x[2] + 0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z -
0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3];
subject to
c1: 19.986 - 0.076 * x[1] + 0.023 * x[2] - 0.027 * x[3] + 0.12 * x[1]^2 - 0.018 * x[1] *
x[2] - 0.006 * x[1] * x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] + 0.072*z*x[2] -
0.037*z*x[3] <= 20.5 ;
c2: 19.986 - 0.076*x[1] + 0.023*x[2] - 0.027*x[3] + 0.12*x[1]^2 - 0.018*x[1]*x[2] -
0.006*x[1]*x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] + 0.072*z*x[2] -
0.037*z*x[3] >= 19.5 ;
c3: 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] + 0.062*x[1]^2 - 0.041*x[1]*x[2] +
0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z - 0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3]
<=0.02 ;
c4: 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] + 0.062*x[1]^2 - 0.041*x[1]*x[2] +
0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z - 0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3]
>=0 ;
options solver bonmin;
option bonmin_options "bonmin.algorithm B-BB";
solve;
display x;
display z;
```

Hybrid branch-and-cut code for the proposed RPD model

```
reset;
var z binary;
var x{1..3} >=-1 <= 1;
minimize mse: (19.986 - 0.076 * x[1] + 0.023 * x[2] - 0.027 * x[3] + 0.12 * x[1]^2 -
0.018 * x[1] * x[2] - 0.006 * x[1] * x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] +
0.072*z*x[2] - 0.037*z*x[3] -20)^2 + 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] +
0.062*x[1]^2 - 0.041*x[1]*x[2] + 0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z -
0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3];
subject to
```

```
c1: 19.986 - 0.076 * x[1] + 0.023 * x[2] - 0.027 * x[3] + 0.12 * x[1]^2 - 0.018 * x[1] *
x[2] - 0.006 * x[1] * x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] + 0.072*z*x[2] -
0.037*z*x[3] <= 20.5 ;
c2: 19.986 - 0.076*x[1] + 0.023*x[2] - 0.027*x[3] + 0.12*x[1]^2 - 0.018*x[1]*x[2] -
0.006*x[1]*x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] + 0.072*z*x[2] -
0.037*z*x[3] >= 19.5 ;
c3: 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] + 0.062*x[1]^2 - 0.041*x[1]*x[2] +
0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z - 0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3]
<=0.02 ;
c4: 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] + 0.062*x[1]^2 - 0.041*x[1]*x[2] +
0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z - 0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3]
>=0 ;

options solver bonmin;
option bonmin_options "bonmin.algorithm B-Hyb";
solve;
display x;
display z;
```

Outer Approximation code for the proposed RPD model

```
reset;
var z binary;
var x{1..3} >=-1 <= 1;
var u;
var n >=0;
minimize mse: n;
subject to
c1: n>=(u)^2 + 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] + 0.062*x[1]^2 -
0.041*x[1]*x[2] + 0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z - 0.01*z*x[1] -
0.034*z*x[2] - 0.05*z*x[3];
c2: u <= 0.5 ;
c3: u >= -0.5 ;
c4: 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] + 0.062*x[1]^2 - 0.041*x[1]*x[2] +
0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z - 0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3]
<=0.02 ;
c5: 0.126 + 0.046*x[1] - 0.057*x[2] - 0.032*x[3] + 0.062*x[1]^2 - 0.041*x[1]*x[2] +
0.02*x[1]*x[3] + 0.031*x[2]*x[3] + 0.006*z - 0.01*z*x[1] - 0.034*z*x[2] - 0.05*z*x[3]
>=0 ;
c6: 19.986 - 0.076 * x[1] + 0.023 * x[2] - 0.027 * x[3] + 0.12 * x[1]^2 - 0.018 * x[1] *
x[2] - 0.006 * x[1] * x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] + 0.072*z*x[2] -
0.037*z*x[3]-20<=u;
```

```
c7: 19.986 - 0.076 * x[1] + 0.023 * x[2] - 0.027 * x[3] + 0.12 * x[1]^2 - 0.018 * x[1] *
x[2] - 0.006 * x[1] * x[3] - 0.03*x[2]*x[3] + 0.03*z - 0.076*z*x[1] + 0.072*z*x[2] -
0.037*z*x[3]-20>=u;

options solver bonmin;
option bonmin_options "bonmin.algorithm B-OA";
solve;
display x;
display z;
display u;
display n;
```

Appendix C

MATLAB Codes and JMP Procedures in Chapter Five

Nonlinearly-constrained irregular experimental design space codes/procedures

MATLAB Codes

The proposed algorithm

The first iteration

```
nfactors=2;
nruns=12;
f1=@(x) [x]*[0.707;0.707]<1|[x]*[0;1]<1|[x]*[1;0]<1; %The linearized constraints
bnds=[-1 -1;1 1];
x=sortrows(cordexch(nfactors,nruns,'quadratic',’tries’,100000,'bounds',bnds,'levels',101,'e
xcl',f1))
```

The second iteration

```
nfactors=2;
nruns=12;
f2=@(x) [x]*[0.414;1]<1.082|[x]*[2.414;1]<2.613|[x]*[0;1]<1|[x]*[1;0]<1;
bnds=[-1 -1;1 1];
x=sortrows(cordexch(nfactors,nruns,'quadratic','tries',100000,'bounds',bnds,'levels',101,'e
xcl',f2))
```

The third iteration

```
nfactors=2;
nruns=12;
f3=@(x)
[x]*[0.198;1]<1.020|[x]*[0.667;1]<1.203|[x]*[1.497;1]<1.801|[x]*[5.025;1]<5.128|[x]*[0
;1]<1|[x]*[1;0]<1;
bnds=[-1 -1;1 1];
x=sortrows(cordexch(nfactors,nruns,'quadratic','tries',100000,'bounds',bnds,'levels',101,'e
xcl',f3))
```

The fourth iteration

```
nfactors=2;
nruns=12;
f4=@(x)
[x]*[0.0974;1]<1.005|[x]*[0.303;1]<1.046|[x]*[0.534;1]<1.135|[x]*[0.820;1]<1.293|[x]*[
1.217;1]<1.577|[x]*[1.870;1]<2.123|[x]*[3.297;1]<3.448|[x]*[10.153;1]<10.204|[x]*[0;1
]<1|[x]*[1;0]<1;
bnds=[-1 -1;1 1];
```

```
x=sortrows(cordexch(nfactors,nruns,'quadratic','tries',100000,'bounds',bnds,'levels',101,'e
xcl',f4))
```

The fifth iteration

```
nfactors=2;
nruns=12;
f5=@(x)
[x]*[0.0651;1]<1.003|[x]*[0.198;1]<1.020|[x]*[0.339;1]<1.057|[x]*[0.493;1]<1.116|[x]*[
0.667;1]<1.203|[x]*[0.877;1]<1.331|[x]*[1.139;1]<1.517|[x]*[1.497;1]<1.801|[x]*[2.027
;1]<2.262|[x]*[2.947;1]<3.115|[x]*[5.025;1]<5.128|[15.338;1]<15.384|[x]*[0;1]<1|[x]*[1
;0]<1;
bnds=[-1 -1;1 1];
x=sortrows(cordexch(nfactors,nruns,'quadratic','tries',100000,'bounds',bnds,'levels',101,'e
xcl',f5))
```

JMP Procedure

The proposed algorithm

1. Select DOE>Custom Design
2. Select Custom Design>Optimality Criterion>Make D-Optimal Design
3. Select Custom Design>Number of Starts and then enter “100000”
4. Add the number of input variables and click continue
5. Select Define Factor Constraints>Specify Linear Constraints Then Enter the outer linear constraints
6. Select Model>RSM
7. Select Design Generation>Number of Runs and then Enter the number of points defined
8. Click Make Design
9. Select Design Evaluation>Run Order>Keep the Same>Make Table
10. Check the optimality and feasibility conditions
    a. If the design is optimal, then stop.
    b. Otherwise go to Step 1.

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