NEW APPROACHES TO DESIRABILITY FUNCTIONS BY NONSMOOTH AND NONLINEAR OPTIMIZATION

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ABSTRACT

NEW APPROACHES TO DESIRABILITY FUNCTIONS
BY NONSMOOTH AND NONLINEAR OPTIMIZATION

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Desirability Functions continue to attract attention of scientists and researchers working in the area of multi-response optimization. There are many versions of such functions, differing mainly in formulations of individual and overall desirability functions. Derringer and Suich's desirability functions being used throughout this thesis are still the most preferred ones in practice and many other versions are derived from these. On the other hand, they have a drawback of containing nondifferentiable points and, hence, being nonsmooth. Current approaches to their optimization, which are based on derivative-free search techniques and modification of the functions by higher-degree polynomials, need to be diversified considering opportunities offered by modern nonlinear (global) optimization techniques and related softwares. A first motivation of this work is to develop a new efficient solution strategy for the maximization of overall desirability functions which comes out to be a nonsmooth composite constrained optimization problem by nonsmooth optimization methods.

We observe that individual desirability functions used in practical computations are of min-type, a subclass of continuous selection functions. To reveal the mechanism that gives rise to a variation in the piecewise structure of desirability functions used in practice, we concentrate on a component-wise and generically piecewise min-type functions and, later on, max-type

functions. It is our second motivation to analyze the structural and topological properties of desirability functions via piecewise max-type functions.

In this thesis, we introduce adjusted desirability functions based on a reformulation of the individual desirability functions by a binary integer variable in order to deal with their piecewise definition. We define a constraint on the binary variable to obtain a continuous optimization problem of a nonlinear objective function including nondifferentiable points with the constraints of bounds for factors and responses. After describing the adjusted desirability functions on two well-known problems from the literature, we implement modified subgradient algorithm (MSG) in GAMS incorporating to CONOPT solver of GAMS software for solving the corresponding optimization problems. Moreover, BARON solver of GAMS is used to solve these optimization problems including adjusted desirability functions. Numerical applications with BARON show that this is a more efficient alternative solution strategy than the current desirability maximization approaches.

We apply negative logarithm to the desirability functions and consider the properties of the resulting functions when they include more than one nondifferentiable point. With this approach we reveal the structure of the functions and employ the piecewise max-type functions as generalized desirability functions (GDFs). We introduce a suitable finite partitioning procedure of the individual functions over their compact and connected interval that yield our so-called GDFs. Hence, we construct GDFs with piecewise max-type functions which have efficient structural and topological properties. We present the structural stability, optimality and constraint qualification properties of GDFs using that of max-type functions.

As a by-product of our GDF study, we develop a new method called two-stage (bilevel) approach for multi-objective optimization problems, based on a separation of the parameters: in $\mathbf{y}$-space (optimization) and in $\mathbf{x}$-space (representation). This approach is about calculating the factor variables corresponding to the ideal solutions of each individual functions in $\mathbf{y}$, and then finding a set of compromised solutions in $\mathbf{x}$ by considering the convex hull of the ideal factors. This is an early attempt of a new multi-objective optimization method. Our first results show that global optimum of the overall problem may not be an element of the set of compromised solution.

The overall problem in both $\mathbf{x}$ and $\mathbf{y}$ is extended to a new refined (disjunctive) generalized semi-infinite problem, herewith analyzing the stability and robustness properties of the objective function. In this course, we introduce the so-called robust optimization of desirability functions for the cases when response models contain uncertainty. Throughout this thesis, we give several modifications and extensions of the optimization problem of overall desirability functions.

Keywords: desirability functions, nonsmooth optimization, nonlinear programming, differential topology, multi-objective optimization

ÖZ

ÇEKİCİLİK FONKSİYONLARINA PÜRÜZLÜ VE DOĞRUSAL OLMAYAN OPTİMİZASYON YÖNTEMLERİ İLE YENİ YAKLAŞIMLAR

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Çekicilik fonksiyonları, çok yanıtlı optimizasyon alanında çalışan bilim adamları ve araştırmacıların ilgisini çekmeye devam etmektedir. Tekil ve toplam çekicilik fonksiyonlarının farklı formülasyonu ile elde edilmiş çok çeşitli çekicilik fonksiyonu vardır. Derringer ve Suich tarafından geliştirilen ve bu tezde kullanılan fonksiyonlar hala pratikte en çok tercih edilen ve farklı versiyonları türetilmiş fonksiyonlardır. Diğer taraftan bunlar türevlenemeyen noktalar içermektedir ve bu nedenle pürüzlü fonksiyonlardır. Bu fonksiyonların optimizasyonu için türevsiz arama teknikleri ve türevlenemeyen noktalarını gidermek için o noktada yüksek dereceli polinomlarla değiştirilmeleri gibi yaklaşımlar mevcuttur. Bu yaklaşımların modern doğrusal olmayan optimizasyon teknikleri ve ilgili yazılımlarla çeşitlendirilmesi gerekmektedir.

Bu tezin çıkış noktası pürüzlü birleşik kısıtlı bir optimizasyon problemi olan toplam çekicilik fonksiyonunu en büyüklenmesi icin yeni etkili bir çözüm yolu geliştirmekir. İkinci önemli nokta pratikte kullanılan fonksiyonların çeşitliliğine neden olan parçalı yapıyı açığa çıkarmak tır. Bu amaçla min-tipi ve max-tipi fonksiyonlar üzerinde yoğunlaşılmıştır.

Bu tezde, tekil çekicilik fonksiyonlarının parçalı yapısının yarattığı zorluğu gidermek amacıyla, problemin ikili bir tam sayı ile yeniden formüle edilmesine dayanan ayarlı çekicilik fonksiyonları tanıtılmıştır. Bu değişiklikler yapıldıktan sonra, doğrusal olmayan amaç fonksiyonu türevlenemeyen noktalar içeren ve faktörlerin ve yanıtların sınırları ile, ikili değişkene ait bir kısıt içeren sürekli bir optimizasyon problemi elde edilir. Ayarlı çekicilik fonksiyonlarını iki çok bilinen örnek üzerinde açıklandıktan sonra, optimizasyon problemini çözmek icin Değiştirilmiş Altgradyan Algoritması, GAMS ortamında yazılarak CONOPT çözücüyle birlikte kullanılmıştır. GAMS ortamının BARON çözücüsü de bu problemlerdeki ayarlı çekicilik fonksiyonlarının optimizasyonu için çalıştırılmıştır. Bu iki örnek üzerinde BARON kullanılarak yapılan uygulama ile bu yaklaşımın var olan çekicilik fonksiyonu maximizasyonu yaklaşımlarımdan daha etkili bir alternatif çözüm yöntemi olduğu gösterilmiştir.

Toplam çekicilik fonksiyonlarının optimizasyon problemlerinin bazı değişik formülasyonları gösterilmiş ve sonra sonlu bir ayrıştırma yöntemi geliştirilerek genelleştirilmiş çekicilik fonksiyonları elde edilmiştir. Bu fonksiyonları oluşturmada parçalı max-tipi fonksiyonlar kullanılmış ve bunların bazı yapısal ve topolojik özellikleri tanımlanmıştır.

Bunlara ek olarak, çok yanıtlı optimizasyon problemleri için İki Aşamalı Yaklaşım yöntemi önerilmiştir. Bu yöntem parametrelerin ayrıştırılması ile toplam problemin optimizasyon (y-uzayında) ve temsil (x-uzayında) şeklinde ayrıştırılmasına dayanmaktadır. Toplam problem genelleştirilmiş yarı-sonsuz bir problem haline getirilerek yanıtlı modellerindeki belirsizliğe karşı sağlamlaştırılmıştır.

Anahtar Kelimeler: çekicilik fonksiyonları, pürüzlü optimizasyon, doğrusal olmayan programlama, diferansiyel topoloji, çok amaçlı optimizasyon

To Caner Öztürk

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"Every day I remind myself that my inner and outer life are based on the labors of other men,
living and dead, and that I must exert myself in order to give in the same measure
as I have received and am still receiving."
Albert Einstein

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PREFACE

After dealing with nonsmoothness in some important data mining models, initially nonsmooth optimization and later nonsmooth analysis became two of my major research interests. This thesis is about our nonsmooth optimization facilities on a specific type of function from multi-response optimization called as desirability functions.

When we observed that nonsmoothness was a challenging issue in desirability functions and nonsmooth optimization had never been considered for maximizing these functions, this study began. We considered to carry out an application with BARON, a global optimization solver of GAMS for nonconvex and nonsmooth problems, which is shown to be very suitable for our problems. By some inquiries, we understood that an application with modified subgradient algorithm (MSG), a nonsmooth and nonconvex approach, could have been a good alternative to our application with BARON and results would be explained in comparison. As a next step to this application, we considered optimization of desirability functions including more than one nondifferentiable functions by employing our adjusted desirability functions approach.

Another observation about desirability functions was their min-type character. This gave born to the idea of analyzing a suitable abstract class of piecewise smooth functions that would be considered as a generalization of desirability functions. This is shown to be possible generically. As a by-product of this idea, based on this generalization process, we proposed a new approach which yields a set of compromised solutions for multi-response problems.

With this study, we extend the theory of desirability functions with nonsmooth, nonlinear and semi-infinite optimization. During this study, Morse theory, differential topology, robust optimization and multi-objective optimization entered in our scope. There are interesting future works with these topics to go beyond of our current study.

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CHAPTER 1

INTRODUCTION

Most industrial processes, products and systems have more than one quality response; they are usually conflicting but should be optimized concurrently and concertedly. For quality improvement, optimal levels of product, process or system variables (input variables, or factors) are searched which give the best synthesis of these responses (output variables). This problem is known as a *multi-response optimization problem*. In quality terminology, decision variables are called factors and dependent variables are called responses of the problem.

In fields other than quality, instead of the word response, different words such as property, criteria, characteristic or objective are used to refer to the output variables. According to these words, the problem of simultaneously optimizing the output variables is called *multi-criteria optimization* (MCO), *multi-objective optimization* (MOO) or *vector optimization* problem. In some scientific communities, special names were introduced, such as *Tikhonov regularization* which have a similar meaning, too. All of these problems under different names and their solution strategies have common properties and can be seen as special cases of each other.

Most commonly used approaches to solve the multi-response problems include *response surface methodology* (*RSM*), *Taguchi method*, *loss functions*, *Mahalanobis distance* and *desirability functions* [57, 70, 75, 77]. Each of these approaches has its own strengths and limitations.

One of the main steps in multi-response optimization is experimental design [77], which is commonly used to collect data for developing products and processes, robust to different sources of variability. It is important to plan and conduct experiments to analyze the resulting data in such a manner that valid and effective conclusions are obtained. In an experimental design, the first step consists of defining the problem, then the factors together with their ranges and specific levels, at which experiments runs will be made, are chosen. The next step is the selection of the responses according to the information they provide. Finally, the choice of an appropriate experimental design is made.

Throughout an experimental design, data are collected and the estimated response models are obtained that relate the factors to the responses. The most common way of obtaining the response models is *regression* by means of *polynomial fitting* or *spline fitting*. For the cases where polynomial fitting is not capable of modeling the quantitative and qualitative responses, *artificial neural networks* have became highly preferred, too.

By optimizing all response functions of a process or product simultaneously, we expect to find the best trade-off within these responses. Here, a difficulty arises because as one response is improved, it is often done at the expense of one or more other responses. This is the reason for the definition of optimality in multi-response optimization being different from the one used in a single-response case.

Another issue arising in computations during optimization of responses at the same time is that each of them may have a different measurement scale. The so-called *scalarization techniques* offer ways to handle different scales of responses by transforming them to scale-free values and then converting multiple objectives into a single objective called the *overall desirability* by an aggregation technique. *Linear scalarization* techniques are sum-based aggregations, in fact, usually convex combinations of different objectives [32]. Desirability functions approach is a *nonlinear scalarization* technique converting a multi-objective problem into a maximization problem with a single objective of the overall desirability which is the geometrical mean of the individual desirability values of different objectives [25, 44].

In this thesis, although we deal with multi-response problems, multi-response optimization is accepted as a multi-objective optimization and we combine notions from each of these areas when necessary in our analyses and method developments. We are mainly interested in revealing mathematical infrastructure of desirability functions to propose alternative methods for their optimization.

Scalarization with *desirability functions* is based on the following idea: when one of the responses of an industrial process or product or a system with many responses is not in the desired limits, then the overall response of the system is not desirable. In this thesis, we focus on different aspects of optimization of desirability functions of Derringer and Suich's [25] type. The optimization problem of these functions is a constrained problem with bounds of factors and responses. This optimization is a challenging task because of the fact that the overall desirability function is a composite, nonsmooth and nonlinear function of a multiplicative form.

The studies about finding optimal points of *nonsmooth functions*, explaining their foundations and topological properties, have been noticeable in the area of nonsmooth optimization. These functions are usually nonsmooth at some points, i.e., we do not have the gradient information of these functions at those points so that the gradient-based optimization methods like steepest-descent methods, Newton methods, and so on, are not applicable for solving the optimization problems including these functions. Some important classes of nonsmooth functions such as (nondifferentiable) convex functions and Lipschitz continuous functions have the concept of directional derivative, giving rise to the subgradient information as a set-valued derivative replacing the gradient information [17, 86].

Nonsmooth optimization methods such as subgradient method and bundle methods are applicable on these classes. When we do not have convexity and local Lipschitzness, there is a rich theory of optimization of nonsmooth functions with very few assumptions [4, 6, 14, 48, 56, 78, 87]. In practical application, it becomes important to choose the most suitable method for the optimization of functions lacking "nice" properties such as convexity and local Lipschitzness.

1.1 Preliminaries

In this study, $\mathbb{R}^n$ represents the n-dimensional real Euclidean space with the usual inner (i.e., scalar) product $< \mathbf{x}, \mathbf{y} >= \mathbf{x}^T\mathbf{y} = \sum_{i=1}^{n} x_i y_i$ and the Euclidean norm $||\mathbf{x}||_2 = \sqrt{(\mathbf{x}, \mathbf{x})} = (\mathbf{x}^T\mathbf{x})^{\frac{1}{2}}$, where "$T$" stands for transpose, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ where $x_i, y_i \in \mathbb{R}$ are the ith components of the vectors $\mathbf{x}$ and $\mathbf{y}$, respectively. We denote by $\mathbf{0}_m = (0, 0, \ldots, 0)^T$ and $\mathbf{1}_m = (1, 1, \ldots, 1)^T$ the zero vector and the one vector, respectively, of some dimension m according to the context. All the vectors are considered as column vectors. The space of continuously differentiable real-valued functions will be represented by $C^1(\mathbb{O})$, while $C^2(\mathbb{O})$ will comprise the 2-times continuously differentiable real-valued functions, and $C^k(\mathbb{O})$ is the space of the k-times continuously differentiable real-valued functions f on $\mathbb{O}$ ($k \geq 1$) with $\mathbb{O} \subseteq \mathbb{R}^n$ being some given, nonempty and open set.

We stay in $\mathbb{R}^n$ throughout our study mainly because many optimization problems in practice are defined in $\mathbb{R}^n$ or can be approximated by a problem defined in $\mathbb{R}^n$. Moreover, our functions will be scalar-valued and our treatment will be with first- and second-order differentiability notions. The vector-valued functions and differentiability notions of higher order makes the problem more complicated and cannot be discussed in this framework.

1.2 Outline of the Thesis

This thesis is about dealing with nonsmoothness of desirability functions with nonsmooth optimization approaches. We make necessary modifications in the desirability maximization problem and apply suitable methods which consider the nondifferentiability in our functions. We show all the details of our modifications and the efficiency of our approach on numerical experiments.

Min-type character of the individual desirability functions which are being used in practical applications and then max-type logarithmic individual functions are studied. We analyze main topological properties, structural stability of our functions, optimality conditions and constraint qualifications within an abstract class of piecewise smooth functions. This is a kind of generalization process of the individual desirability functions and is shown to be possible generically. Based on this process, we propose a new approach which results with a set of compromised solutions for multi-response problems.

In Chapter 2, we present the necessary background information for our computational, structural and topological methods. We provide a reasoning for our interest in *Derringer and Suich's desirability functions* and their optimization with a mathematical point of view as well as an overview of the current approaches to their optimization problems. There are different research groups working on nonsmooth optimization, as a result, there are many theories to handle the nonsmooth function classes and their problems. We have deeply studied most of these theories and analyzed their problem solving potential related with our research, rigorously discussed and tried to find the best methods and approaches for the applications on desirability optimization problem. A summary of the existing nonsmooth optimization approaches with the derivative tools on which they are based is given. This background information related with desirability functions and nonsmooth optimization is necessary for Chapters 3 and 4.

In Chapter 3, we show that by taking the convex combination of the "sides" of an individual desirability function, one can get rid of the piecewise formulation of the function. This is done by a binary integer variable representing the activeness of the sides of the function and we call an individual desirability function expressed like this an *adjusted individual desirabil-*

ity functions. Then, we convert the formulation of the overall desirability maximization from a $0-1$ *mixed-integer nonlinear problem* to a continuous one by adding a constraint for the binary variable. The resulting problem with the constraints of bounds for factors and responses together with the constraint for the binary variable is a nonlinear continuous optimization problem with an objective function including nondifferentiable points. We demonstrate details of this approach on two classical multi-response problems taken from the literature: one of which includes only two-sided desirability functions and the other includes both one-sided and two-sided functions. We reformulate the overall desirability functions for both problems and solve the resulting optimization problems by *BARON* solver of *GAMS* and *modified subgradient algorithm* (*MSG*) implemented in GAMS together with *CONOPT* solver. We compare and discuss the results.

In Chapter 4, we analyze the weighted desirability functions using concepts and approaches of nonsmooth optimization. Two techniques are proposed for preventing the responses from being undesirable. The first technique forms the basis for ϵ-individual desirability functions. By employing this technique, we transform the multiplicative form of overall desirability functions into an additive form by applying the natural logarithm and make some modifications of the optimization problem of overall desirability functions. The second technique is about locally cutting-off the undesirable points from the interval of a response by a $\epsilon - \delta$ argument. We show the advantage of the first and the disadvantage of the second method in transforming our problem into an additive form for our further analysis. We write the optimization problem of overall desirability function when individual desirability functions include a finite number of nondifferentiable points as in adjusted desirability functions. By using the separability of this overall function together with the Chain Rule for nonsmooth Lipschitz functions, we give a necessary optimality condition for the global optimal of the overall problem using *Clarke subdifferential* for this new problem. Moreover, we analyze the Pareto-optimality of the global solution of the weighted additive overall problem.

In Chapter 5, we propose and develop a finite partitioning procedure of the individual desirability functions over their compact and connected interval which leads to the definition of *generalized desirability functions* (GDFs). We call the negative logarithm of an individual desirability function having a max-type structure and including a finite number of nondifferentiable points as a *generalized individual desirability function*. By introducing *continuous selection functions* into desirability functions and, especially, employing *piecewise max-type* *functions*, it is possible to describe some structural and topological properties of these generalized functions. Our aim with this generalization is to show the mechanism that gives rise to a variation and extension in the structure of functions used in classical desirability approaches. Moreover, we propose a new method called as two-stage (bilevel) approach for multi-response optimization problems based on a separation of the parameters as **y**-space (optimization) and **x**-space (representation). We obtain a set of compromised solution for multi-response problems with this method, however, globality is not guaranteed yet. This new method may be seen as an early attempt of a future study

In Chapter 6, we consider the effects and scientific opportunities of employing semi-infinite max-type functions on the structure of the generalized individual functions instead of the finite max-type continuous selections. Furthermore, the overall problem in both **x** and **y** are shown to be extended to a refined *generalized semi-infinite problem*, herewith analyzing the stability and robustness properties of the objective function. In this context, we introduce the so-called *robust desirability functions* for the cases when response models contain uncertainty, and we study the structure of the response functions.

In Chapter 7, our conclusions and outlook to future works can be found. Further aspects of Morse theory for piecewise max-type functions and a characterization of structural stability of the optimization problem in the variable **x** may proceed. It will be interesting to analyze the reformulated and extended desirability functions which we present throughout this thesis, through a multi-objective optimization research.

CHAPTER 2

A SURVEY OF DESIRABILITY FUNCTIONS AND NONSMOOTH OPTIMIZATION

2.1 Desirability Functions Approach

Desirability functions approach is the general name used for methods of multi-response problems which assign a scale-free value to all responses in the problem by the so-called *individual desirability functions* and then aggregate these values by taking their geometric mean to obtain the overall desirability function yielding a single objective problem. This approach was originally introduced by Harrington [44]. Then another version was developed by Derringer and Suich [25] which has been the one widely used in the literature, although it has the drawback of containing nondifferentiable points. In that study, the overall desirability function, namely, the geometric mean of linear individual desirability functions, is optimized by a univariate search technique which does not use any derivative information of the function. Later, a weighted case of these desirability functions was proposed by Derringer [25].

Castillo et al. [19] demonstrate a modified version of the Derringer and Suich's desirability functions for the linear case based on polynomial approximations of the individual desirability functions at their nondifferentiable points. Then, the optimization problem of the overall desirability function obtained from the geometric mean of the smoothed functions is solved by a generalized reduced gradient (GRG) method.

Other than these conventional desirability function studies, there are also approaches based on different formulations of desirability functions. The one introduced by Kim and Lin [59] solves a *maxmin* problem of maximizing the minimum degree of satisfaction which is based on an alternative formulation of the individual desirability functions. In the approach proposed by Ch'ng et al. [16], an aggregation technique is used different than the geometric mean to compute the overall desirability function from the individual ones including no non-differentiable points by a change of variables in the functions.

Jeong and Kim recently introduced interactive desirability functions approach in [49] which takes into account the preference of the decision maker on the trade-offs among the responses or on the shape, bound and target of a desirability function. The approach delivered in Khuri and Conlon [58] is similar to desirability functions in the sense of transforming the problem to look for a compromised optimum, which is called as the *generalized distance approach*.

The philosophy behind the desirability functions approach is that when one of the quality characteristics of an industrial process or product with many characteristics is not in the desired limits, then the overall quality of the industrial process or the product is not desirable. In this section, we provide a mathematical point of view on desirability functions with a survey of the current approaches to their optimization problem.

2.1.1 Desirability Functions of Derringer and Suich Type

In a multi-response optimization problem, a response $Y(\mathbf{x})$ is a function $Y : \mathbb{R}^n \rightarrow \mathbb{R}$ of vector of controllable factors or independent variables $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$, where $x_i \in \mathbb{R}$ $(i = 1, 2, \ldots, n)$. An individual desirability function $d(Y(\mathbf{x}))$ scales a response into the interval $[0, 1]$, i.e., $d : \mathbb{R} \rightarrow [0, 1]$. This means that the function d becomes 0 for completely undesirable values of response, and it becomes 1 for totally desirable values of the response.

We notice that desirability functions are composite functions, and we denote desirability functions by d as a function of y and d^Y as a function of $\mathbf{x}$, according to the needs of the context:

$$d^Y(\mathbf{x}) := d(Y(\mathbf{x})) = d(y), \tag{2.1}$$

where $y := Y(\mathbf{x})$ with $y : \mathbb{R} \rightarrow \mathbb{R}$ and $d^Y : \mathbb{R}^n \rightarrow [0, 1]$. There are two types of them, *one-sided* and *two-sided* ones [25]:

$$d(y) := \begin{cases} 0, & \text{if} \quad y \leq l, \\ (\frac{y-l}{u-l})^r, & \text{if} \quad l < y \leq u, \\ 1, & \text{if} \quad y > u, \end{cases} \tag{2.2}$$

$$d(y) := \begin{cases} 0, & \text{if} \quad y \leq l, \\ (\frac{y-l}{t-l})^{s_1}, & \text{if} \quad l < y \leq t, \\ (\frac{y-u}{t-u})^{s_2}, & \text{if} \quad t < y \leq u, \\ 0, & \text{if} \quad y > u. \end{cases} \tag{2.3}$$

Here, l is the minimum and u is the maximum acceptable value of y, and t is the most desirable value of y which could be selected anywhere between l and u. The value of r used in equation (2.2) should be specified by the user. The larger the r is, the more desirable the y values closer to u, and vice versa. s_1 and s_2 in equation (2.3) have a similar meaning.

There can be three different optimization goals for a response: maximization, minimization or target value. If a response is *maximum-is-the-best* type, then its desirability is as in the first graphic of Figure 2.1 and second graphic in the same figure shows desirability of *target-is-the-best* type.

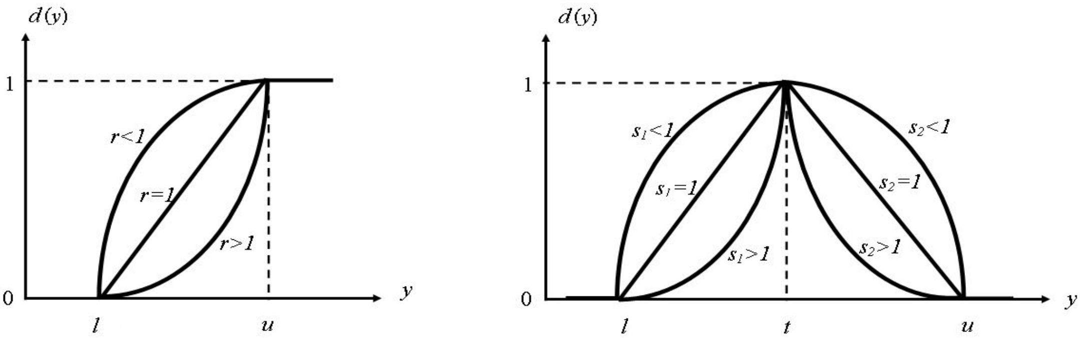

Figure 2.1: One-sided and Two-sided Individual Desirability Functions of Derringer and Suich's type

One of the main properties of these functions: they are flexible in the sense that the functions can assume a variety of shapes [19, 25]. Although, the two-sided individual desirability function in Figure 2.1 seem symmetric, asymmetric specifications are possible with these functions as in Figure 2.2.

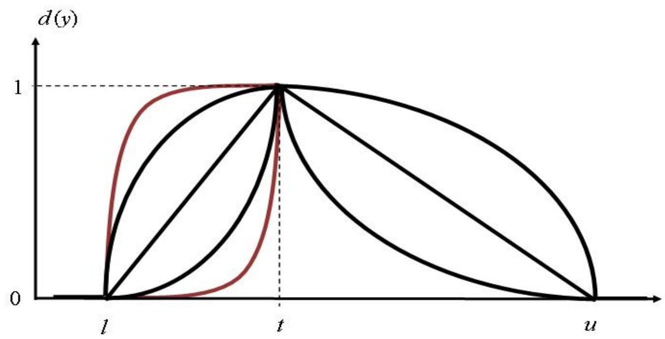

Figure 2.2: Asymmetric Individual Desirability Functions

We assume that there are m many responses in a multi-response optimization problem. After calculating the desirabilities of all responses by corresponding functions given in (2.2) and (2.3), overall desirability $D(\mathbf{y}) : \mathbb{R}^m \to [0,1]$ is calculated using the geometric mean [25]:

$$D(\mathbf{y}) := (d_1(y_1) \cdot d_2(y_2) \cdot \ldots \cdot d_m(y_m))^{\frac{1}{m}}, \tag{2.4}$$

where $\mathbf{y} := \mathbf{Y}(\mathbf{x})$ and $\mathbf{Y}(\cdot) := (Y_1, Y_2, \ldots, Y_m)^T(\cdot)$. Here, it is obvious that $D(\mathbf{y})$ will have a value in $[0,1]$. We denote the overall desirability as a function of $\mathbf{x}$ by $D^Y : \mathbb{R}^n \to [0,1]$ and define it by $D^Y(\mathbf{x}) := D(\mathbf{Y}(\mathbf{x}))$, i.e., $D^Y(\mathbf{x}) := \left(d_1^Y(\mathbf{x}) \cdot d_2^Y(\mathbf{x}) \cdot \ldots \cdot d_m^Y(\mathbf{x})\right)^{\frac{1}{m}}$.

Employing geometric mean to compute the overall desirability from individual desirabilities gives rise to the main property of desirability functions as an approach. If a desirability d of a response y becomes 0 at a factor value $\bar{\mathbf{x}}$, the overall desirability becomes 0 at this $\bar{\mathbf{x}}$, independently from the values of other individual desirabilities at that point. In this formulation of desirability functions, possible correlations between the responses are not taken into account and hence, it is assumed that the responses are independent of each other.

When the importance of individual desirability functions may differ in computing the overall desirability functions, a weighting strategy is possible [26]:

$$D(\mathbf{y}) := \left(\prod_{j=1}^{m} d_j(y_j)^{w_j}\right)^{\frac{1}{\sum_{j=1}^{m} w_j}}. \tag{2.5}$$

Weighted overall desirability has similar properties to the non-weighted one. Again, if one of the responses is undesirable at a factor vector $\bar{\mathbf{x}}$, then the overall desirability is zero at that point, i.e., $D(\mathbf{Y}(\bar{\mathbf{x}})) = 0$, without considering desirabilities of other responses at that point. Its values again range between 0 and 1. These weights can be specified by a decision maker next to the shapes of the curves of desirability functions. Obviously, when deciding about the weights it would be better to take into account relative importance of the product, process and system responses with respect to each other.

2.1.2 Optimization of Overall Desirability Function

The overall desirability function $D(\mathbf{y})$ is a continuous function of the individual desirabilities $d_j(y)$ from equation (2.4) and we see that each function d is continuous up to y from (2.2) and (2.3). In this thesis, a response Y is assumed to be a continuous function of the vector of factors, $\mathbf{x}$. Therefore, the overall desirability function D^Y is a continuous function of the factor vector $\mathbf{x}$.

The optimization of overall desirability functions becomes a complicated task when there are two-sided individual desirability functions in the problem. In the two-sided desirability functions formulation (2.3), the target value is attained at a nondifferentiable point, and hence, the function is not smooth at this point. It follows that a suitable single objective optimization method shall be chosen to solve the optimization problem of maximizing the continuous but nondifferentiable overall desirability function, i.e., we want $D(\mathbf{y})$ as close to unity as possible.

To optimize the overall desirability function given in (2.4) involving two-sided desirabilities, one way is to use the optimization techniques that do not employ the derivative information to find the optimum. Another way is to modify the individual desirability functions by approximation approaches to smooth them and then use the gradient-based methods. Herewith, the problem takes the following form:

$$\begin{aligned} &\text{maximize} \quad D(\mathbf{Y}(\mathbf{x})) \\ &\text{subject to} \\ &\quad \text{i. bounds of the factors } x_i \quad (i = 1, 2, \ldots, n), \\ &\quad \text{ii. bounds and targets of the responses } Y_j(\mathbf{x}) \quad (j = 1, 2, \ldots, m), \end{aligned} \tag{2.6}$$

Here, $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ is the vector of factors with the constraint set (a parallelepiped)

$$[\mathbf{l}_x, \mathbf{u}_x] := \mathop{\times}_{i=1}^{n} [l_{x_i}, u_{x_i}], \tag{2.7}$$

where l_{x_i} is the lower limit and u_{x_i} is the upper limit of x_i $(i = 1, 2, \ldots, n)$. First constraint group of the problem (2.6), i.e., the bounds for the factors, are decided during the experimental design, and hence, they are known during the optimization procedure. In computation, the bounds for the factor levels are usually standardized to $[-1, 1]$.

Second constraint group, i.e., bounds and targets of the responses $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_m)^T$, are determined by the problem owners and experts. These bounds l_j and u_j for $Y_j(\mathbf{x})$ are in fact functions of $\mathbf{x}$, decided during experimental design, usually as 95 percent confidence interval. In computations, nonnegativity constraints for the individual desirability functions are also needed, which are in fact redundant for the algorithms to stop at values quite near to 0 from below, are usually occurring in numerical calculations.

2.1.2.1 Direct Search Optimization Methods

As its name implies, a *direct search method* is used to look for the best solution through a series of comparison of each trial solution with the current best one by looking at the function values. This name is firstly coined by Hooke and Jeeves [47] and their method is called *Hooke-Jeeves direct search method*.

Although many advanced numerical optimization tools are developed, direct search methods are still in use in practice. A first reason for this is that direct search methods have fairly good convergence results. Secondly, they are usually successfully applicable to many complicated nonlinear optimization problems where other methods usually fail. Thirdly, they are user-friendly and easy to implement. Besides their simplicity, flexibility and reliability, they are also robust. To get more information about direct search methods, a recent review paper [69] may be consulted.

A common point of these methods is that they do not use the derivative information of the function in the optimization process. The estimated responses $\hat{Y}(\mathbf{x})$ $(j = 1, 2, \ldots, m)$ are continuous functions of the factors $\mathbf{x}$, the individual desirabilities $d(\hat{Y}(\mathbf{x}))$ of the estimated responses are also continuous functions of the factors $\mathbf{x}$, and hence, the overall desirability function $D(\mathbf{Y}(\cdot))$ is a continuous function of the factors $\mathbf{x}$. Therefore, direct search methods can be used to optimize the overall desirability over the domain of the factors.

In the study of Derringer and Suich [25], firstly, second degree polynomials are fitted by regression to some data collected through experimentation to model the relations between the responses and the factors. Then, the individual desirabilities of these responses and overall desirability functions are calculated. For each set of factor levels, an overall desirability value is obtained. After all factor levels are searched, an optimal point that maximizes the overall desirability is found by a direct search method similar to that of Hooke and Jeeves [47].

2.1.2.2 Modified Desirability Functions

The idea in the modification approach is to smooth the two-sided desirability functions by a local polynomial approximation at their nondifferentiable points and being able to use the gradient based methods, which are widely available and more popular. Castillo et al. [19] proposed a smoothing technique and showed for on the linear case $(s_1 = s_2 = 1)$ of the two-sided individual desirability functions to get rid of the nondifferentiable points. Then the optimization of overall desirability function becomes a nonlinear optimization problem which can be solved by a gradient based method.

The nondifferentiable point of a two-sided desirability function is at t where the optimal value of the function is attained. The approximation function has to be a polynomial of degree 4 for each response $y\ (= y_j)\ (j = 1, 2, \ldots, m)$:

$$p(y) := A + By + Cy^2 + Dy^3 + Ey^4 \tag{2.8}$$

with 5 unknowns A, B, C, D and E, since it has to satisfy the following five conditions for each j:

1. the desirability value of the approximating function at t has to be equal to the value of the nondifferentiable desirability function at t;

2. the desirability value of the approximating function at $t - \delta$ has to be equal to the value of the nondifferentiable desirability function at $t - \delta$, where δ is the half size of a small neighborhood around t;

3. the desirability value of the approximating function at $t + \delta$ has to be equal to the value of the nondifferentiable desirability function at $t + \delta$;

4. the derivative of the approximating function at $t - \delta$ has to be equal to the derivative of the nondifferentiable desirability function at $t - \delta$;

5. the derivative of the approximating function at $t + \delta$ has to be equal to the derivative of the nondifferentiable desirability function at $t + \delta$.

These five conditions are expressed as a system of 5 linearly independent equations with 5 unknowns, A, B, C, D and E for each $j = 1, 2, \ldots, m$. Therefore, generically, we have a unique solution on this system.

Herewith, the approximated individual desirability function $d^{\mathrm{appr}}(y)$ is defined by

$$d^{\mathrm{appr}}(y) := \begin{cases} a + by, & \text{if} \quad l < y \leq t - \delta, \\ p(y), & \text{if} \quad t - \delta < y \leq t + \delta, \\ c + dy, & \text{if} \quad t + \delta < y \leq u, \\ 0, & \text{otherwise}, \end{cases} \tag{2.9}$$

with coefficients a, b for the function on $[l, t - \delta)$ and coefficients c, d for the function $(t + \delta, u]$ for the case of a single nondifferentiable point at t. Here, δ defines a small neighborhood around the nondifferentiable point, the value of $\delta = (u - t)/50$ is used in [19], and it is reported that smaller values of δ did not effect the solution.

After modifying all individual desirability functions in this way to get rid of the nondifferentiable points, the overall desirability function is computed with these modified, and hence, smoothed functions. Castillo et al. [19] used GRG2 [65] which is a generalized reduced gradient method provided by Microsoft Excel to optimize the overall desirability function.

This approach is widely used in comparison with other approaches to desirability functions. However, it is not an easy method to implement, especially, when the number of responses increases. Many polynomial approximations and, hence, numerous calculations included in this approach, which may lead to an inaccurate result for some inexperienced users.

2.1.2.3 Optimization Softwares for Desirability Functions

We mentioned of the two existing solution strategy being used for solving optimization problem (2.6) of desirability functions: direct search methods and modified desirability functions approach. Most optimization softwares for desirability functions are working based on these two approaches. It is common to find an optimization method for desirability functions under the category of multi-response optimization techniques of a *software package*.

First implementation of a direct search algorithm for desirability functions is conducted by Derringer and Suich with FORTRAN language [25]. A widely used software called Design-Expert [21] has a module which is also based on direct search approach for desirability maximization. A recent software with direct search implementation, which uses Nelder-Mean simplex method, is available under the name Package Desirability maintained by Max Kuhn [63].

Modified desirability functions of Castillo et al. [19] is carried out in Excel Solver of Microsoft Office using a special generalized reduced gradient method, namely, GRG2 [65]. In SAS Institute and MINITAB, there are design of experiments softwares which execute desirability functions for multi-response optimization problems. Corresponding software of SAS is called JMP [90]. The mentioned sofware in MINITAB is called *Response Optimization* which employs a reduced gradient algorithm with multiple starting points for maximizing the overall desirability function [76].

Many of these software have advanced graphing opportunities for the users of desirability functions. It is also important to note that since most of these softwares we mention above have commercial licenses, the details of the algorithms and specific optimization tricks in their solution strategies are not wholly known.

2.2 Nonsmooth Optimization

2.2.1 Introduction

Optimization of a *smooth function* $f : \mathbb{O} \to \mathbb{R}$ with $\mathbb{O} \subseteq \mathbb{R}^n$ for which we have the gradient information at all points of the domain of the function to find a descent direction that will direct us to an optimal point, is a relatively easy task than the optimization of a *nonsmooth* function. The fact that a nonsmooth function $f : \mathbb{O} \to \mathbb{R}$ ($\mathbb{O} \subseteq \mathbb{R}^n$) is not everywhere differentiable in its domain makes it necessary to develop other tools than gradient-based ones for its optimization [23].

Nonsmooth optimization bases on nonsmooth calculus (nonsmooth analysis) and is mainly about the theories developed to locate the extremum points of nonsmooth functions. The latter ones include a variety of classes of functions, having different analytical, structural and topological properties. Initial studies in this area focus on *convex* functions which include nondifferentiable points but have the convex directional derivatives at these points. This gives rise to a convex set of subgradients, i.e., the *subdifferential*, as a set-valued derivative replacing the gradient information [13, 82, 100, 79, 86].

If a function is *nonconvex*, then the subdifferential may be defined but it does not necessarily become a convex set, and a calculus finally resulting in optimality conditions may not be available. However, the differential theory for nonsmooth functions lacking convexity was able to be developed by generalizations of the notions of convex optimization. Based on the tools to handle the nondifferentiable points of a convex function, new approaches to treat the Lipschitz functions, directionally differentiable functions, semismooth and semicontinuous functions, and so on, have been developed. Hence, nonsmooth optimization has become a separate field, and today it is extended to several different types of nonsmooth function classes with different tools.

With the doctoral thesis of Clarke, a generalized subgradient called as *Clarke subgradient* and a convex subdifferential called as *Clarke subdifferential*, which is the closed convex hull of all limit points of the known gradients at points converging to the considered nondifferentiable point, are presented for *locally Lipschitz continuous* functions [17]. Other subdifferentials are suggested for locally Lipschitz continuous functions, such as *Michel-Penot subdifferential* and *Shor subdifferential* [72, 73, 95].

There are many subdifferentials proposed for nonconvex functions, such as *approximate sub-*

differentials of Ioffe [48], and *weak subdifferentials* based on supporting conic surfaces as a generalization of supporting hyperplanes, proposed by Azimov and Gasimov [4]. Among the subdifferentials for the set-valued nonconvex functions we can count the *coderivatives* of Mordukhovich [78] and *radial epiderivatives* proposed by Gasimov [56].

For non-Lipschitz but *lower semicontinuous functions*, smooth local approximations from below led to the concept of *viscosity subdifferentials* [14], *proximal subdifferentials* [87], suitable directional limits led to *Fréchet subdifferentials* (equivalent to proximal subdifferentials in reflexive Banach spaces) and *Clarke's subdifferential on Banach spaces* are the most common subdifferentials.

Another important class of functions are quasidifferentiable functions which have sublinear and continuous directional derivatives giving rise to the notion of *quasidifferential* mainly developed and studied by Demyanov, Rubinov, Pshenichnyi, Bagirov, and so on, [6, 22, 84]. *Discrete gradients* proposed by Bagirov [7] are used to approximate subgradients of a broad class of nonsmooth functions.

These constructions we mention here are some of the tools that lead to an effective calculus and optimality conditions for different general classes of nonsmooth functions, such as, (non-differentiable) convex, Lipschitz continuous, lower semicontinuous, quasidifferentiable functions, and, so on. Some of these classes include certain subclasses like *semismooth* functions [74], *semiconvex* functions [74] or *regular* functions in Clarke's sense [17] that are widely studied in the nonsmooth optimization area. There are also studies on classes of generalized derivative objects such as *Warga's derivate containers* [103].

2.2.2 Some Classes of Nonsmooth Functions

In this subsection, we review definitions and properties of some nonsmooth function classes which are necessary for this thesis, such as, convex, Lipschitz continuous, semismooth and max-type functions. To study nonsmooth functions and presenting the tools for handling the nonsmoothness, it is appropriate to use the *extended-valued* functions $f : \mathbb{O} \to \overline{\mathbb{R}}$ with $\overline{\mathbb{R}} := [-\infty, \infty] = \mathbb{R} \cup \{\pm\infty\}$ and $\mathbb{O} \subseteq \mathbb{R}^n$. Connected to this, the *proper* functions are introduced: a function $f : \mathbb{O} \to \overline{\mathbb{R}}$ is said to be *proper*, if $f(\mathbf{x}) > -\infty$ for all $\mathbf{x} \in \mathrm{dom} f$, where

$$\mathrm{dom} f := \{\mathbf{x} \in \mathbb{O} \mid f(\mathbf{x}) < \infty\} \tag{2.10}$$

is nonempty.

2.2.2.1 Convex Functions

Let $\mathbb{O} \subseteq \mathbb{R}^n$, a nonempty convex set, be given. A function $f : \mathbb{O} \to \mathbb{R}$ is called *convex* [86] on $\mathbb{O}$ if

$$f(\lambda\mathbf{x} + (1-\lambda)\mathbf{y}) \leq \lambda f(\mathbf{x}) + (1-\lambda)f(\mathbf{y}) \tag{2.11}$$

for any $\mathbf{x}, \mathbf{y} \in \mathbb{O}$ and $\lambda \in [0,1]$. The geometrical interpretation of a convex function says that the values of a convex function at the values on the line segment $\lambda\mathbf{x} + (1-\lambda)\mathbf{y}$, i.e., $f(\lambda\mathbf{x} + (1-\lambda)\mathbf{y})$, are less than or equal to the height of the chord joining the points $(\mathbf{x}, f(\mathbf{x}))$ and $(\mathbf{y}, f(\mathbf{y}))$, i.e., $\lambda f(\mathbf{x}) + (1-\lambda)f(\mathbf{y})$. In general, convex functions are quite important for optimization theory because of the fact that every local minimum of a convex function is a global minimum.

At a nondifferentiable point of a convex function the gradient does not exist, but we have a set of generalized gradients, i.e., subgradients. A vector $\boldsymbol{\xi} \in \mathbb{R}^n$ is called a *subgradient* of a nonsmooth proper convex function f at a nondifferentiable point $\mathbf{x} \in \text{dom}f$ if it satisfies the *subgradient inequality*, i.e.,

$$f(\mathbf{y}) \geq f(\mathbf{x}) + < \boldsymbol{\xi}, \mathbf{y} - \mathbf{x} > . \tag{2.12}$$

The set of all subgradients of a nonsmooth convex function $f : \mathbb{O} \to \overline{\mathbb{R}}$ at a nondifferentiable point $x \in \text{dom}f$ is called the *subdifferential* of f at $\mathbf{x}$, and is denoted by $\partial f(\mathbf{x})$:

$$\partial f(\mathbf{x}) := \{\boldsymbol{\xi} \in \mathbb{R}^n \mid f(\mathbf{y}) \geq f(\mathbf{x}) + < \boldsymbol{\xi}, \mathbf{y} - \mathbf{x} > \ \ \forall \mathbf{y} \in \mathbb{R}^n\}. \tag{2.13}$$

If $\mathbf{x}$ is in the interior of dom$f$, then it is guaranteed that the subdifferential $\partial f(\mathbf{x})$ is nonempty, convex, closed and bounded. For $\mathbf{x}$ in the relative interior of dom$f$, the subdifferential is nonempty, convex and closed. In general, the set $\partial f(\mathbf{x})$ is only guaranteed to be closed if $\mathbf{x} \in \text{dom}f$, because it may be empty or unbounded (i.e., f is not subdifferentiable) at the relative boundary points of dom$f$.

Although the gradient does not exist at a nondifferentiable point $\mathbf{x}$ of a nonsmooth convex function, we have the one-sided directional derivative at this point. The subgradients at this point can be characterized by means of this directional derivative:

$$f'(\mathbf{x}; \mathbf{v}) = \sup_{\boldsymbol{\xi} \in \partial f(\mathbf{x})} < \boldsymbol{\xi}, \mathbf{v} > . \tag{2.14}$$

The directional derivative of a proper convex function is a proper lower semicontinuous sublinear function of its direction. As we already noted, if $\mathbf{x}$ is in the interior of dom$f$ then the subdifferential $\partial f(\mathbf{x})$ is compact (closed and bounded) and, moreover, by this equality, the directional derivative is finite. Thus, one can write the subdifferential in relation with the directional derivative:

$$\partial f(\mathbf{x}) = \{\boldsymbol{\xi} \in \mathbb{R}^n \mid f'(\mathbf{x};\mathbf{v}) \geq <\boldsymbol{\xi}, \mathbf{v}> \ \ \forall \mathbf{v} \in \mathbb{R}^n\}. \tag{2.15}$$

The subdifferential admits every calculus rule like the sum rule and chain rule. This makes it possible to study the optimality conditions of convex functions at their nonsmooth critical points.

2.2.2.2 Lipschitz Continuous Functions

A function $f : \mathbb{O} \to \mathbb{R}$ is said to satisfy *Lipschitz condition* [17] on $\mathbb{O}$ if for some nonnegative scalar K, called the Lipschitz constant (or Lipschitz rank), one has

$$|f(\mathbf{y}) - f(\mathbf{z})| \leq K\|\mathbf{y} - \mathbf{z}\|_2 \tag{2.16}$$

for any $\mathbf{y}, \mathbf{z} \in \mathbb{O}$. Also, f is said to be Lipschitz near $\mathbf{x}_0 \in \mathbb{O}$ if for some $\epsilon > 0$, f satisfies a Lipschitz condition within the relative ϵ-neighborhood $\mathbb{B}(\mathbf{x}_0, \epsilon) \cap \mathbb{O}$ where $\mathbb{B}(\mathbf{x}_0, \epsilon) := \{\mathbf{x} \in \mathbb{R}^n \mid \|\mathbf{x} - \mathbf{x}_0\|_2 < \epsilon\}$ of $\mathbf{x}_0$. Functions which satisfy the Lipschitz condition near a point $\mathbf{x}_0$ are called *locally Lipschitz* or *locally Lipschitzian*, where K is called as the Lipschitz rank of f at $\mathbf{x}_0$. For functions of a real variable, Lipschitzness means the existence a finite upper bound for the gradient, this implies that the function is not "too step".

These functions are differentiable almost everywhere meaning that the set of nondifferentiable points has a measure of zero in Lebesgue sense (Rademacher's Theorem) [85], i.e., their gradient set $\nabla f(x)$ is measurable in $\mathbb{O}$. A function which is locally Lipschitz near a point may neither be differentiable there nor admit directional derivatives in the classical sense. The theory for optimizing the locally Lipschitz functions is worked out by Clarke [17] based on his generalizations of directional derivative, subgradient and subdifferential. He called his theory as nonsmooth optimization, and since then the theory has been named by this term

In his book [17], Clarke presents the theory and calculus of subgradients for locally Lipshitz functions. He shows that the relation between *Clarke subgradient* and *Clarke subdifferential* has a duality with the geometric notions of normal and tangent cones. Clarke directional derivative $f'_C(\mathbf{x};\mathbf{v})$ is a generalized directional derivative developed for Lipschitz functions. Given $f : \mathbb{O} \to \overline{\mathbb{R}}$ locally Lipschitzian, *Clarke subdifferential* $\partial_C f(\mathbf{x})$ of f at $\mathbf{x} \in \mathbb{O}$ can be defined as

$$\partial_C f(\mathbf{x}) := \{\boldsymbol{\xi} \in \mathbb{R}^n \mid f'_C(\mathbf{x};\mathbf{v}) \geq < \boldsymbol{\xi}, \mathbf{v} > \ \ \forall \mathbf{v} \in \mathbb{R}^n\}. \tag{2.17}$$

The set $\partial_C f(\mathbf{x})$ is nonempty, convex and compact for each $\mathbf{x} \in \mathbb{R}^n$. As set-valued map, $\partial_C f(\mathbf{x})$ is locally bounded and has a closed graph; hence, it is upper-semicontinuous. Furthermore, $f'_C(\mathbf{x};\mathbf{v})$ is the support function of $\partial_C f(\mathbf{x})$. This is because closed convex sets are characterized by their support function:

$$f'_C(\mathbf{x};\mathbf{v}) = \sup_{\boldsymbol{\xi} \in \partial_C f(\mathbf{x})} < \boldsymbol{\xi}, \mathbf{v} > . \tag{2.18}$$

When it comes to calculate the Clarke subdifferentials numerically from the definitions we wrote, this does not turn out to be a simple task. By using the idea that nondifferentiable points of a locally Lipschitz function f forms a set of zero measure, Clarke suggests to define the today so-called *Clarke subdifferential* as

$$\partial_C f(\bar{\mathbf{x}}) := \mathrm{co}\{\boldsymbol{\xi} \in \mathbb{R}^n \mid \boldsymbol{\xi} = \lim_{k \to \infty} \nabla f(\mathbf{x}_k),\ \mathbf{x}_k \to \bar{\mathbf{x}}\ (k \to \infty), \mathbf{x}_k \in D\ (k \in \mathbb{N})\}, \tag{2.19}$$

where the notation “co” respresents the convex hull. Here, $D \subseteq \mathbb{O}$ is the set where the function is differentiable.

Theorem 2.2.1. *[17]* Let $f : \mathbb{O} \to \overline{\mathbb{R}}$ be locally Lipschitzian. The *Mean Value Theorem* for Clarke subdifferentials $\boldsymbol{\xi}$ says, where $\mathbf{x}, \mathbf{y} \in \mathbb{O}$ [66]:

$$f(\mathbf{y}) - f(\mathbf{x}) =< \boldsymbol{\xi}, \mathbf{y} - \mathbf{x} > . \tag{2.20}$$

By using this Mean Value Theorem, the nonsmooth Sum and Chain Rules with respect to Clarke subdifferential is elaborated in the following way:

Theorem 2.2.2. *[17]* Let $F(\cdot) = (f_1(\cdot), f_2(\cdot), \ldots, f_m(\cdot))^T$ be a vector-valued function of the variable $\mathbf{x} \in \mathbb{O}$, where each $f_i : \mathbb{O} \to \mathbb{R}$ $(i = 1, 2, \ldots, m)$ is locally Lipschitz. Let $g : \mathbb{R}^m \to \mathbb{R}$ be locally Lipschitz. Then $g \circ F : \mathbb{O} \to \mathbb{R}$ is locally Lipschitz and for any $\mathbf{x} \in \mathbb{R}^n$ one has

$$\partial_C(g \circ F)(\mathbf{x}) \subseteq \mathrm{co}\left\{ \sum_{i=1}^{m} \boldsymbol{\xi}_i \mu^i \mid \boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_m)^T \in \partial_C g(F(\mathbf{x})),\ \mu^i \in \partial_C f_i(\mathbf{x})\ (i = 1, 2, \ldots, m) \right\}. \tag{2.21}$$

Remark 2.2.3. In Theorem 2.2.2, if each f_i $(i = 1, 2, \ldots, m)$ and g are regular (we explain below), and $\partial_C g(F(\mathbf{x})) \subseteq \mathbb{R}_+$, where $\mathbb{R}_+$ is the set of nonnegative numbers, then equality holds in the above inclusion.

2.2.2.3 Semismooth Functions

Some functions which are locally Lipschitz have a directional derivative, i.e., their Clarke derivative $f'_C(\mathbf{x};\mathbf{v})$ is equal to the directional derivative $f'(\mathbf{x};\mathbf{v})$; this means: $f'_C(\mathbf{x};\mathbf{v}) = f'(\mathbf{x};\mathbf{v})$. These functions are called *regular*. As we see in the theorems above, regularity is quite important in calculus of Clarke's subdifferential to have the equality in the formulations.

The most important example of regular functions are *semismooth* functions which constitute a quite wide class, containing also the piecewise smooth (or piecewise continuously differentiable) functions. A function $f : \mathbb{O} \to \mathbb{R}$ is called *semismooth* at $\mathbf{x} \in \mathbb{O}$ if it is locally Lipschitz at $\mathbf{x}$ and for direction $\mathbf{v} \in \mathbb{R}^n$, the following limit exists [7, 74]:

$$\lim_{\substack{\boldsymbol{\xi}\in\partial f(\mathbf{x}+\alpha\mathbf{u})\\ \mathbf{u}\to\mathbf{v}\\ \alpha\to+0}} <\boldsymbol{\xi},\mathbf{u}> . \tag{2.22}$$

Max-type and *min-type* functions are functions which are nondecreasing in some variables and nonincreasing in the others. Their optimization problem involves *maximinimization* or *minimaximization* rather than simple minimization or maximization:

$$\underset{\mathbf{x}\in\mathbb{O}}{\text{minimize}} \quad \max_{1\le i\le m} f_i(\mathbf{x}). \tag{2.23}$$

The max- and min-type function classes are so wide that often a certain max-type or min-type form is chosen to study the differential properties. Let be given functions $f_i : \mathbb{O} \to \mathbb{R}$ $(i = 1, 2, \ldots, m)$. A common class of max-type functions is

$$f(\mathbf{x}) = \max\,\{f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_m(\mathbf{x})\}, \tag{2.24}$$

defining a function $f : \mathbb{O} \to \mathbb{R}$, where each f_i $(i = 1, 2, \ldots, m)$ is continuously differentiable. Such a function is a *regular locally Lipschitz* function [17]. By using Theorem 2.2.2, we calculate the Clarke subdifferential $\partial_C f(\mathbf{x})$:

$$\partial_C f(\mathbf{x}) \subseteq \operatorname{co}\left\{ \bigcup_{i\in I_0(\mathbf{x})} \partial_C f_i(\mathbf{x}) \right\}, \tag{2.25}$$

where $I_0(\mathbf{x}) := \{i \in \{1, 2, \ldots, m\} \mid f(\mathbf{x}) = f_i(\mathbf{x})\}$. If each f_i is regular, then equality holds in the above inclusion.

2.2.3 Methods for Nonsmooth Optimization Problems

From the application side, a nonsmooth method may work fine for some type of problem, however, it is possible that it may fail for another type. This means that none of the methods is good for all types of problems. The main groups of nonsmooth optimization methods are *subgradient* methods [24, 96, 99, 111] and *bundle* methods [67, 68, 111]. They have advantages and disadvantages according up to the specific properties optimization problem. In practice, main disadvantage of both subgradient and bundle methods is related with finding appropriate software. Existing ones are developed for immediate purposes of the researchers, not targeting users with different needs. Hence, getting ready nonsmooth softwares for a different problem is not usually a practical issue. Besides these methods, there are *global optimization*, *derivative free* and *nonlinear optimization* techniques which are useful when the objective function of the problem is nonsmooth [83, 93].

In this thesis, we use two methods for solving our desirability maximization problem as a *nonsmooth composite constrained problem*. The first one (*i*) is called *Modified Subgradient Algorithm* (*MSG*) [36], it is based on the duality framework obtained by sharp augmented Lagrangian; this method belongs to the category of subgradient methods. MSG is implemented in *General Algebraic Modeling System* (*GAMS*) together with *CONOPT* [18, 92] which is a provided solver within GAMS. CONOPT is based on the *generalized reduced gradient* (GRG) approach.

The second method (*ii*) is *Branch and Reduce Optimization Navigator* (*BARON*) [8, 93, 91] which is provided as a solver within GAMS and it is based on the branch and reduce approach. BARON is an element of the category of global, nonlinear and nonsmooth methods. In this background section, we give reviews of these two methods.

2.2.3.1 Modified Subgradient Algorithm (MSG)

For solving constrained optimization problems, one of the efficient ways is considering the duality relations provided by the *augmented Lagrangian* framework introduced by Rockafellar and Wets in [88]. Augmented Lagrangian is obtained by an augmentation of the classical Lagrange function with a certain augmenting function. When this function is $\sigma(z) := |z|$, it is called as the *sharp augmented Lagrangian*. MSG developed by Kasımbeyli [36] uses this idea in solving a nonsmooth optimization problem. We give the details of MSG algorithm with respect to the needs of our numerical examples in Chapter 3. Here, let us briefly introduce the dual problem by Sharp Augmented Lagrangian. Let us consider the nonlinear programming problem

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{x} \in \mathbb{X}, \\ & \boldsymbol{h}(\mathbf{x}) = \mathbf{0}_m, \end{aligned} \tag{2.26}$$

where $\mathbb{X}$ is compact and the functions $f : \mathbb{R}^n \to \mathbb{R}$ and $\boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^m$ are continuous. The *sharp augmented Lagrangian* $L : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}_+ \to \mathbb{R}$ associated with problem (2.26) is defined by

$$L(\mathbf{x}, \mathbf{u}, c) := f(\mathbf{x}) + c\|\boldsymbol{h}(\mathbf{x})\|_2 - \mathbf{u}^T \boldsymbol{h}(\mathbf{x}). \tag{2.27}$$

Here, $\mathbf{x} \in \mathbb{R}^n$ is the decision variable of the primal problem (2.26) and decision variables for the dual problem are $\mathbf{u} \in \mathbb{R}^m$ and the scalar $c \in \mathbb{R}_+$, where $\mathbb{R}_+$ is the set of nonnegative numbers; $\|\cdot\|_2$ is the Euclidean norm. The dual function $H : \mathbb{R}^m \times \mathbb{R}_+ \to \mathbb{R}$ can be defined as the minimum of the augmented Lagrangian which we introduced above with respect to the dual parameters:

$$H(\mathbf{u}, c) := \min_{\mathbf{x} \in \mathbb{X}} \quad f(\mathbf{x}) + c\|\boldsymbol{h}(\mathbf{x})\|_2 - \mathbf{u}^T \boldsymbol{h}(\mathbf{x}). \tag{2.28}$$

The dual problem which is the maximization of the dual function is

$$\underset{(\mathbf{u}, c) \in \mathbb{R}^m \times \mathbb{R}_+}{\text{maximize}} \quad H(\mathbf{u}, c). \tag{2.29}$$

This problem is typically a nonsmooth convex problem and hence, nonsmooth minimization techniques can be used for solving it. For our case, the advantage of MSG over other nonsmooth methods is that it has quite limited requirements: the objective and constraints should be continuous, the set $\mathbb{X}$ of variables needs to be compact, and constraints should be of equality type. Namely, we do not pose any differentiability and convexity conditions on the objective and constraints functions in the dual formulation.

MSG uses an ϵ-subgradient search direction [96] in order to strictly improve the value of the dual function $H(\mathbf{u}, c)$ and the sequence of dual function values is convergent. In contrast with the penalty or multiplier methods, for improving the value of the dual function, one does not need to take the "penalty like parameter". We can be sure about the zero duality gap if the objective and constraints functions of the corresponding problem are locally Lipschitz continuous [36].

One drawback of this method is its strict dependence on parameter selection to find the optimal point. Main parameters, which should be initially put in the method, are the step-size parameter and an upper bound for the sharp augmented Lagrangian. These parameters are usually decided by trial and error. For more information on zero duality gap, saddle point properties and different step size formulations, we refer to [15, 36, 38, 55].

2.2.3.2 GAMS: BARON and CONOPT

The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization. It consists of a language compiler and a stable of integrated high-performance solvers. For solving a real-world problem, the data need to be organized and corresponding codes have to be written; this transforms the data into the form required by the solution procedures of mathematical programming. Eliminating errors in these codes is not easy because these programs are available only to the ones who wrote them. GAMS was developed to improve this situation by

- providing a high-level language for the compact representation of large and complex models,
- allowing changes to be made in model specifications simply and safely,
- allowing unambiguous statements of algebraic relationships, and
- permitting model descriptions that are independent of solution algorithms.

The design of GAMS has incorporated ideas drawn from relational database theory and mathematical programming and has attempted to merge these ideas to suit the needs of strategic modelers. Relational database theory provides a structured framework for developing general data organization and transformation capabilities. Mathematical programming provides a way of describing a problem and a variety of methods for solving it. All data transformations are specified concisely and algebraically. This means that all data can be entered in their most elementary form and that all transformations made in constructing the model and in reporting are available for inspection. For the inputs, outputs and other details of a GAMS program we refer to the documents provided in [34], also demo downloads can be found in this source.

In GAMS, there are many solution procedures, which are called models in our study and we will be interested in three of these:

- NLP: for nonlinear programming,

- DNLP: for nonlinear programming with discontinuous derivatives, and
- MINLP: for mixed integer nonlinear programming.

NLP procedures are defined as models in which all functions which appear with endogenous arguments, i.e., arguments that depend on model variables, are smooth with smooth derivatives. DNLP models can in addition use functions that are smooth but have discontinuous derivatives. The solvers differ in the methods which they use, in whether they find a globally optimal solution with proven optimality, in the size of models that they can handle, and in the format of models which they accept. For NLP models, the default solver of GAMS is CONOPT and for DNLP models the suitable solver is BARON.

The algorithm used in CONOPT is based on the GRG algorithm first suggested by Abadie and Carpentier [2]. The actual implementation has many modifications to make it efficient for large models and for models written in the GAMS language. Details on the algorithm can be found in Drud [27, 28, 29, 30]. There are different versions of CONOPT in GAMS implementing different algorithms, in our version, GAMS includes CONOPT3 implementing a generalized reduced gradient method.

BARON is a computational system for solving *mixed-integer nonlinear nonconvex* optimization problems to global optimality. BARON implements deterministic global optimization algorithms of the branch-and-bound type that are guaranteed to provide global optima under fairly general assumptions. While traditional NLP and MINLP algorithms converge only under certain convexity assumptions, BARON provides global optima under fairly general assumptions for DNLP models. These include the availability of finite lower and upper bounds on the variables and their expressions in the NLP or MINLP to be solved.

BARON implements algorithms of the branch-and-bound type enhanced with a variety of constraint propagation and duality techniques for reducing ranges of variables in the course of the algorithm. BARON implements branch-and-bound algorithms involving convex relaxations of the original problem. Branching takes place not only on discrete variables, but also on continuous ones which are nonlinearly involved. Users can specify branching priorities for both discrete and continuous variables.

CHAPTER 3

A COMPUTATIONAL APPROACH TO DESIRABILITY FUNCTIONS BASED ON NONLINEAR AND NONSMOOTH OPTIMIZATION

We present the current approaches to desirability maximization in Chapter 2: direct search methods and modified desirability functions. As explained in that chapter, these methods have some serious drawbacks related with computational time and ease of use. As an alternative, we propose a new approach for the optimization of desirability functions: after a reformulation of the individual desirability functions to deal with their piecewise definition, we employ nonsmooth optimization methods to solve the resulting overall desirability function. For reformulation of individual functions, a binary variable is introduced into the function as a coefficient showing the activeness of a "side". Using this binary variable helps us overcome the difficulty in expressing the piecewise definition. We call the reformulated function as *adjusted individual desirability functions*.

Optimization of the overall desirability function calculated from the adjusted individual ones becomes a $0-1$ mixed-integer nonlinear optimization problem. This problem includes the binary integer variables showing a side is active or inactive at a factor value and continuous factor variables. The overall desirability function is a nonlinear mapping as the geometric mean of the reformulated individual functions. Then, we convert this mixed-integer problem to a continuous one by adding a constraint for the binary variable. The resulting continuous problem is a nonlinear constrained optimization problem of an objective function including nondifferentiable points together with the constraints of bounds for factors, responses and the constraints of binary variables.

We describe our approach on two classical multi-response problems taken from the literature, one of which includes only two-sided linear desirability functions and the other includes both one-sided and two-sided linear desirability functions. We have reformulated the overall desirability functions for both problems and solved the resulting optimization problems by two different nonsmooth methods. Firstly, the problems are defined as DNLP models and solved with BARON solver of GAMS. Secondly, we implement MSG which is based on writing the convex dual of the problem with the Sharp Augmented Lagrangian. We define the dual problems as NLP and solve them with CONOPT solver of GAMS.

3.1 Adjusted Individual Desirability Functions

Adjusted desirability functions are obtained by a reformulation of the original ones. This reformulation is best explained on two-sided individual desirability functions including one nondifferentiable point [1]. These functions are made of two "sides" (in competition), one of which becomes active depending on the response value of factor levels. Since for each combination of factor levels, there exists a single response value, one side of a two-sided individual function becomes active.

Let us assume that there are m many responses in a multi-response optimization problem, we denote by p the number of responses having one-sided desirabilities and by $m-p$ the number of responses having two-sided desirability functions in a multi-response problem, where $0 \leq p < m$. A two-sided individual desirability function $d\ (= d_j)$ with $l\ (= l_j)$, $t\ (= t_j)$, $u\ (= u_j)$ and $y\ (= y_j = Y_j(\mathbf{x}))$ for each $j = 1, 2, \ldots, m-p$ can be written as:

$$d(y) = \begin{cases} 0, & \text{if} \quad y \leq l, \\ d_1(y), & \text{if} \quad l \leq y \leq t, \\ d_2(y), & \text{if} \quad t \leq y \leq u, \\ 0, & \text{if} \quad y \geq u. \end{cases} \tag{3.1}$$

Here,

$$d_1(y) := (\frac{y-l}{t-l})^{s_1} \quad \text{and} \quad d_2(y) := (\frac{y-u}{t-u})^{s_2} \tag{3.2}$$

are the sides of the *two-sided individual desirability function* $d(\cdot) : \dot{\mathbb{I}} \rightarrow \mathbb{R}$ where $\dot{\mathbb{I}}\ (= \mathbb{I}_j := [l_j, u_j])$. For y in $[l, t]$, the first function (side) $d_1(y)$ is active (on) and the second function (side) $d_2(y)$ is inactive (off). For y in $[t, u]$ this situation is reverse, i.e., $d_1(y)$ is inactive (off) but $d_2(y)$ is active (on) where $l < t < u$. We note that at the target point t, we have $d = d_1 = d_2$.

Based on this discussion, we express each individual function d with a mixed-integer formulation by taking a convex combination of sides d_1 and d_2, using the binary integer variable

$z\ (= z_j)\ (j = 1, 2, \ldots, m - p)$:

$$d(y, z) = zd_1(y) + (1 - z)d_2(y). \tag{3.3}$$

Here, the binary coefficients z becomes 1 when $d_1(y)$ is active (on). Let us remember that we denote desirability functions by d as a function of y and d^Y as a function of $\mathbf{x}$, according to the needs of the context:

$$d^Y(\mathbf{x}) = d(y) = d(Y(\mathbf{x})), \tag{3.4}$$

where $d^Y(\cdot) : \mathbb{X} \to [0, 1]$ with $\mathbb{X} = [\mathbf{l}_x, \mathbf{u}_x]$, in practice. When we are dealing with optimization of the desirability functions, we write and use the functions based on factors $\mathbf{x}$, but we consider the functions in y-space when the shape of desirability functions or calculating their values are being discussed.

By using equation (3.3), we write $d^Y(\mathbf{x}, z) = (zd_1 + (1 - z)d_2)(Y(\mathbf{x}))$, which gives us $d^Y(\mathbf{x}, z) = zd_1(Y(\mathbf{x})) + (1 - z)d_2(Y(\mathbf{x}))$. We define $d_1^Y(\cdot) := d_1(Y(\cdot))$ and $d_2^Y(\cdot) := d_2(Y(\cdot))$ and reach the mixed-integer formulation in $\mathbf{x}$ of an individual desirability function:

$$d^Y(\mathbf{x}, z) = zd_1^Y(\mathbf{x}) + (1 - z)d_2^Y(\mathbf{x}). \tag{3.5}$$

Here, when $z = 1$, $d^Y(\mathbf{x}, z) = d_1^Y(\mathbf{x})$ and, when $z = 0$, $d^Y(\mathbf{x}, z) = d_2^Y(\mathbf{x})$, according to the activeness of the sides as explained above.

3.1.1 Optimization of Adjusted Overall Desirability

By *adjusted overall desirability function* shown by $D^Y(\cdot) := D(\mathbf{Y}(\cdot))$ we mean that all two-sided individual desirability functions included in the problem are reformulated as above:

$$D^Y(\mathbf{x}, \mathbf{z}) := \left[\prod_{j=1}^{p} d_j^Y(\mathbf{x})^{w_j} \cdot \prod_{j=p+1}^{m} d_j^Y(\mathbf{x}, z_j)^{w_j} \right]^{\frac{1}{\sum_{j=1}^{m} w_j}}, \tag{3.6}$$

for $\mathbf{x} := (x_1, x_2, \ldots, x_n)^T$ and $\mathbf{z} := (z_1, z_2, \ldots, z_p)^T$. The optimization problem of the reformulated overall desirability function can be stated as follows:

$$\begin{aligned}
&\text{maximize} \quad D^Y(\mathbf{x}, \mathbf{z}) \\
&\text{subject to} \\
&\quad \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x], \\
&\quad \mathbf{0}_p \leq \boldsymbol{d}^Y(\mathbf{x}) \leq \mathbf{1}_p, \\
&\quad \mathbf{0}_{m-p} \leq \boldsymbol{d}^Y(\mathbf{x}, \mathbf{z}) \leq \mathbf{1}_{m-p}, \\
&\quad \mathbf{h}(\mathbf{z}) = \mathbf{0}_{m-p}.
\end{aligned} \tag{3.7}$$

In our computations, the bounds $[\mathbf{l}_x, \mathbf{u}_x]$ for the factor levels are standardized to $[\mathbf{-1}_n, \mathbf{1}_n]$. Moreover, instead of the bound constraints $[l_j, u_j]$ $(j = 1, 2, \ldots, m)$ of the responses, we use the contraint of being between $\mathbf{0}$ and $\mathbf{1}$ for both one-sided individual desirability functions $\boldsymbol{d}^{\boldsymbol{Y}}(\mathbf{x}) := (d_1^Y(\mathbf{x}), d_2^Y(\mathbf{x}), \ldots, d_p^Y(\mathbf{x}))^T$ and two-sided individual desirability functions $\boldsymbol{d}^{\boldsymbol{Y}}(\mathbf{x}, \mathbf{z}) := (d_{p+1}^Y(\mathbf{x}, z_{p+1}), d_{p+2}^Y(\mathbf{x}, z_{p+2}), \ldots, d_m^Y(\mathbf{x}, z_m))^T$ for coding purposes.

Remark 3.1.1. If we had used the bounds of the responses in our problem, then these constraints for the values of desirability functions would have become redundant. We note that these two different constraints can be used interchangeably. □

The constraint $\mathbf{h}(\mathbf{z}) = \mathbf{0}_{m-p}$ is to ensure that the variable z $(= z_j)$ becomes binary for all $j = 1, 2, \ldots, p$:

$$\mathbf{h}(\mathbf{z}) := (h(z_1), h(z_2), \ldots, h(z_{m-p}))^T \quad \text{where} \quad h(z) := (z - z^2)\ (z \in \mathbb{R}). \tag{3.8}$$

For convenience of notation, we use the "dummy" notation $\mathbf{0}$ and $\mathbf{1}$ for the 0 and 1 vectors, suppressing the dimensions, which we can easily understand from the context.

3.1.2 Two Problems

We use adjusted desirability function to reformulate two of the most common multi-response problems in the literature: wire bonding process optimization problem [19] and tire-tread compound problem [25, 49]. The first problem is described in Appendix (A) and the second problem is presented in Appendix (B).

These problems are used to introduce and explain the methods of modified desirability functions and direct search optimization for desirability functions.

Wire Bonding Process Optimization (***Problem 1***): There are 3 control factors, x_1, x_2, x_3, each of which is scaled to -1 and 1. Hence, $\mathbf{x} = (x_1, x_2, x_3)^T$ with $\mathbf{x} \in [\mathbf{-1}, \mathbf{1}]$. There are six responses $Y_j(\mathbf{x})$ $(j = 1, 2, \ldots, 6)$, all of which have two-sided linear desirabilities, and we reformulate according to the formula given in (3.5).

The maximization of overall desirability for wire bonding process optimization looks as follows:

$$\begin{aligned}
&\text{maximize} \quad D^Y(\mathbf{x},\mathbf{z}) \\
&\text{subject to} \\
&\quad \mathbf{x} \in [\mathbf{-1},\mathbf{1}]\,, \\
&\quad \mathbf{0} \le \boldsymbol{d}^Y(\mathbf{x},\mathbf{z}) \le \mathbf{1}, \\
&\quad \mathbf{h}(\mathbf{z}) = \mathbf{0},
\end{aligned} \tag{3.9}$$

where the objective function is

$$D^Y(\mathbf{x},\mathbf{z}) = \prod_{j=1}^{6} \left(z_j d^Y_{j,1}(\mathbf{x}) + (1 - z_j) d^Y_{j,2}(\mathbf{x}) \right). \tag{3.10}$$

The constraint functions are $\mathbf{h}(\mathbf{z}) := (z_1 - z_1^2, z_2 - z_2^2, \ldots, z_6 - z_6^2)^T$ and $\boldsymbol{d}^Y(\mathbf{x},\mathbf{z}) := (d^Y_1(\mathbf{x}, z_1), d^Y_2(\mathbf{x}, z_2), \ldots, d^Y_6(\mathbf{x}, z_6))^T$. For the graphics of the individual desirability functions of the problem and other details, see Appendix (A) and Figure (A.1).

Tire Tread Compound Optimization (***Problem 2***): Again, there are 3 control factors, x_1, x_2, x_3, each of which is between -1 and 1. Hence, $\mathbf{x} = (x_1, x_2, x_3)^T$ with $\mathbf{x} \in [\mathbf{-1},\mathbf{1}]$. There are four responses $Y_j(\mathbf{x})$: for $j = 1, 2$, responses have one-sided linear desirabilities, and for $j = 3, 4$, responses have two-sided linear desirabilities. We reformulate individual desirabilities for responses $j = 3, 4$ according to the formula given in (3.5).

Our present example is different from the first problem of wire bonding process optimization since this one includes both one-sided and two-sided individual desirabilities. The maximization of overall desirability for tire tread compound looks as follows:

$$\begin{aligned}
&\text{maximize} \quad D^Y(\mathbf{x},\mathbf{z}) \\
&\text{subject to} \\
&\quad \mathbf{x} \in [\mathbf{-1},\mathbf{1}]\,, \\
&\quad \mathbf{0} \le \boldsymbol{d}^Y(\mathbf{x},\mathbf{z}) \le \mathbf{1}, \\
&\quad \mathbf{0} \le \boldsymbol{d}^Y(\mathbf{x}) \le \mathbf{1}, \\
&\quad \mathbf{h}(\mathbf{z}) = \mathbf{0},
\end{aligned} \tag{3.11}$$

where the objective function is

$$D^Y(\mathbf{x},\mathbf{z}) = \prod_{j=1}^{2} d^Y_j(\mathbf{x}) \cdot \prod_{j=3}^{4} \left(z_j d^Y_{j,1}(\mathbf{x}) + (1 - z_j) d^Y_{j,2}(\mathbf{x}) \right). \tag{3.12}$$

Moreover, the constraint functions are $\mathbf{h}(\mathbf{z}) := (z_3 - z_3^2, z_4 - z_4^2)^T$, $\boldsymbol{d}^Y(\mathbf{x},\mathbf{z}) := (d^Y_3(\mathbf{x}, z_3), d^Y_4(\mathbf{x}, z_4))^T$ and $\boldsymbol{d}^Y(\mathbf{x}) := (d^Y_1(\mathbf{x}), d^Y_2(\mathbf{x}))^T$. For the graphics of the individual desirability functions of the problem and other details, see Appendix (B) and Figure (B.1).

3.2 Numerical Experiments

3.2.1 Introduction

As we explain in Chapter 2, the conventional individual and overall desirability functions are continuous functions of the factors $\mathbf{x}$. Let us examine the continuity of the objective mappings and constraints of problems (3.9) and (3.11). In view on the formula (3.6), we say that the objective mappings are continuous functions of $\mathbf{x}$ and $\mathbf{z}$. The constraints functions $\boldsymbol{d}^Y(\mathbf{x},\mathbf{z})$ and $\boldsymbol{d}^Y(\mathbf{x})$ are the continuous maps of $\mathbf{x}$ and $\mathbf{z}$ from (3.3) together with (3.1). The constraint function $\mathbf{h}(\mathbf{z})$ is a continuous map of $\mathbf{z}$ from (3.8). Hence, in both problems, we have continuous objective and constraint functions.

Here, we explain the implementation of two nonsmooth optimization methods which we find appropriate for the optimization of our problems. Further mathematical properties of our problems are given Chapter 4. Our preference is based on the fact that they do not need assumptions like smoothness and convexity and they do not calculate derivatives or subdifferentials at every step to find the optimal point.

In the first method, the duals of problems (3.9) and (3.11) are constructed with respect to the sharp augmented Lagrangian and MSG is implemented together with CONOPT/GAMS for NLP models. With the second method, primal problems (3.9) and (3.11) are solved by BARON/GAMS as DNLP models. We remember that these models are some solution procedures of GAMS as explained in Chapter 2.

3.2.2 Implementation of MSG with GAMS solver of CONOPT

MSG is proposed by Gasimov [36] for solving the dual problems constructed with respect to sharp augmented Lagrangian functions for primal problems including only equality constraints. MSG is convergent and capable of yielding a zero duality gap when the appropriate parameter selection is done, without any assumption of convexity on the functions of the problem which are all need to be continuous. The objectives of (3.9) and (3.11) are continuous functions of $\mathbf{x}$ and $\mathbf{z}$ including points of nondifferentiability to which MSG becomes successfully applied.

Since MSG requires equality constraints, we need to convert the box constraints of our problems (3.9) and (3.11), given as inequality constraints, into the equality ones. For this aim, one can introduce slack variables which in fact increase the number of variables in the problem.

Another way is to consider the max-type functions which cause constraint functions to be nonsmooth. In application, we have preferred slack variables to keep the smoothness.

The dual problems obtained by the Sharp Augmented Lagrangian are solved by MSG as an NLP model together with CONOPT. For both problems, the general sketch of the algorithm is given, the sharp augmented Lagrangian is constructed, inequality constraints are converted to equality ones and appropriate parameters are selected.

3.2.2.1 Dual for Problem 1

In this part, we turn the inequality constraints of problem (3.9) into equality constraints to apply MSG. The vectorial constraint for the integers $\mathbf{h}(\mathbf{z}) = \mathbf{0}$ is already a system of equality constraints. By introducing slack variables $a_j \geq 0$ and $b_j \geq 0$, we have the equality constraint functions for all $j = 1, 2, \ldots, 6$:

$$\begin{aligned} d_j^{c,a}(\cdot) &:= d_j^Y(\cdot) - a_j = 0 \quad \text{for} \quad 0 \leq d_j^Y(\cdot), \quad \text{and} \\ d_j^{c,b}(\cdot) &:= d_j^Y(\cdot) - 1 + b_j = 0 \quad \text{for} \quad d_j^Y(\cdot) \leq 1. \end{aligned} \tag{3.13}$$

Let us define

$$\boldsymbol{h}(\mathbf{x}, \mathbf{z}) := (\mathbf{h}^T(\mathbf{z}), (\boldsymbol{d}^{c,a})^T(\mathbf{x}, \mathbf{z}), (\boldsymbol{d}^{c,b})^T(\mathbf{x}, \mathbf{z}))^T = \mathbf{0} \tag{3.14}$$

as the extended vector of equality constraints, where

$$\boldsymbol{d}^{c,a}(\cdot) := (d_j^{c,a}(\cdot))_{j=1,2,\ldots,6}^T, \quad \text{and} \quad \boldsymbol{d}^{c,b}(\cdot) := (d_j^{c,b}(\cdot))_{j=1,2,\ldots,6}^T. \tag{3.15}$$

Remark 3.2.1. As we have noted, instead of using slack variables for convertion into equality constraints, one can employ the max operator for $0 \leq d_j^Y(\cdot)$ and for $d_j^Y(\cdot) \leq 1$ ($j = 1, 2, \ldots, 6$), respectively, as follows:

$$\max\{0, -d_j^Y(\cdot)\} = 0 \quad \text{and} \quad \max\{0, d_j^Y(\cdot) - 1\} = 0. \tag{3.16}$$

□

The sharp augmented Lagrangian of (3.9) in vector notation is

$$L(\mathbf{x}, \mathbf{z}, c, \mathbf{u}) := D^Y(\mathbf{x}, \mathbf{z}) + c\|\boldsymbol{h}(\mathbf{x}, \mathbf{z})\|_2 - \mathbf{u}^T \boldsymbol{h}(\mathbf{x}, \mathbf{z}). \tag{3.17}$$

Explicitly we can write this mapping $L(\mathbf{x}, \mathbf{z}, c, \mathbf{u})$ by

$$
\begin{aligned}
L(\mathbf{x}, \mathbf{z}, c, \mathbf{u}) := & \prod_{j=1}^{6} \left(z_j d_{j,1}^Y(\mathbf{x}) + (1 - z_j) d_{j,2}^Y(\mathbf{x}) \right) \\
& + c \sqrt{ \left(\sum_{j=1}^{6} \left(z_j - z_j^2 \right) \right)^2 + \left(\sum_{j=1}^{6} \left(d_j^Y(\mathbf{x}, z_j) - a_j \right) \right)^2 + \left(\sum_{j=1}^{6} \left(d_j^Y(\mathbf{x}, z_j) - 1 + b_j \right) \right)^2 } \\
& - u_1 \left(\sum_{j=1}^{6} \left(z_j - z_j^2 \right) \right) - u_2 \left(\sum_{j=1}^{6} \left(d_j^Y(\mathbf{x}, z_j) - a_j \right) \right) - u_3 \left(\sum_{j=1}^{6} \left(d_j^Y(\mathbf{x}, z_j) - 1 + b_j \right) \right),
\end{aligned}
\tag{3.18}
$$

where $\mathbf{u} := (u_1, u_2, u_3)^T$ with $u_1, u_2, u_3 \in \mathbb{R}$ and $c \in \mathbb{R}$ being the Lagrange multipliers, and $L : \mathbb{R}^3 \times \mathbb{R}^6 \times \mathbb{R} \times \mathbb{R}^3 \to \mathbb{R}$. The dual function is given by

$$
H(\mathbf{u}, c) := \min_{(\mathbf{x}, \mathbf{z}) \in \mathbb{R}^3 \times \mathbb{R}^6} L(\mathbf{x}, \mathbf{z}, c, \mathbf{u}). \tag{3.19}
$$

Then, the dual problem of (3.9) having decision variables $(\mathbf{u}, c)$ with respect to the sharp Augmented Lagrangian is

$$
\underset{(\mathbf{u}, c) \in \mathbb{R}^3 \times \mathbb{R}_+}{\text{maximize}} \quad H(\mathbf{u}, c). \tag{3.20}
$$

3.2.2.2 Dual for Problem 2

In this part, we turn the inequality constraints of problem (3.11) into equality constraints for applying MSG. The vectorial constraint for the integers $\mathbf{h}(\mathbf{z}) = \mathbf{0}$ is already a system of equality constraints. By introducing slack variables $a_j \geq 0$ and $b_j \geq 0$, we have the equality constraint functions for all $j = 1, 2, 3, 4$:

$$
\begin{aligned}
d_j^{c,a}(\cdot) := d_j^Y(\cdot) - a_j = 0 \quad & \text{for} \quad 0 \leq d_j^Y(\cdot), \quad \text{and} \\
d_j^{c,b}(\cdot) := d_j^Y(\cdot) - 1 + b_j = 0 \quad & \text{for} \quad d_j^Y(\cdot) \leq 1 \quad .
\end{aligned}
\tag{3.21}
$$

Let

$$
\boldsymbol{h}(\mathbf{x}, \mathbf{z}) := (\mathbf{h}^T(\mathbf{z}), (\boldsymbol{d}^{c,a})^T(\mathbf{x}, \mathbf{z}), (\boldsymbol{d}^{c,b})^T(\mathbf{x}, \mathbf{z}), (\boldsymbol{d}^{c,a})^T(\mathbf{x}), (\boldsymbol{d}^{c,b})^T(\mathbf{x}))^T = \mathbf{0} \tag{3.22}
$$

be the extended vector of equality constraints, where

$$
\boldsymbol{d}^{c,a}(\cdot) := (d_j^{c,a}(\cdot))_{j=1,2,3,4}, \quad \text{and} \quad \boldsymbol{d}^{c,b}(\cdot) := (d_j^{c,b}(\cdot))_{j=1,2,3,4}. \tag{3.23}
$$

Hence, the sharp augmented Lagrangian of (3.11) is

$$
L(\mathbf{x}, \mathbf{z}, c, \mathbf{u}) := -D^Y(\mathbf{x}, \mathbf{z}) + c \|\boldsymbol{h}(\mathbf{x}, \mathbf{z})\|_2 - \mathbf{u}^T \boldsymbol{h}(\mathbf{x}, \mathbf{z}). \tag{3.24}
$$

In other words,

$$
\begin{aligned}
L(\mathbf{x},\mathbf{z},c,\mathbf{u}) :=& \prod_{j=1}^{2} d_j^Y(\mathbf{x}) \cdot \prod_{j=3}^{4}\left(z_j d_{j,1}^Y(\mathbf{x}) + (1-z_j) d_{j,2}^Y(\mathbf{x})\right)\\
&+c\sqrt{\left(\sum_{j=1}^{2}\left(d_j^Y(\mathbf{x})-a_j\right)\right)^2+\left(\sum_{j=1}^{2}\left(d_j^Y(\mathbf{x})-1+b_j\right)\right)^2+\left(\sum_{j=3}^{4}\left(z_j-z_j^2\right)\right)^2+\left(\sum_{j=3}^{4}\left(d_j^Y(\mathbf{x},z_j)-a_j\right)\right)^2+\left(\sum_{j=3}^{4}\left(d_j^Y(\mathbf{x},z_j)-1+b_j\right)\right)^2}\\
&-u_1\left(\sum_{j=1}^{2}\left(d_j^Y(\mathbf{x})-a_j\right)\right)-u_2\left(\sum_{j=1}^{2}\left(d_j^Y(\mathbf{x})-1+b_j\right)\right)-u_3\left(\sum_{j=3}^{4}\left(z_j-z_j^2\right)\right)\\
&-u_4\left(\sum_{j=3}^{4}\left(d_j^Y(\mathbf{x},z_j)-a_j\right)\right)-u_5\left(\sum_{j=3}^{4}\left(d_j^Y(\mathbf{x},z_j)-1+b_j\right)\right),
\end{aligned}
\tag{3.25}
$$

where $\mathbf{u} := (u_1,u_2,u_3,u_4,u_5)^T$ with $u_1,u_2,u_3,u_4,u_5 \in \mathbb{R}$ and $c \in \mathbb{R}$ are the Lagrange multipliers, and $L : \mathbb{R}^3 \times \mathbb{R}^2 \times \mathbb{R} \times \mathbb{R}^5 \to \mathbb{R}$. The dual function is defined by

$$H(\mathbf{u},c) := \min_{(\mathbf{x},\mathbf{z})\in\mathbb{R}^3\times\mathbb{R}^2} L(\mathbf{x},\mathbf{z},c,\mathbf{u}). \tag{3.26}$$

Then, the dual problem of (3.11) having the state variables $(\mathbf{u},c)$ with respect to the sharp Augmented Lagrangian is

$$\underset{(\mathbf{u},c)\in\mathbb{R}^5\times\mathbb{R}_+}{\text{maximize}} \quad H(\mathbf{u},c). \tag{3.27}$$

3.2.2.3 MSG Algorithm for Problems

We program the following algorithm in GAMS for solving our problems:

Step 1. Set $k = 1$ and choose initial values of dual parameters $\mathbf{u}_k$ and c_k, i.e., $\mathbf{u}_0$ and c_0, respectively.

Step 2. Solve

$$
\begin{aligned}
&\underset{(\mathbf{x},\mathbf{z})}{\text{minimize}} \quad L(\mathbf{x},\mathbf{z},c_k,\mathbf{u}_k)\\
&\text{subject to} \quad L(\mathbf{x},\mathbf{z},c_k,\mathbf{u}_k) \le \bar{H}.
\end{aligned}
\tag{3.28}
$$

Let $(\mathbf{x}_k,\mathbf{z}_k)$ be the solution. If $||\boldsymbol{h}(\mathbf{x}_k,\mathbf{z}_k)||_2 = \mathbf{0}$, then STOP.

Otherwise, go to Step 2.

Step 3. Set step size s_k and update formulas for $\mathbf{u}_{k+1}$, c_{k+1}

$$s_k = \frac{\delta(\alpha(\bar{H} - L(\mathbf{x}_k,\mathbf{z}_k,c_k,\mathbf{u}_k)) + (\bar{c}-c)||\boldsymbol{h}(\mathbf{x}_k,\mathbf{z}_k))||_2}{(\alpha^2 + (1+\alpha)^2)||\boldsymbol{h}(\mathbf{x}_k,\mathbf{z}_k)||_2^2}, \tag{3.29}$$

$$\mathbf{u}_{k+1} := \mathbf{u}_k - \alpha s_k \boldsymbol{h}(\mathbf{x}_k,\mathbf{z}_k), \tag{3.30}$$

$$c_{k+1} := c_k + (1+\alpha) s_k ||\boldsymbol{h}(\mathbf{x}_k,\mathbf{z}_k)||_2. \tag{3.31}$$

Set $k = k+1$ and go to Step 2.

For this algorithm, only initial values that have to be entered at the beginning of the program are of dual parameters $\mathbf{u}$ and c, i.e., $\mathbf{u}_0$ and c_0, respectively. There are fixed input parameters choosen specific to the problem: α, δ and $\bar{H}$. As seen in the algorithm, $\bar{H}$ is an upper bound for the sharp augmented Lagrangian $L(\mathbf{x}, \mathbf{z}, c_k, \mathbf{u}_k)$ and parameters α, δ are necessary for calculating the step size parameters. Some restrictions for these parameters are $\delta \in (0, 2)$ and $\alpha > 0$.

The combination of parameters α, δ and $\bar{H}$ is not unique, they are found by trial and error, and, especially, *learning*. During implementation in GAMS, we suggest to define $\bar{H}$ as an upper bound for the sharp augmented Lagrangian L, not as an inequality constraint as in the equation (3.28). This is because we do not want to break the rule in MSG, i.e., all inequality constraints have to turned in equality ones and then imported in the dual function via augmented Lagrangians.

Anyway, using $\bar{H}$ is very crucial for MSG algorithm to find the solution. In Table 3.1, we present a set of appropriate parameters for our problems with $\mathbf{0}_3 = (0, 0, 0)^T$:

Table 3.1: Values of MSG Parameters.

	$(\mathbf{u}_0, c_0)$	α	δ	$\bar{H}$
Problem 1	$(\mathbf{0}_3, 0)$	1	2	63
Problem 2	$(\mathbf{0}_3, 0)$	4	1.15	210

Remark 3.2.2. There are different formulations for step size s_k suggested in the literature [15, 37]. We note that in our problems these step sizes do not have a significant influence on the computation time, and so on. They all work fine, and we found the global optima for both problems. □

The minimization problem stated in Step 1 of MSG algorithm is a nonlinear optimization problem. A suitable model, i.e., solution procedure of GAMS for this problem is NLP and its related solver is CONOPT solver of GAMS.

Remark 3.2.3. The subproblem in Step 1 of MSG algorithm can be solved as an NLP model by CONOPT solver of GAMS or as a MINLP model by DICOPT solver of GAMS. For MINLP model, one needs to define the vector $\mathbf{z}$ not as a variable, but as a binary variable in GAMS notation. With both models we arrive at the optimal solution and there is no superiority between these models in our problems. In fact, when NLP model is used in a GAMS programme, CONOPT is the default solver and when MINLP model is used DICOPT is the default solver. This means that an OPTION statement is not necessary for calling the solver, just defining the model type in the SOLVE statement is enough:

$$
\begin{gathered}
\textit{SOLVE xz USING nlp MINIMIZING L} \\
\textit{SOLVE xz USING minlp MINIMIZING L}
\end{gathered} \tag{3.32}
$$

3.2.3 DNLP Model with BARON

Optimization problems of two example problems are stated in (3.9) and (3.11). In these problems, the first-order derivatives of the objective functions are discontinuous at nondifferentiable points, occurring at target values of responses having two-sided desirability. For this type of objectives, the best model type of GAMS is called DNLP, and the appropriate solver for these models is BARON. BARON only needs the availability of finite lower and upper bounds on the variables and no modifications in the constraints.

3.3 Results

All runs are conducted on a computer with Intel (R) Core (TM) 2 Duo CPU T 7300 @ 2.00 GHz processor. We present optimization results of three different problems: (*i*) wire bonding process optimization problem (i.e., problem 1), (*ii*) a special case of wire bonding process optimization problem with 3 responses, and (*iii*) tire tread compound problem (i.e., problem 2).

In Table 3.2, we present our results in comparison with the existing results from the literature for problem 1. In Castillo et al.'s work [19], the optimal solutions for this problem are obtained from a kind of generalized reduced gradient algorithm (GRG2) in Ms Excel Solver and Hooke-Jeeves (HJ) univariate search. Moreover, in the study of Chang et al. [16], the same problem is solved by a new approach as explained in the previous chapter.

We compare our results obtained from CONOPT solver applied on the dual problems of MSG and from BARON solver applied on the primal problem with the ones of Castillo et al. and Chang et al.. The optimal solution as indicated in Castillo et al. [19] is the only optimal one in the region of interest. All of the points given in the table are basically the same solution points because they give close desirability values, except that of Ch'ng in row 3.

In Table 3.3, we present results related with the special case of the wire bonding process optimization problem with 3 responses models. Considering highly correlated responses

y_2, y_3, y_5 and y_6 as a single response in wire bonding process optimization problem (problem 1), Castillo et al. [19] provide a new mutual model for all of these responses. The details of these models are given in Appendix A. Since optimal response combination calculated by the individual and overall desirability functions proposed by Ch'ng et al. [16] is not available in their study corresponding row of Table 3.3 (i.e., in row 2) is includes missing values.

In Table 3.4, we present our results in comparison with the existing results from the literature for problem 2. In Derringer and Suich's (DS) work [25], the optimal points for this problem are obtained by a search technique similar to the one of Hooke and Jeeves. Moreover, in the study of Jeong and Kim (JK) [49], this same problem is solved by a new approach as explained in Chapter 2. We compare our results obtained from CONOPT solver applied on the dual problems of MSG and BARON solver applied on the primal problem with the ones of Derringer and Suich and Jeong and Kim.

By looking at the overall desirability, we conclude that these results can be accepted as the same solution, except that of JK in row 2.

Table 3.2: Optimal solutions of the wire bonding problem.
Numbers in the first column: 1: GRG2, 2: HJ, 3: Ch'ng, 4: BARON, and 5: MSG+CONOPT.

	$(\bar{x}_1, \bar{x}_2, \bar{x}_3)$	$(\bar{y}_1, \bar{y}_2, \bar{y}_3, \bar{y}_4, \bar{y}_5, \bar{y}_6)$
1	$(0.1039, 1.0000, 0.7988)$	$(186.0249, 174.5222, 172.0592, 192.6354, 173.0744, 185.0036)$
2	$(0.1078, 1.0000, 0.7988)$	$(186.0475, 174.5247, 172.0582, 192.6998, 173.0913, 184.9979)$
3	$(-0.0435, 1.0000, 0.8654)$	$(185.0000, 174.5786, 172.3065, 190.0000, 172.4829, 185.4201)$
4	$(0.1050, 1.0000, 0.7980)$	$(186.0368, 174.5178, 172.0518, 192.6509, 173.0732, 184.9922)$
5	$(0.1050, 1.0000, 0.7980)$	$(186.0368, 174.5178, 172.0518, 192.6509, 173.0732, 184.9922)$

	$(d_1(\bar{y}_1), d_2(\bar{y}_2), d_3(\bar{y}_3), d_4(\bar{y}_4), d_5(\bar{y}_5), d_6(\bar{y}_6))$	$\bar{D}$
1	$(0.2050, 0.3015, 0.1373, 0.4729, 0.2050, 1.0006)$	0.3061
2	$(0.2095, 0.3016, 0.1372, 0.4600, 0.2016, 1.9999)$	0.3061
3	$(0.0000, 0.3663, 0.1845, 1.0000, 0.1986, 1.2336)$	0.1079
4	$(0.2074, 0.3012, 0.1368, 0.4698, 0.2049, 1.0008)$	0.3061
5	$(0.2074, 0.3012, 0.1368, 0.4698, 0.2049, 1.0008)$	0.3061

Table 3.3: Optimal solutions of the wire bonding problem with 3 responses.
Numbers in the first column: 1: GRG2, 2: Ch'ng, 3: BARON, and 4: MSG+CONOPT.

	$(\bar{x}_1, \bar{x}_2, \bar{x}_3)$	$(\bar{y}_1, \bar{y}_2, \bar{y}_3, \bar{y}_4, \bar{y}_5, \bar{y}_6)$
1	$(-0.0074, 1.0000, 0.7417)$	$(186.9027, 173.0484, 170.1249, 190.0137, 170.9173, 182.4345)$
2	$(0.0977, 0.9296, 0.7539)$	$(186.1, 172.3, 170.0, 190.0, 170.8, 182.6)$
3	$(0.0000, 1.0000, 0.7140)$	$(187.3287, 172.7017, 170.0000, 189.9982, 170.5568, 181.7580)$
4	$(-0.0020, 1.0000, 0.7210)$	$(187.2210, 172.7885, 170.0000, 189.9995, 170.6464, 181.9277)$

	$(d_1(\bar{y}_1), d_2(\bar{y}_2), d_3(\bar{y}_3), d_4(\bar{y}_4), d_5(\bar{y}_5), d_6(\bar{y}_6))$	$\bar{D}$
1	$(0.3805, 0.2032, 0.0083, 1.0027, 0.0612, 0.8290)$	0.1789
2	–	–
3	$(0.4657, 0.1801, 0.0010, 0.9996, 0.0371, 0.7839)$	0.1160
4	$(0.4442, 0.1859, 0.0010, 0.9999, 0.0431, 1.7952)$	0.1189

Table 3.4: Optimal solutions of the tire tread compound problem.
Numbers in the first column: 1: DS, 2: JK, 3: BARON, and 4: MSG+CONOPT.

	$(\bar{x}_1, \bar{x}_2, \bar{x}_3)$	$(\bar{y}_1, \bar{y}_2, \bar{y}_3, \bar{y}_4)$
1	$(-0.050, 0.145, -0.868)$	$(129.4333, 1300.0000, 465.7313, 68.0051)$
2	$(-0.157, 1.219, -0.604)$	$(139.82, 1239.10, 446.51, 73.93)$
3	$(-0.052, 0.148, -0.869)$	$(129.4252, 1300.2000, 465.9318, 68.0207)$
4	$(-0.067, 0.186, -0.862)$	$(129.7169, 1299.9, 465.9420, 68.2421)$

	$(d_1(\bar{y}_1), d_2(\bar{y}_2), d_3(\bar{y}_3), d_4(\bar{y}_4))$	$\bar{D}$
1	$(0.1887, 1.0000, 0.6573, 0.9327)$	0.5832
2	$(0.3966, 0.7974, 0.4647, 0.1424)$	0.3803
3	$(0.1885, 1.0006, 0.6593, 0.9306)$	0.5833
4	$(0.1943, 0.9997, 0.6594, 0.9010)$	0.5829

3.4 Discussion and Conclusion

With this chapter, we suggest an alternative solution procedure for maximization of desirability functions. It can be said that this approach is solely different from the current optimization techniques. The efficiency of coding and implementing this new procedure is demonstrated with numerical experiments. The two problems used in experiments are the "lab animals" for testing almost all new desirability optimization approaches. Moreover, they contain both one-sided and two-sided individual desirability functions arising in multi-response problems.

Main superiority of our procedure including two different strategies for the optimization stage lies in its independence from properties of the problem like convexity and differentiability. Although our first strategy which includes implementing MSG with CONOPT may need mathematical knowledge related with Sharp Augmented Lagrangians, the second strategy with BARON yields a practical and efficient approach together with adjusted desirability functions.

We propose this second application with BARON as a strong alternative to the traditional methods and softwares mentioned in Chapter 2 for desirability maximization. Let us summarize our suggestion: (*i*) write the overall optimization problem of desirability functions based on adjusted desirability functions in GAMS environment, (*ii*) solve the overall problem by nonsmooth optimization methods, especially, BARON solver of GAMS.

Let us recall from Chapter 2, the original problem of desirability functions given in (2.6), together with overall desirability given in (2.4), and individual desirabilities introduced in (2.2) and (2.3). A careful eye would observe that it is possible to obtain the convex formulation of our two optimization problems from experiments by applying the negative logarithm to the overall desirability. This would result with convex individual desirability functions which are originally concave and the overall desirability function would be a convex combination of individual ones. Eventually, the resulting problem would have been a convex composite nonsmooth optimization, where nonsmoothness come from the nondifferentiable points occurring in the target point of individual desirability functions. Then, one can solve this problem by a software from convex optimization, without any assumption on differentiability.

We don't suggest convex way. Firstly, for implementation of convex optimization softwares, some tricks like introducing equality constraints into the problem and some reformulations of the constraints would be needed. Secondly, convex approach would not work when individual desirability functions are not concave as in the cases where superscripts s_1 and s_2 in the formulation of individual desirability (2.2) and (2.3) are greater than 1 or when there are more than one nondifferentiable points in an individual desirability function.

Our approach including BARON safe for all of these cases. Moreover, besides having no assumption on convexity and differentiability, one does not need to worry about the initial point selection and reformulating constraints. This is a straightforward, easy to implement and less computational method.

CHAPTER 4

AN ANALYSIS OF WEIGHTED DESIRABILITY FUNCTIONS BASED ON NONSMOOTH OPTIMIZATION

4.1 Introduction

In this chapter, we apply logarithm on desirability functions which result with an equivalent additive (separable) optimization problem to the original overall desirability maximization. By using theoretical opportunities of this new formulation, we analyze some aspects of desirability functions like their nonsmooth characters and Pareto-optimality of the global solutions of the overall problems. This will also be a preparation for the next chapter where we present a general class of functions to explain the structure of desirability functions used in practice. In applications, shape of an individual desirability function is chosen by decision maker who decides the parameters such as bounds and targets of the responses, and so on. A one-sided individual desirability function $d(\cdot)$ $(= d_j) : [l, u] \to [0, 1]$ is either linear or nonlinear but smooth and monotone on $[l, u]$ $(= \mathbb{I}_j = [l_j, u_j])$ and a two-sided function $d(\cdot) : [l, u] \to [0, 1]$ is either piecewise linear or nonlinear but piecewise monotone and nonsmooth at its target point.

One important property of the functions employed in practice for assessing desirability of a response is that these functions are *min-type* functions containing at most one nondifferentiable points. However, a decision maker can choose a two-sided desirability functions including more than one nondifferentiable point according to the desired behavior of function around its target point as mentioned in Castillo et al. [19]. Based on this idea, we improve the theory of desirability functions accordingly. In this context, optimality properties of the optimization problem including desirability functions with a finite number of nondiffferentiable points are analyzed.

In this chapter, we apply negative logarithm on weighted case of desirability functions which result with an equivalent additive (separable) optimization problem to the original overall desirability maximization. By using theoretical opportunities of this new formulation, we analyze some aspects of desirability functions including a finite number of nondifferentiability points related with their nonsmooth characters and Pareto-optimality of the global solutions of the overall problems. Content of this chapter is also a preparation for Chapter 5 where we elaborate *max-type* character of the negative logarithm applied GDFs by a general class of functions ,i.e., *continuous selection functions*.

4.2 Weighted Desirability Functions

Weighted desirability functions make it possible to write the overall desirability from the viewpoint of the response trade-offs. In practice, weights are assigned by decision makers according to importance levels of different responses in the overall desirability.

The weighted overall desirability function is defined by:

$$D(\mathbf{Y}(\mathbf{x})) = \left(\prod_{j=1}^{m} d_j(\mathbf{Y}(\mathbf{x}))^{w_j} \right)^{\frac{1}{\sum_{j=1}^{m} w_j}} \tag{4.1}$$

where $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_m)^T$ is the vector of responses, $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ is the vector of factors, m is the number of responses and $w_j \geq 0$ are the weights $(j = 1, 2, \ldots, m)$. The function D is a continuous function of $\mathbf{x}$, bounded by 0 from below and by 1 from above. We remember that $D^Y(\mathbf{x}) = D(\mathbf{Y}(\mathbf{x})) = D(\mathbf{y})$, where $\mathbf{y} = \mathbf{Y}(\mathbf{x})$, and $d_j^Y(\mathbf{x}) = d_j(Y_j(\mathbf{x})) = d_j(y)$, where $y_j = Y_j(\mathbf{x})$, and $\mathbf{y} = (y_1, y_2, \ldots, y_m)^T$ $(j = 1, 2, \ldots, m)$.

The optimization problem of (4.1) can be defined by implicitly defining bound constraints as follows:

$$\begin{array}{ll} \text{maximize} & D^Y(\mathbf{x}) = \left(d_1^Y(\mathbf{x})\right)^{w_1} \cdot \left(d_2^Y(\mathbf{x})\right)^{w_2} \cdot \ldots \cdot \left(d_m^Y(\mathbf{x})\right)^{w_m} \\ \text{subject to} & \mathbf{x} \in \mathbb{X} \cap \mathbb{I}^X, \end{array} \tag{4.2}$$

where the constraint of the problem is introduced and explained below.

Remark 4.2.1. We have assumed that $w_1 + w_2 + \ldots + w_m = 1$ without loss of generality given for $w_j \geq 0$ not all zero at the same time $(j = 1, 2, \ldots, m)$. If all weights were zero at same time, i.e., $w_j = 0$ $(j = 1, 2, \ldots, m)$, then any $y_j \in \mathbb{R}$ would become a solution of the problem (4.2). We notice that any sum of weights, say $\omega_1 + \omega_2 + \ldots + \omega_m = r$ for some $r > 0$, can be reduced to 1 by defining $w_j := \omega_j / r$ $(j = 1, 2, \ldots, m)$. □

We have $\mathbf{x} \in \mathbb{X} \subset \mathbb{R}^n$ and $x_i \in \mathbb{X}_i$ where $\mathbb{X}$ is the Cartesian product of regions $\mathbb{X}_i$ ($i \in I = 1, 2, \ldots, n$):

$$\mathbb{X} = \bigtimes_{i \in I} \mathbb{X}_i \quad (= \mathbb{X}_1 \times \mathbb{X}_2 \times \ldots \times \mathbb{X}_n). \tag{4.3}$$

We remember that every response y_j is desired in some interval $\mathbb{I}_j = [l_j, u_j]$ ($j = 1, 2 \ldots, m$). Now, we define

$$\mathbb{I}^X := \left\{ \mathbf{x} \in \mathbb{R}^n \mid Y_j(\mathbf{x}) \in \mathbb{I}_j \ (j = 1, 2, \ldots, m) \right\} = \bigcap_{j=1}^{m} \left(Y^{-1} \left([l_j, u_j] \right) \right). \tag{4.4}$$

Here, $\mathbb{I}^X$ is closed as it is the finite intersection of the closed sets $Y^{-1}\left([l_j, u_j]\right) \subset \mathbb{R}^n$. Similarly, $\mathbb{X}$ is closed. As a result $\mathbb{X} \bigcap \mathbb{I}^X$ is compact and $D^Y(\mathbf{x})$, the objective function of (4.2), is continuous, a globally optimal point to the problem (4.2) always exists, but it may not be unique.

4.3 Preventing from Undesirability

A two-sided desirability function $d(Y(\mathbf{x}))$ becomes zero at the lower bound l and upper bound u of the response $Y_j(\mathbf{x})$. To continue our analysis, we need to prevent the individual desirabilities from vanishing and always have them satisfy $d(Y(\mathbf{x})) > 0$. This will be necessary when we want to apply the logarithm to obtain the separable overall function in the next section and save the overall desirability function from being undesirable.

We propose two suitable techniques for preventing two-sided desirability functions from undesirability: one based on cutting-off the interval around the corresponding point and the other one based on perturbing the whole function directly by adding an arbitrarily small constant $\epsilon > 0$.

Cutting-off the interval of y (*Technique 1*): We introduce lower bounds $\delta^l > 0$ and $\delta^u > 0$ (arbitrarily small numbers) for $Y(\mathbf{x}) - l$ and $u - Y(\mathbf{x})$, respectively. This can be interpreted as a cutting-off of a piece of the interval of $Y(\mathbf{x})$ at l of length δ^l and at u of length δ^u. By cutting-off the half neighborhoods $[l, l + \delta^l)$ and $(u - \delta^u, u]$, which are mapped into the intervals $[0, \epsilon^l]$ and $[0, \epsilon^u]$ ($\epsilon^l := d(l + \delta^l)$ and $\epsilon^u := d(u - \delta^u)$ are arbitrarily small numbers), respectively, the function is prevented from entering these intervals and desirabilities never become zero as shown in Figure 4.1.

The new desirability function will be defined on the interval $[l + \delta^l, u - \delta^u]$ and we always have $d(Y(\mathbf{x})) > 0$, whereas it will not be defined on the intervals $[l, l + \delta^l)$ and $(u - \delta^u, u]$.

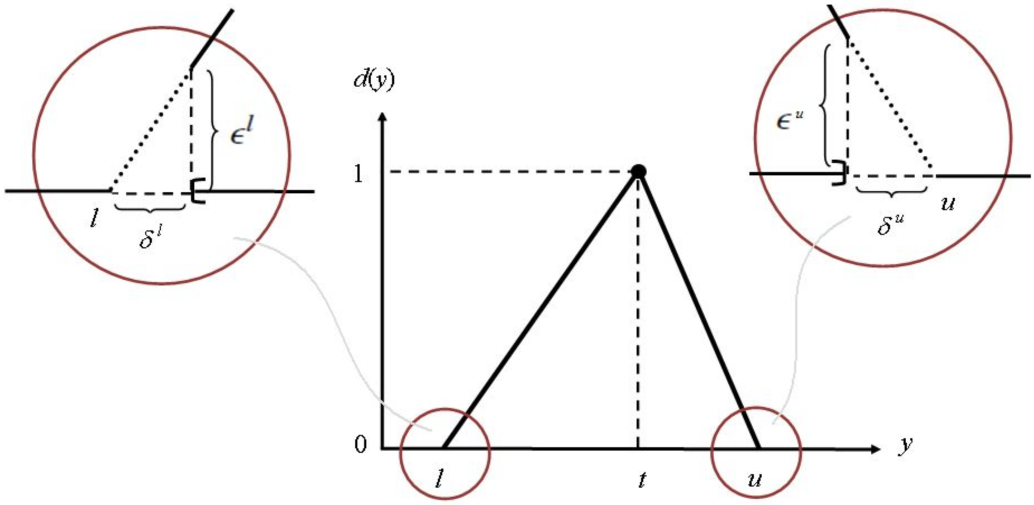

Figure 4.1: Cutting-off of individual desirability functions $d_j(y_j)$ $(j = 1, 2, \ldots, m)$.

In the optimization problem (4.2), we suggest to add two more additional constraints that do not affect the solution but ensure that the two-sided desirabilities never vanish, based on this technique for all $j = 1, 2, \ldots, m$:

$$\begin{aligned} &(Y(\mathbf{x}) - l)^2 \geq (\delta^l)^2, \quad \text{and} \\ &(u - Y(\mathbf{x}))^2 \geq (\delta^u)^2. \end{aligned} \tag{4.5}$$

Shifting the desirability functions (*Technique 2*): We introduce ϵ-individual two-sided desirability functions with $d^\epsilon(Y(\mathbf{x})) := (d + \epsilon)(Y(\mathbf{x}))$, where $\epsilon := \epsilon_{Y(\mathbf{x})} > 0$ (arbitrarily small number) to be a lower bound for ϵ-individual desirabilities, $d^\epsilon(Y(\mathbf{x})) \geq \epsilon$. This can be interpreted as a shift in the function values from $[0, 1]$ to $[\epsilon, 1 + \epsilon]$. Hence, at $Y(\mathbf{x}) = l$ and $Y(\mathbf{x}) = u$, we prevent desirability from being zero; there, it will be $d^\epsilon(Y(\mathbf{x})) = \epsilon$. At $Y(\mathbf{x}) = t$, the desirability will be $d^\epsilon(Y(\mathbf{x})) = 1 + \epsilon$ as shown in Figure 4.2.

By doing this, we change the definition of the individual desirability functions with respect to ϵ as follows:

$$d^\epsilon(y) := \begin{cases} \epsilon, & \text{if} \quad y \leq l, \\ (\frac{y-l}{t-l})^{s_1} + \epsilon, & \text{if} \quad l < y \leq t, \\ (\frac{y-u}{t-u})^{s_2} + \epsilon, & \text{if} \quad t < y \leq u, \\ \epsilon, & \text{if} \quad y > u. \end{cases} \tag{4.6}$$

Remark 4.3.1. Our Techniques 1 and 2 are suitable for both linear and nonlinear versions of individual desirability functions. The small numbers δ^l, δ^u, ϵ^l, ϵ^u and ϵ should be chosen according to this shape of the desirability function near l and u. Moreover, we note that our

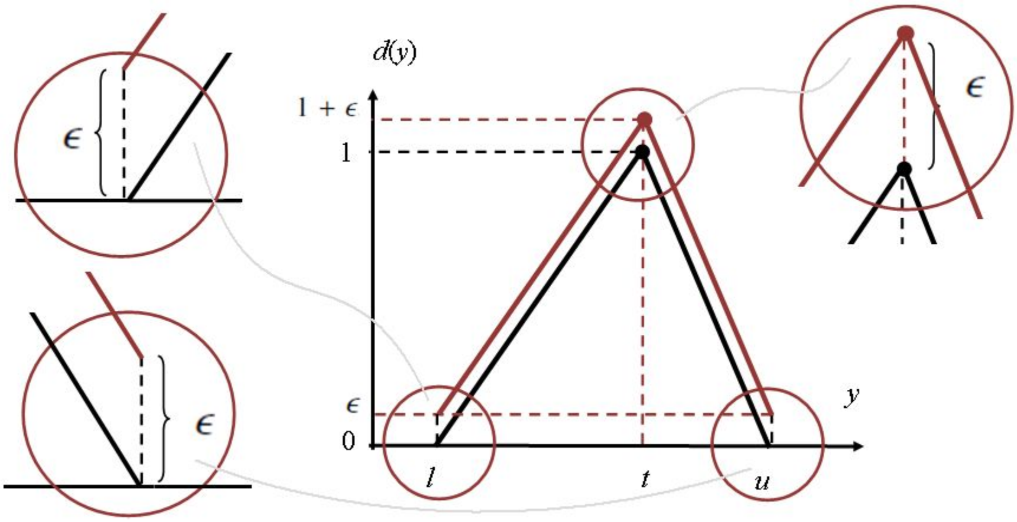

Figure 4.2: Shifting individual desirability functions $d_j(y_j)$ $(j = 1, 2, \ldots, m)$.

original problem is a maximization one whose optimal solution will not be affected by this cutting-off and shifting.

4.4 Additive Overall Desirability Function

We apply negative logarithm to the objective function of (4.2) which is defined explicitly in (4.1) and obtain an additive expression for the overall function $F(\mathbf{Y}(\cdot)) := -\log(D(\mathbf{Y}(\cdot)))$ with respect to the individual desirabilities:

$$F(\mathbf{Y}(\cdot)) := \sum_{j=1}^{m} w_j f_j(Y_j(\cdot)). \tag{4.7}$$

Here, the functions f_j will be the negative logarithm of the individual desirability functions d_j. However, since d_j becomes zero at the lower and upper bound of a two-sided desirability function, we can use techniques introduced in Section (4.3) to make sure that the logarithm is always defined.

We can define function f $(= f_j)$ either on the interval (l, u) based on the Technique 1:

$$f(y) := -\log(d(y)) \quad f(Y(\cdot)) = -\log(d(Y(\cdot))), \tag{4.8}$$

or on the interval $[l, u]$ based on the Technique 2:

$$f(y) := -\log(d^{\epsilon}(y)) \quad f(Y(\cdot)) = -\log(d^{\epsilon}(Y(\cdot))), \tag{4.9}$$

If we apply Technique 1 to individual desirability functions d, then their logarithm will always be defined on the open interval (l, u) of y, where $y_j = Y_j(\mathbf{x})$, for all $j = 1, 2, \ldots, m$.

The functions f_j are of the form $f : (l, u) \to [0, M)$ with

$$M := \max \left\{M^l, M^u\right\}, \tag{4.10}$$

where $M^l := -\log(\epsilon^l) = -\log(d(l + \delta^l))$ and $M^u := -\log(\epsilon^u) = -\log(d(u - \delta^u))$ for positive constants $M \ (= M_j)$, $M^l \ (= M^l_j)$ and $M^u \ (= M^u_j)$.

The domain of f^Y is $[\mathbf{l}_x, \mathbf{u}_x]$ and it will be affected from this cutting-off process. If vectors

$$\mathbf{x}^l := Y^{-1}(\{l\}) \quad \text{and} \quad \mathbf{x}^u := Y^{-1}(\{u\}) \tag{4.11}$$

are uniquely existing (in case of nonuniqueness, i.e., "$\in$": chosen) in $[\mathbf{l}_x, \mathbf{u}_x]$, then by cutting-off the intervals around the bounds l and u of $Y(\mathbf{x})$ will result in a cutting-off from the domain of f^Y around $\mathbf{x}^l$ and $\mathbf{x}^u$, since $Y(\mathbf{x})$ is a continuous function. This will deteriorate the compactness and connectedness of the domain of f^Y. If they are outside of $[\mathbf{l}_x, \mathbf{u}_x]$ together with their corresponding neighborhood, then there will be no change in the definition of f^Y, i.e., $f^Y : [\mathbf{l}_x, \mathbf{u}_x] \to [0, M)$.

Because of this possible deterioration of compactness and connectedness, we choose shifting strategy explained under Technique 2 for our further studies to have the logarithm always be defined. In this case, there will not be a compactness and connectedness problem in the domain of f^Y and the function f will be defined everywhere on $[l, u]$.

4.4.1 Optimization of Additive Overall Desirability Function

The functions obtained by the negative logarithm of desirability functions are again composite functions, and we will denote them by $f \ (= f_j)$ as a function of y and $f^Y \ (= f^Y_j)$ as a function of $\mathbf{x}$, according to the needs of the context:

$$f^Y(\mathbf{x}) := f(y) = f(Y(\mathbf{x})), \quad \text{where} \quad y = Y(\mathbf{x}). \tag{4.12}$$

It is important to note that each $f_j(\cdot) : \mathbb{I}_j \to [0, M_j)$ $(j = 1, 2, \ldots, m)$ is always positive and have an underlying *max-type* structure on the interval $\mathbb{I}_j$ based on their derivation from min-type functions. All the observations we present in this chapter constitute a starting point for the next chapter.

The additive (separable) overall desirability function given in (4.7) as the weighted sum of individual $f_j(Y_j(\mathbf{x}))$ $(j = 1, 2, \ldots, m)$:

$$F^Y(\cdot) = F(\mathbf{Y}(\cdot)) = F(\mathbf{y}), \tag{4.13}$$

where $\mathbf{y} = \mathbf{Y}(\mathbf{x}) = (Y_1, Y_2, \ldots, Y_m)^T(\mathbf{x})$, $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ with $x_i \in \mathbb{R}$ $(i = 1, 2, \ldots, n)$, $Y_j : \mathbb{R}^n \to \mathbb{R}$, $f_j : \mathbb{R} \to \mathbb{R}$ $(j = 1, 2, \ldots, m)$, $F : \mathbb{R}^m \to \mathbb{R}$ and $F^Y : \mathbb{R}^n \to \mathbb{R}$.

The overall desirability function $F(\mathbf{Y}(\mathbf{x}))$ (or $F^Y(\mathbf{x})$), as can be seen in (4.7), is a linear aggregation of the individual functions $f(Y(\cdot)) = -\log(d^{\epsilon}(Y(\cdot)))$, i.e., the negative logarithm of the ϵ-individual desirabilities.

Now, let us write the additive overall optimization problem with the objective function given above in (4.7):

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & F(\mathbf{Y}(\mathbf{x})) \\ \text{subject to} \quad & \mathbf{x} \in \mathbb{X}, \\ & Y_j(\mathbf{x}) \in \mathbb{I}_j \quad (j = 1, 2, \ldots, m). \end{aligned} \tag{4.14}$$

Here, $\mathbf{x} \in \mathbb{X} \subset \mathbb{R}^n$, where the parallelepiped $\mathbb{X}$ given in (4.3) is implicitly defined by a finite number of inequality constraints and $Y_j(\mathbf{x}) \in \mathbb{I}_j \subseteq \mathbb{R}$, where $\mathbb{I}_j$ is an interval.

Remark 4.4.1. We note that this reformulation of the overall problem does not cause any change in the global optimal solution, i.e., the solution of the original problem (4.2) and the one of (4.14) are the same. However, we could not say the same thing for the solution if $F(\mathbf{Y}(\mathbf{x}))$ would have been the weighted sum of the individual desirability functions $d_j(Y_j(\mathbf{x}))$. For a review of different reformulations similar to the desirability function optimization and their solution characteristics, we refer to the study of Park and Kim [81]. □

4.4.2 A Finite Number of Nondifferentiable Points in Desirability Functions

Although in practice two-sided desirability functions include only one nondifferentiable points, there can be more than 1 nondifferentiable point in a two-sided individual desirability function reflecting the desired behavior of function around its target point. In this subsection, we analyze some differentiability properties of individual desirability functions when they are allowed to include a finite number of nondifferentiable points and write the corresponding overall optimization problem. To do this, we follow our idea of *adjusted* individual desirability functions presented in Chapter *3*. In Figure 4.3, an example of an individual desirability function including more than one nondifferentiable point and its possible outcome with applying negative logarithm is shown.

When we look at its shape, we see that the desirability function shown in Figure 4.3 has a similar tendency to target value as in $s_1 < 1$ and $s_2 > 1$ case of a two-sided individual desirability function. Let us assume that there are $\kappa_j - 1$ $(\kappa_j \in \mathbb{R})$ $(j = 1, 2, \ldots, m)$ many nondifferentiable

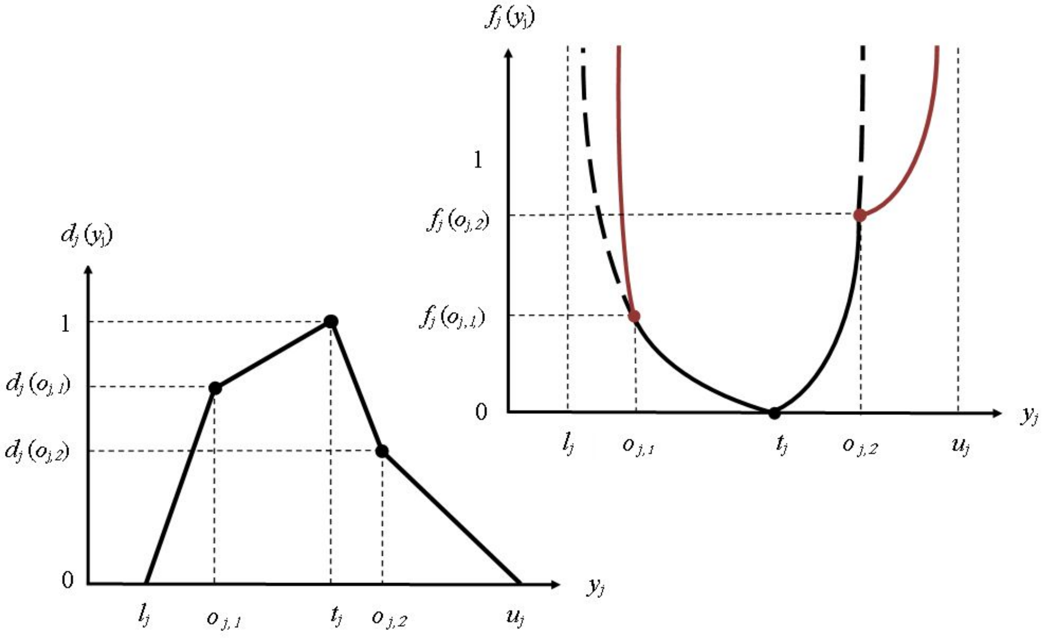

Figure 4.3: Individual desirability functions: $d_j(y_j)$ ($j = 1, 2, \ldots, m$) and $f_j(y_j)$: after negative logarithm applied.

points and hence, k_j "pieces" in individual desirability functions of a multi-response optimization problem. Here, we name the part of the function between any two nondifferenble points by the word "piece". We say this to prevent a possible confusion between the notions of "piece" and "side" for individual desirability functions. In conventional desirability functions including a single nondifferentiable point the meanings of these notions coincide, however when we speak of a finite number of nondifferentiable points they have separate meanings as we explain below.

In a two-sided individual desirability functions, a "side" is the part of the function between lower and target values of the response where in between there can be a finite number of nondifferentiable points. In Figure 4.3, functions have 2 sides but 4 pieces because of 3 nondifferentiable points. Hence, a "piece" is the part of the function lying between consecutive nondifferentiable points. Since a unique response value corresponds to every combination of factor levels, one 'piece' of the function will be active. When a piece of a individual Gdesirability function is active, remaining pieces are inactive. As a result of this side and piece discussion, we can use the similar activeness argument for pieces also as we did for sides in Chapter *3*.

An individual desirability function $f_j^Y (= f_j^Y(\mathbf{x}, \mathbf{z}_j))$ is a continuous function with respect to

$\mathbf{x}$ including $\kappa_j - 1$ many nondifferentiable points. This function can be expressed as follows for $\mathbf{z}_j = (z_{j,1}, z_{j,2}, \ldots, z_{j,\kappa_j})^T$ with $\sum_{\kappa=1}^{\kappa_j} z_{j,\kappa} = 1$ $(j = 1, 2, \ldots, m)$ and $z_{j,\kappa} \in \{0, 1\}$ $(\kappa = 1, 2, \ldots, \kappa_j; j = 1, 2, \ldots, m)$:

$$f_j^Y(\mathbf{x}, \mathbf{z}_j) = \sum_{\kappa=1}^{\kappa_j} z_{j,\kappa} f_{j,\kappa}^Y(\mathbf{x}) \quad (j = 1, 2, \ldots, m). \tag{4.15}$$

Hence, the overall problem given in 4.14 turns into

$$\begin{aligned}
\text{minimize} \quad & \sum_{j=1}^{m} w_j \sum_{\kappa=1}^{\kappa_j} z_{j,\kappa} f_{j,k}^Y(\mathbf{x}) \\
\text{subject to} \quad & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x], \\
& f_{j,\kappa}^Y(\mathbf{x}) \geq 0 \quad (\kappa = 1, 2 \ldots \kappa_j; j = 1, 2, \ldots, m), \\
& \sum_{\kappa=1}^{\kappa_j} z_{j,\kappa} = 1 \quad (j = 1, 2, \ldots, m), \\
& z_{j,\kappa} \in \{0, 1\} \quad (\kappa = 1, 2, \ldots, \kappa_j; j = 1, 2, \ldots, m).
\end{aligned} \tag{4.16}$$

This is a minimization of an additive objective function which is a convex combination of nonconvex functions $f_j^Y(\mathbf{x}, \mathbf{z}_j)$ with $w_j \geq 0 \quad (j = 1, 2, \ldots, m)$ and $\sum_{j=1}^{m} w_j = 1$. We note that each functions $f_{j,\kappa}^Y$ is assumed to be a C^2-function $f_{j,\kappa}^Y : \mathbb{R}^n \to \mathbb{R}$. Here, $z_{j,\kappa}$ is the indicator of the active piece $f_{j,\kappa}^Y$ of f_j^Y:

$$z_{j,\kappa} = \begin{cases} 1, & \text{if} \quad f_j^Y(\mathbf{x}) = f_{j,\kappa}^Y(\mathbf{x}), \\ 0, & \text{otherwise.} \end{cases} \tag{4.17}$$

The constraint $z_{j,\kappa} \in \{0, 1\}$ can be equivalently stated as $z_{j,\kappa} - z_{j,\kappa}^2 = 0$ as we used in Chapter *3* and $\mathbf{z}_j = (z_{j,1}, z_{j,2}, \ldots, z_{j,\kappa_j})^T$ is a unit vector of length κ_j. Problem (4.16) is a global optimization problem of the nonconvex and nonsmooth objective function with possibly many local minima and maxima. By using nonsmooth and nonconvex optimization we state the special case of this problem with max-type functions:

$$\begin{aligned}
\text{minimize} \quad & F^Y(\mathbf{x}) \; (= \sum_{j=1}^{m} w_j \max_{\kappa=1,2,\ldots,\kappa_j} f_{j,\kappa}^Y(\mathbf{x})) \\
\text{subject to} \quad & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x], \\
& F^Y(\mathbf{x}) \geq \mathbf{0},
\end{aligned} \tag{4.18}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_m)^T$ and the objective function is a convex combination of the max-type functions f_{j,κ_j}^Y.

Here, our aim is to establish the link of the individual desirability functions to max-type functions. By using this link, we propose a topological approach to a class of piecewise max-type functions motivated by desirability functions including stability and further structural insights, in fact, generic results presented in Chapter 5.

We complete this part by giving a necessary condition for the global optimal of the additive overall problem (4.14) based on *Clarke subdifferential*. We write and evaluate the Clarke subdifferential and the Clarke directional derivative [17] of the objective function of (4.14) $F^Y(\mathbf{x}) = \sum_{j=1}^{m} w_j(f_j \circ Y_j)(\mathbf{x})$ for the cases when f_j is Lipschitz continuous and Y_j is continuously differentiable for all $j = 1, 2, \ldots, m$. We notice that f_j may contain a finite number of non-differentiable points as far as Lipschitzness is not deteriorated for Clarke subdifferential and optimality condition to be valid.

Then, we use the Chain Rule and the Sum Rule at any corresponding point $\mathbf{x} \in \mathbb{R}^n$. Then, we give a necessary optimality condition for the problem (4.14).

a. *Clarke Subdifferential* $\partial f^Y(\mathbf{x})$ for $f^Y(\mathbf{x})$:

$$\begin{aligned}\partial F^Y(\mathbf{x}) &= \partial_C\left(\sum_{j=1}^{m} w_j(f_j \circ Y_j)(\mathbf{x})\right) \subseteq \sum_{j=1}^{m} w_j \partial_C(f_j \circ Y_j)(\mathbf{x}) \subseteq \sum_{j=1}^{m} w_j \partial f_j(Y_j(\mathbf{x}))\nabla Y_j(\mathbf{x}) \\ &\subseteq \operatorname{co}\left\{\sum_{j=1}^{m} w_j \upsilon_j \nabla Y_j(\mathbf{x}) \mid \upsilon_j \in \partial f_j(Y_j(\mathbf{x}))\ (j = 1, 2, \ldots, m)\right\},\end{aligned} \tag{4.19}$$

where $\partial f_j(Y_j(\mathbf{x}))$ is the Clarke subdifferential of f_j at $Y_j(\mathbf{x})$ $(j = 1, 2, \ldots, m)$.

b. Moreover, for the cases when $f_j : [l_j, u_j] \to \mathbb{R}$ is convex, the *Clarke directional derivative* [17] of the composition $(f_j \circ Y_j)'_C(\mathbf{x}; v_j)$ exists for all $\mathbf{x} \in \mathbb{R}^n$, and all $j = 1, 2, \ldots, m$, $\mathbf{v} := (v_1, v_2, \ldots, v_n)^T \in \mathbb{R}^n$ and it satisfies

$$(f_j \circ Y_j)'_C(\mathbf{x}; v_j) \leq f_j(Y_j(\mathbf{x}) + \nabla Y_j(\mathbf{x}) v_j) - f_j(Y_j(\mathbf{x})). \tag{4.20}$$

Then, the Clarke directional derivative $(f^Y)'_C(\mathbf{x}; \mathbf{v})$ of $f^Y(\mathbf{x}) := \sum_{j=1}^{m} w_j(f_j \circ Y_j)(\mathbf{x})$ exists for all $\mathbf{x}$ and $\mathbf{v}$ in $\mathbb{R}^n$:

$$\left(\sum_{j=1}^{m} w_j(f_j \circ Y_j)\right)'_C(\mathbf{x}; v_j) \leq \sum_{j=1}^{m} w_j (f_j \circ Y_j)'_C(\mathbf{x}; v_j) \leq \sum_{j=1}^{m} w_j \left[f_j(Y_j(\mathbf{x}) + \nabla Y_j(\mathbf{x}) v_j) - f_j(Y_j(\mathbf{x}))\right]. \tag{4.21}$$

We define $\mathbf{c}_y^l$, $\mathbf{c}_y^u$, $\mathbf{c}_x^l$ and $\mathbf{c}_x^u$ encompassing the following coordinate functions, respectively: $(c_y^l)_j(\mathbf{x}) := Y_j(\mathbf{x}) - l_j$, $(c_y^u)_j(\mathbf{x}) =: u_j - Y_j(\mathbf{x})$, $(c_x^l)_i(\mathbf{x}) := x_i - l_{x_i}$ and $(c_x^u)_i(\mathbf{x}) =: u_{x_i} - x_i$ for all $i = 1, 2, \ldots, n$, and $j = 1, 2, \ldots, m$.

Let us suppose that $\overline{\mathbf{x}} \in [\mathbf{l}_x, \mathbf{u}_x]$ is a solution of the overall problem (4.2), the functions $Y_j, \mathbf{c}_y^l, \mathbf{c}_y^u, \mathbf{c}_x^l$, and $\mathbf{c}_x^u$, are continuously differentiable, the functions f_j $(j = 1, 2, \ldots, m)$ are Lipschitz continuous and that *Mangasarian Fromovitz constraint qualification* (*MFCQ*) [51] holds at $\overline{\mathbf{x}}$.

We know that then there exist *Lagrange multiplier* vectors $\overline{\boldsymbol{\mu}}^l, \overline{\boldsymbol{\mu}}^u, \overline{\boldsymbol{\tau}}^l, \overline{\boldsymbol{\tau}}^u$ with components $\overline{\mu}_j^l, \overline{\mu}_j^u, \overline{\tau}_i^l, \overline{\tau}_i^u$ $(i = 1, 2, \ldots, n;\ j = 1, 2, \ldots, m)$, such that the following stationary condition is satisfied at $(\overline{\mathbf{x}}, \overline{\boldsymbol{\mu}}^l, \overline{\boldsymbol{\mu}}^u, \overline{\boldsymbol{\tau}}^l, \overline{\boldsymbol{\tau}}^u)$:

$$\begin{aligned}\mathbf{0} \in \ & \sum_{j=1}^{m} w_j \partial f_j(Y_j(\overline{\mathbf{x}})) \nabla Y_j(\overline{\mathbf{x}}) - \sum_{j \in (J_0)_y^l(\overline{\mathbf{x}})} \overline{\mu}_j^l \nabla (c_y^l)_j(\overline{\mathbf{x}}) - \sum_{j \in (J_0)_y^u(\overline{\mathbf{x}})} \overline{\mu}_j^u \nabla (c_y^u)_j(\overline{\mathbf{x}}) \\ & - \sum_{i \in (J_0)_x^l(\overline{\mathbf{x}})} \overline{\tau}_i^l \nabla c_x^l(\overline{\mathbf{x}}) - \sum_{i \in (J_0)_x^u(\overline{\mathbf{x}})} \overline{\tau}_i^u \nabla c_i^u(\overline{\mathbf{x}}),\end{aligned} \tag{4.22}$$

together with the complementary conditions

$$\overline{\mu}_j^l (c_y^l)_j(\overline{\mathbf{x}}) = 0 \quad \text{and} \quad \overline{\mu}_j^u (c_y^u)_j(\overline{\mathbf{x}}) = 0,$$

$$\overline{\tau}_i^l (c_x^l)_i(\overline{\mathbf{x}}) = 0 \quad \text{and} \quad \overline{\tau}_i^u (c_x^l)_i(\overline{\mathbf{x}}) = 0,$$

where i and j are active. Here, at some feasible $\overline{\mathbf{x}}$, $(J_0)_y^l(\overline{\mathbf{x}})$ is the set of the *active* indices with $Y_j(\overline{\mathbf{x}}) = l_j$, so that $\nabla (c_y^l)_j(\overline{\mathbf{x}}) = \nabla Y_j(\overline{\mathbf{x}})$, and $(J_0)_y^u(\overline{\mathbf{x}})$ is the set of the *active* indices with $Y_j(\overline{\mathbf{x}}) = u_j$, so that $\nabla (c_y^u)_j(\overline{\mathbf{x}}) = -\nabla Y_j(\overline{\mathbf{x}})$. Moreover, $(J_0)_x^l(\mathbf{x})$ is the set of *active* indices, with $(c_x^l)_i(\overline{\mathbf{x}}) = 0$, and $(J_0)_x^u(\overline{\mathbf{x}})$ is the set of the *active* indices, with $(c_x^u)_i(\overline{\mathbf{x}}) = 0$. Hence, (4.22) becomes

$$\mathbf{0} \in \sum_{j=1}^{m} w_j \partial f_j(Y_j(\overline{\mathbf{x}})) \nabla Y_j(\overline{\mathbf{x}}) - \sum_{j \in (J_0)_y^l(\overline{\mathbf{x}})} \overline{\mu}_j^l \nabla Y_j(\overline{\mathbf{x}}) + \sum_{j \in (J_0)_y^u(\overline{\mathbf{x}})} \overline{\mu}_j^u \nabla Y_j(\overline{\mathbf{x}}). \tag{4.23}$$

Remark 4.4.2. In the above formulations, the inclusions turn to equality if the functions are *Clarke regular* [17]. Although we may have Clarke regularity in some cases of desirability functions, calculating subgradients of the overall function, which is a weighted sum of individual functions and a composite function, will not be an efficient strategy for optimization of these functions. We can conclude that the calculation of the subgradients of the function $f^Y(\mathbf{x})$ is a very difficult task, and therefore, the application of methods of nonsmooth optimization requiring a subgradient evaluation at each iteration, including bundle method and its variations [67], cannot be very effective. This is a validation of our selection of methods in the previous chapter for our numerical experiments. □

4.5 Desirability Functions as a Scalarization Method of Multi-Objective Problems

One way of solving a multi-objective optimization problem is to transform it into a single objective problem by a suitable *scalarization method* [75]. There are *linear* and *nonlinear* scalarization methods according to the aggregation strategy applied to combine the individual objectives. For a linear scalarization, it is possible to take the convex combination of the different objectives and obtain a sum-based aggregation function. The desirability function approach is in the category of a *nonlinear* scalarization method since geometric mean operation is used to aggregate the individual desirabilities. However, as we showed in the previous section, desirability functions can be converted to a sum-based aggregation strategy by applying the natural logarithm. Then, the objective function becomes a convex combination of the logarithm applied individual functions. Considering the relations between multi-response optimization and multi-objective optimization, it can be said that these weights work in a way that certain regions of the Pareto front could be preferred and worked on [98, 101] within desirability functions approach.

Let us write the *associated multi-objective optimization problem* formulation for our problem 4.14:

$$\begin{aligned} \text{minimize} \quad & (f_1(Y_1(\mathbf{x})), f_2(Y_2(\mathbf{x})), \ldots, f_m(Y_m(\mathbf{x}))) \\ \text{subject to} \quad & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x], \\ & Y_j(\mathbf{x}) \in [l_j, u_j] \quad (j = 1, 2, \ldots, m). \end{aligned} \tag{4.24}$$

For the cases where a set of solutions $\{\bar{\mathbf{y}}_1, \bar{\mathbf{y}}_2, \ldots, \bar{\mathbf{y}}_\tau\}$ of multi-objective optimization problem (4.24) is looked rather than for a single optimal solution, the so-called *Pareto optimization methods* may be prefered. Within these methods, different solutions are compared by using the notion of *Pareto dominance*, which is good for multi-objective comparisons and introduced by Vilfredo Pareto [32]. Another important property for an *optimal* point $\bar{\mathbf{y}}$ from the set of solutions of a multi-objective optimization problem is its being *non-dominated* or *Pareto optimal*. This means that there is no other solution in the set which dominates it. We note that these definitions are for the $\mathbf{y}$-space. An optimal solution $\bar{\mathbf{x}}$ that satisfies $\bar{\mathbf{y}} = \mathbf{Y}(\bar{\mathbf{y}})$ is called *efficent* or *Pareto optimal in factor space*. The set of all non-dominated solutions is called the *Pareto front*. We note that it is an important task in multi-objective optimization to identify the Pareto front. A best solution from the Pareto front can be selected via some interactive procedures with decision makers.

Now, the feasible set $\mathcal{F}$ of (4.24) can be written in terms of the constraints given in (4.2):

$$\mathcal{F} := \left\{ \mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \in \mathbb{X} \cap \mathbb{I}^X \right\}. \tag{4.25}$$

The set of Pareto-optimal solutions of (4.24) is denoted by $\mathcal{P}$. For each vector of weights $\mathbf{w} \in \mathbb{R}^m$, where $\mathbf{w} := (w_1, w_2, \ldots, w_m)^T$, the solution set $\mathcal{S}_w$ of the scalar problem (4.14) is

$$\mathcal{S}_w := \left\{ \mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x],\ \sum_{j=1}^{m} w_j f_j(Y_j(\mathbf{x})) = \min_{\tilde{\mathbf{x}} \in \mathcal{F}} \sum_{j=1}^{m} w_j f_j(Y_j(\tilde{\mathbf{x}})) \right\}. \tag{4.26}$$

In a study of Jeyakumar [50], the relation between the Pareto-optimal set of convex composite multi-objective problems and the feasible set of a weighted sum-based scalarization of that problem is presented. In our case, we do not guarantee the convexity of individual functions f_j for example when they include more than one nondifferentiable points.

In [101], it is proven that the global solution obtained from the conventional desirability maximization without weights is a Pareto-optimal point. We present the similar theorem for the global optimal of the weighted additive overall problem (4.14). This shows that the global optimization of the additive overall functions result in an Pareto optimal point in factor space.

Theorem 4.5.1. A global optimal solution $\bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_m)^T$ of problem (4.14) is Pareto-optimal.

Proof. Assume that $\bar{\mathbf{x}}$ is not Pareto-optimal. Then there exists a point $\mathbf{x}^*$ such that

$$f_s(Y_s(\mathbf{x}^*)) < f_s(Y_s(\bar{\mathbf{x}})),$$

for some $s \in \{1, 2, \ldots, m\}$ and

$$f_k(Y_k(\mathbf{x}^*)) \leq f_k(Y_k(\bar{\mathbf{x}})),$$

for $k = 1, 2, \ldots, m$ $(k \neq j)$. Herewith,

$$F(\mathbf{Y}(\mathbf{x}^*)) = \left(\sum_{j=1}^{m} w_j f_j(\mathbf{Y}(\mathbf{x}^*)) \right) < F(\mathbf{Y}(\bar{\mathbf{x}})) = \left(\sum_{j=1}^{m} w_j f_j(\mathbf{Y}(\bar{\mathbf{x}})) \right). \tag{4.27}$$

This is a contradiction to the assumption of $\bar{\mathbf{x}}$ minimizing $F(\cdot)$. Thus, $\bar{\mathbf{x}}$ must be Pareto-optimal. □

CHAPTER 5

A NEW APPROACH TO DESIRABILITY FUNCTIONS: GENERALIZED DESIRABILITY FUNCTIONS AND TWO-STAGE (BILEVEL) METHOD

5.1 Introduction

In a desirability function approach, each response is scaled into same interval to have a unitless value, called its desirability, assigned by its individual desirability function. During this process, determining the suitable desirability function for a response turns out to be a difficult task for decision makers. We remember that there are three type of responses: (i) target-is-the best responses, which need two-sided individual desirability functions, having lower bound, target value and upper bound specifications, (ii) smaller-the-best and (iii) upper-the-best responses, which need a one-sided individual desirability function, with lower and upper bound specifications. There are many functions suggested to be used as individual desirability functions like Harrington's, Derringer and Suich's, etc. [25, 44]. As we mentioned before, when Derringer and Suich's desirability functions are meant, there is no nondifferentiable point in a one-sided function, whereas a two-sided function contains at least one nondifferentiable point which occurs at the target point.

We observe that the individual desirability functions used in practice (see for example [49, 59]) are simplistic elements of a special type, among the wide subclass of continuous selection functions [3, 9, 51, 64], called min-type functions. Again, we have in mind Derringer and Suich's desirability functions, especially, the two-sided ones in our analysis throughout this chapter. However, these results can easily be extended to other desirability functions. In the previous chapter, we applied the negative logarithm to the overall desirability function which was the geometric mean of ϵ-individual desirabilities defined for the two-sided desirability functions without loss of generality to overcome vanishing of these functions at the lower and upper bounds. We remember that our individual functions after taking the negative logarithm, f_j ($j = 1, 2, \ldots, m$), are always positive and have an underlying *max-type continuous selection* structure, by definition as functions of $y_j = Y_j(\cdot)$ on the intervals $\mathbb{I}_j$.

5.2 Structural Configuration of Desirability Function

Additive separability of the objective function $F(\mathbf{Y}(\mathbf{x}))$ obtained in the previous chapter enables us to consider each $f(Y(\mathbf{x}))$ ($= f_j(Y_j(\mathbf{x}))$) separately in exploring the qualitative insights for this overall optimization problem. By introducing continuous selection functions into desirability function approach, we aim to reveal the properties of the whole class of functions that our individual $f(y)$ ($f_j(y)$) is a member of, by its underlying max-type structure. This situation leads to the definition of *generalized desirability functions (GDFs)*. We call the negative logarithm of an individual desirability function as a *generalized individual desirability function* and denote it with f^g: $f^g(\cdot) := f(Y(\cdot))$, where $f(y)$ is a piecewise smooth function containing any finite number of nondifferentiable points and Y is a smooth function of $\mathbf{x}$. We notice that like conventional individual desirability functions, generalized functions f^g are also nonsmooth composite functions [10, 109] for any $j = 1, 2, \ldots, m$:

$$f^g = f \circ Y.$$

Therefore, our functions f^g are generalized in the sense that the conventional two-sided individual desirability functions used in practice are a special case of them by including only one nondifferentiable point and generalized individual desirability functions f^g are again in the category of two-sided individual desirability functions.

The overall function $F(\cdot)$ of the vector $\mathbf{y} = (y_1, y_2, \ldots, y_m)^T$, where $\mathbf{y} = \mathbf{Y}(\mathbf{x})$ satisfies $F(\mathbf{y}) := \sum_{j=1}^{m} w_j f_j(y_j)$ for $f_j : \mathbb{I}_j \to \mathbb{R}$ ($j = 1, 2 \ldots, m$). The intervals $\mathbb{I}_j = [l_j, u_j]$ ($j = 1, 2 \ldots, m$) can be disjoint for all j, intersecting or even being the same for some or all j. We notice that the graph of F in $\mathbf{y}$ can be connected or disconnected according to the positions of these intervals; usually it is disconnected, and it can be connected only if all responses have the same interval for all j. If we consider the optimization of F with respect to $\mathbf{y}$, we have the following constrained minimization:

$$\begin{aligned} \underset{\mathbf{y}}{\text{minimize}} \quad & F(\mathbf{y}) = w_1 f_1(y_1) + w_2 f_2(y_2) + \ldots + w_m f_m(y_m) \\ \text{subject to} \quad & y_j \in \mathbb{I}_j \quad (j = 1, 2, \ldots, m), \end{aligned} \tag{5.1}$$

where $w_1 + w_2 + \ldots + w_m = 1$ with $w_j \geq 0$ ($j = 1, 2, \ldots, m$) representing the convex combinations of the individual desirability functions f. By the additive structure of the objective function, the optimal (global) solution of this problem $\mathbf{t}$ will be a vector of the (global) optimal solutions of $f_j(y)$, say t_j ($j \in J$): $\mathbf{t} := (t_1, t_2, \ldots, t_m)^T$, i.e., the vector of what we called the *target point* before. This vector $\mathbf{t}$ is usually named as the *ideal point* of the overall problem (4.14); it lies in the m-dimensional cube $\mathbb{I} \subset \mathbb{R}^m$:

$$\mathbb{I} = \bigtimes_{j \in J} \mathbb{I}_j \quad (= \mathbb{I}_1 \times \mathbb{I}_2 \times \ldots \times \mathbb{I}_m). \tag{5.2}$$

In this formulation, we think each f as a *max-type* function of C^2-differentiable functions having a global minimum corresponding to the target point and many nondifferentiable points, and hence, many "pieces". However, instead of being max-type, we may assume that each f has a *piecewise max-type* structure as shown in Figure 5.1 to consider a more generalized case, (ideally but not necessarily) with a unique global minimum and with several local minima.

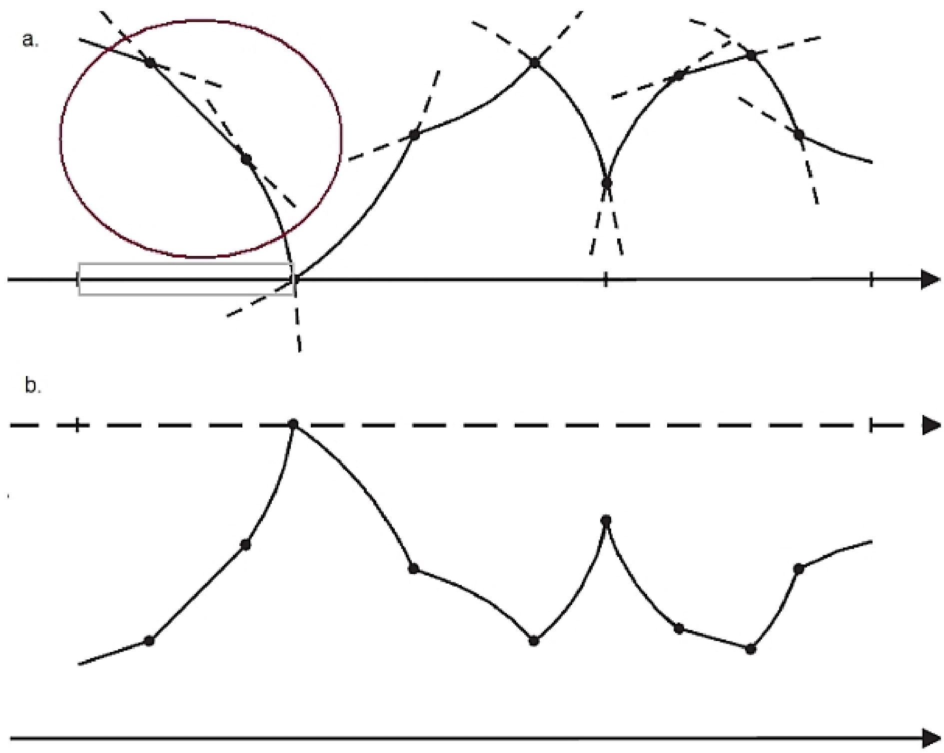

Figure 5.1: Example of a. piecewise min-type (red circle contains a min-type function) and b. piecewise max-type functions.

In this study, we propose a procedure to obtain these piecewise max-type individual functions f_j ($j = 1, 2, \ldots, m$) from the conventional individual desirability functions which include only one nondifferentiable point: a suitable partitioning of the compact and connected interval $\mathbb{I}_j$

into a finite number of subintervals, at each subinterval employing a max-type continuous selection function composed of C^2-differentiable functions. We present the structural and topological properties of partitioned functions f, where such a subdivision into a family of subintervals is guaranteed in some *generic* sense. In fact, the *finiteness* of our piecewise structure given by max-type functions can be guaranteed by the generic conditions which are called *transversality*. Moreover, we will introduce generic conditions in the context of (structural) stability. By focusing on the minimax problem of each f, we analyze the critical points of f after partitioning and state the constraint qualifications by *Morse theory*. For this aim, we consider the equivalent *smooth* problem by a reformulation of the minimax problem of our max-type functions in higher dimension, i.e., $\mathbb{R}^2$ (or in $\mathbb{R}^{n+1}$). We discuss the structural stability of the considered minimax problem via *perturbation analysis*. We consider the affects of employing *semi-infinite* max-type functions on the structure of the generalized individual desirability functions instead of the finite max-type continuous selections.

By different formulations of individual desirability functions, different structures like the ones in [49, 59, 81] from Derringer and Suich's, arise and make it possible to calculate the degree of satisfaction or degree of regretfullness besides desirability. With our generalization, we shed light on the mechanism that gives rise to a variation in the structure of functions used in desirability approaches and we present a source of functions useful for the task of assigning a suitable desirability function. Moreover, this kind of generalized individual functions with a finite number of nondifferentiable points occurs in the approximation of a nonlinear conventional desirability function with linear or affine functions as shown in Figure 5.2. *Generalized overall desirability function* is applied as a name for any convex combination of the individual ones where at least one of them is generalized.

5.3 A Finite Partitioning of Individual Desirability Functions

Using the assumption on the existence of a *finite* partitioning of the interval $\mathbb{I}_j$ ($j = 1, 2, \ldots, m$), we will construct the generalized individual desirability function f_j as a piecewise-smooth function by employing max-type functions at each *subinterval*. The *generic* (topological) justification of our assumption on piecewise structure in terms of transversality will also be explained and made a bit algorithmical. Concerning the genericity of the max- and min-type functions in the sense of composition and coordinate transformation we refer to [51, 52, 53]. In fact, for a suitable finite partitioning of the interval of the conventional individual desir-

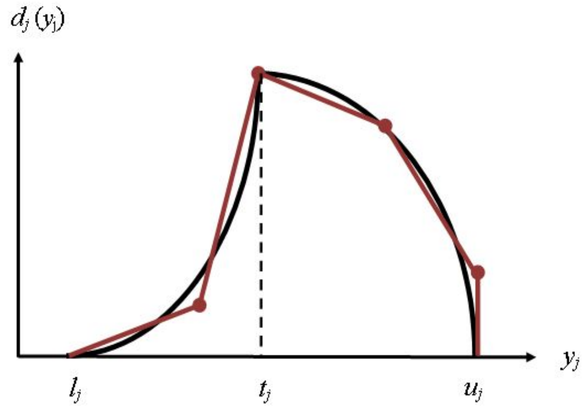

Figure 5.2: A conventional desirability function $d_j(y_j)$ ($j = 1, 2, \ldots, m$) including a finite number of nondifferentiable points.

ability functions, we perform two steps. Let us first define the index sets that will be used throughout this chapter:

- for the number of individual functions f_j and intervals $\mathbb{I}_j$:
  $J = \{1, 2 \ldots, m\}$ with elements $j \in J$,
- for the number of subintervals of $\mathbb{I}_j$:
  $K_j = \{1, 2, \ldots, \kappa_j\}$ with elements $\kappa \in K_j$,
- for the number of function pieces at each subinterval κ:
  $Z_{j,\kappa} = \{1, 2, \ldots, \zeta_{j,\kappa}\}$ with elements $\zeta \in Z_{j,\kappa}$,
- for the total number of function pieces for each j:
  $Z_j = \{1, 2, \ldots, \zeta_j\}$ with elements $\varsigma \in Z_j$.

We choose a sufficiently large interval $\mathbb{I}_j := [l_j, u_j]$ for the variable $y_j \in \mathbb{I}_j$ ($j \in J$). We partition this interval $\mathbb{I}_j$ into κ_j many subintervals, i.e., $\mathbb{I}_j = \bigcup_{\kappa=1}^{\kappa_j} \mathbb{I}_{j,\kappa}$, where $\mathbb{I}_{j,\kappa} := [l_{j,\kappa}, u_{j,\kappa}]$ is the interval with lower bound $l_{j,\kappa}$ and upper bound $u_{j,\kappa}$ ($\kappa \in K_j, j \in J$). Furthermore, we assume that neighboring subintervals have just boundary points in common: $u_{j,\kappa} = l_{j,\kappa-1}$ ($\kappa \in K_j \setminus \{1\}, j \in J$). At each subintervals $\mathbb{I}_{j,\kappa}$, the function is called $f_{j,\kappa}$, where

$$f_{j,\kappa} := f_j \mid_{\mathbb{I}_{j,\kappa}} \quad (\kappa \in K_j, j \in J). \tag{5.3}$$

By partitioning the interval $\mathbb{I}_j$ into κ_j subintervals, we are able to employ piecewise max-type functions to structure generalized individual desirability function f_j, piecewise consisting of max-type functions $f_{j,\kappa}$.

A second partitioning is made for the interval $\mathbb{I}_{j,\kappa}$ by a number of $\zeta_{j,\kappa}$ subintervals, i.e., $\mathbb{I}_{j,\kappa} = \bigcup_{\zeta=1}^{\zeta_{j,\kappa}} \mathbb{I}_{j,\kappa}^{\zeta}$, where $\mathbb{I}_{j,\kappa}^{\zeta} := [l_{j,\kappa}^{\zeta}, u_{j,\kappa}^{\zeta}]$ is the interval with lower bound $l_{j,\kappa}^{\zeta}$ and upper bound $u_{j,\kappa}^{\zeta}$ ($\zeta \in Z_{j,\kappa}, \kappa \in K_j, j \in J$). Here, $u_{j,\kappa}^{\zeta} = l_{j,\kappa}^{\zeta-1}$ ($\zeta \in Z_{j,\kappa} \setminus \{1\}, \kappa \in K_j, j \in J$). At each subinterval $\mathbb{I}_{j,\kappa}^{\zeta}$, the function is called $f_{j,\kappa}^{\zeta}$, where

$$f_{j,\kappa}^{\zeta} := f_{j,\kappa}\,|_{\mathbb{I}_{j,\kappa}^{\zeta}} \qquad (\zeta \in Z_{j,\kappa}, \kappa \in K_j, j \in J). \tag{5.4}$$

By this second partitioning at each subinterval $\mathbb{I}_{j,\kappa}$, we structure $f_{j,\kappa}$ as max-type functions composed of C^2-differentiable functions $f_{j,\kappa}^{\zeta}$ as in Figure 5.3. We denote the total number of functions $f_{j,\kappa}^{\zeta}$ for each individual f_j on $\mathbb{I}_j$ by ζ_j: $\zeta_j := \sum_{\kappa=1}^{\kappa_j} \zeta_{j,\kappa}$.

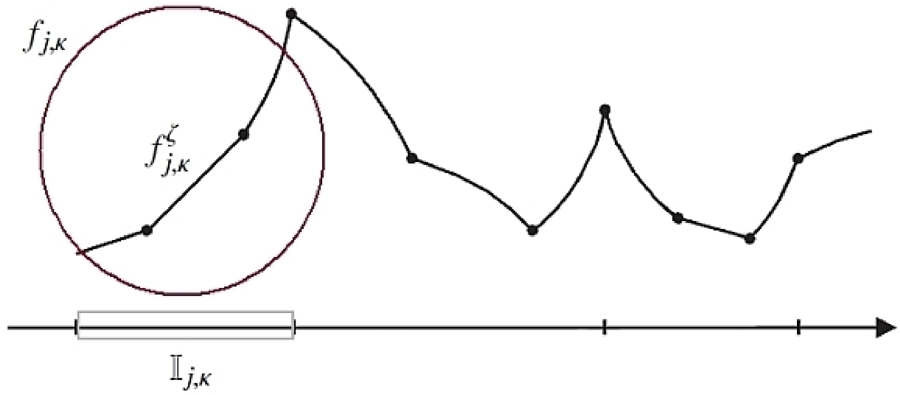

Figure 5.3: A piecewise max-type function obtained from our partitioning procedure.

After these two steps of partitioning, we arrive at the generalized desirability functions consisting of the following functions:

- the C^2-smooth functions $f_{j,\kappa}^{\zeta}(\cdot) : \mathbb{I}_{j,\kappa}^{\zeta} \to \mathbb{R}$ ($\mathbb{I}_{j,\kappa}^{\zeta} \subset \mathbb{R}$) which we call *generating desirability functions*,
- piecewise smooth $f_{j,\kappa}(\cdot) : \mathbb{I}_{j,\kappa} \to \mathbb{R}$ ($\mathbb{I}_{j,\kappa} \subset \mathbb{R}$) of $\zeta_{j,\kappa}$ many $f_{j,\kappa}^{\zeta}$ functions,
- piecewise max-type functions $f_j(\cdot) : \mathbb{I}_j \to \mathbb{R}$ ($\mathbb{I}_j \subset \mathbb{R}$) which we call *generalized individual desirability functions*, composed of κ_j many functions $f_{j,\kappa}$,
- additive function $F(\cdot) : \mathbb{I} \to \mathbb{R}$, which we call *generalized overall desirability function*, i.e., the weighted sum of the generalized individual desirability functions where $\mathbb{I} \subset \mathbb{R}^m$ is defined as in (5.2).

Remark 5.3.1. In this study, we consider all the functions f_j, $f_{j,\kappa}$ and $f_{j,\kappa}^{\zeta}$ ($\zeta \in Z_{j,\kappa}, \kappa \in K_j, j \in J$) to be globally defined on $\mathbb{R}$. Our various model functions were originally defined on wider open sets which include our considered intervals and parallelepipeds. They came from regression, experimental design and global optimization with its critical manifolds. Then, they have become restricted. We note that all the analysis, which we present in this chapter, can be used for the conventional desirability functions and their optimization problems by putting $\kappa = 1$ for one-sided individual desirability functions, $\kappa = 2$ for two-sided individual desirability functions, and $\zeta_{j,\kappa} = 1$ for both cases. □

5.3.1 Optimization

The minimization of functions $f_{j,\kappa}$ in y for a fixed $\kappa \in K_j$ and for a fixed $j \in J$ is a finitely constrained nonsmooth minimax problem:

$$\begin{aligned} \underset{y}{\text{minimize}} \quad & f_{j,\kappa}(y) \\ \text{subject to} \quad & y \in \mathbb{I}_{j,\kappa}, \end{aligned} \tag{5.5}$$

and, in other words,

$$\underset{y \in \mathbb{I}_{j,\kappa}}{\text{minimize}} \quad \underset{\zeta \in Z_{j,\kappa}}{\text{maximize}}\, f^{\zeta}_{j,\kappa}(y). \tag{5.6}$$

Let the solutions of (5.5) be called $t_{j,\kappa}$ ($\kappa \in K_j$) for each $j \in J$. Now, the minimization of generalized individual desirability functions $f_j(y)$ is a *discrete* optimization problem, actually, an *enumeration problem*, over all κ, for each regarded j:

$$\min_{y \in \mathbb{I}_j} f_j(y) \;:=\; \min\{f_{j,1}(t_{j,1}), f_{j,2}(t_{j,2}), \ldots, f_{j,\kappa_j}(t_{j,\kappa_j})\} = \min_{\kappa \in K_j} f_{j,\kappa}(t_{j,\kappa}). \tag{5.7}$$

By solving these problems to find the minimum of $f_j(y)$ per given $j \in J$, we will obtain a set of solutions, say t_j, which are, in fact, $t_j := t_{j,\bar{\kappa}_j}$ at a certain $\bar{\kappa}_j \in K_j$. These solutions are the target points as we discussed before. Hence, the vector $\mathbf{t} := (t_1, t_2, \ldots, t_m)^T$ is the *ideal point* of the overall problem (4.14) that lies in the m-dimensional cube $\mathbb{I}$.

The piecewise smooth structure of the generalized individual desirability functions $f_j(\cdot)$ together with the additive separability (also called: linearity) of the regarded generalized overall desirability function $F(\cdot)$ enable us to be concerned about the local properties of the max-type functions $f_{j,\kappa}(\cdot)$ and their optimization problem (5.5), to achieve results and gain qualitative insights into the full-dimensional problem (5.1) in $\mathbf{y}$.

5.3.2 Structural and Topological Analysis

Our max-type function $f_{j,\kappa}$ can be constructed through a mechanism called *continuous selection* from the generating functions $f^{\zeta}_{j,\kappa}$ ($\zeta \in Z_{j,\kappa}, \kappa \in K_j, j \in J$), which can be linear or nonlinear, convex or nonconvex but C^2-differentiable, and hence, Lipschitz continuous. The set of all continuous selections of C^2-functions $f_{j,\kappa}^{\zeta}$ may be represented by

$$\mathrm{CS}(f_{j,\kappa}^{1}, f_{j,\kappa}^{2}, \ldots, f_{j,\kappa}^{\zeta_{j,\kappa}}). \tag{5.8}$$

For structuring max-type functions $f_{j,\kappa}$, we apply the special type continuous selection, called the *max-type* based on functions $f_{j,\kappa}^{\zeta}$:

$$f_{j,\kappa}(y) := \max_{\zeta \in Z_{j,\kappa}} f_{j,\kappa}^{\zeta}(y), \tag{5.9}$$

and its particular index set

$$(Z_0)_{j,\kappa}(y) := \{\zeta \in Z_{j,\kappa} | \, f_{j,\kappa}^{\zeta}(y) = f_{j,\kappa}(y)\}, \tag{5.10}$$

where $y \in \mathbb{I}_{j,\kappa}$, $\kappa \in K_j$ and $j \in J$. This finite set $(Z_0)_{j,\kappa}(y)$ is called the *active index set* of $f_{j,\kappa}$ at the point y. We have

$$f_{j,\kappa}(y) = f_{j,\kappa}^{\zeta_y}(y), \quad \text{where} \quad \zeta_y \ (= \zeta_{y,j,\kappa}) \in (Z_0)_{j,\kappa}(y). \tag{5.11}$$

Because of the finiteness and compactness of $Z_{j,\kappa}$, the maximum is attained in (5.10), and $|(Z_0)_{j,\kappa}(y)| \geq 1$ for all $y \in \mathbb{I}_{j,\kappa}$.

These max-type functions $f_{j,\kappa}$ are nondifferentiable but Lipschitz continuous by Hager's Theorem [43] and they are almost everywhere differentiable in the sense of Lebesgue measure, i.e., a set of Lebesgue-measure 0 by Rademacher's Theorem [85]. Moreover, they are positive and bounded by 0 from below, piecewise smooth generically and not necessarily convex. Although they may lack convexity, we can call the structure of them as *convex-like* since, via a pathfollowing [41] along y, we select as *active* the function which has the biggest slope (derivative).

Our entire piecewise max-type function f_j is a piecewise continuous selection nonsmooth function which may not be convex and Lipschitz continuous but again is almost everywhere differentiable (in the sense of Lebesgue measure), since ζ_j and κ_j are finite for each $j \in J$. Moreover, we can say the set of all nondifferentiable points of f_j is a *nowhere dense* set.

We can represent the *Clarke subdifferential* at every point $y \in \mathbb{I}_{j,\kappa}$ of $f_{j,\kappa}$ by

$$\mathrm{co}\, \{\nabla f_{j,\kappa}^{\zeta}(y) \mid \zeta \in (Z_0)_{j,\kappa}(y)\}, \tag{5.12}$$

where $(Z_0)_{j,\kappa}(y)$ $(\kappa \in K_j, j \in J)$ is the active index set given in (5.10). Each function $f_{j,\kappa}$ is directionally differentiable, and its directional derivative $(f_{j,\kappa})'(y; v)$ at a given point $y \in \mathbb{R}$ in the direction $v \in \mathbb{R}$ is a max-type continuous selection of the linear functions $(f^{\zeta}_{j,\kappa})'$, i.e., the first-order derivative of $(f^{\zeta}_{j,\kappa})$ with respect to y:

$$(f_{j,\kappa})'(y; v) := \max_{\zeta \in Z_{j,\kappa}(y)} (f^{\zeta}_{j,\kappa})'(y)v. \tag{5.13}$$

We can treat our piecewise max-type function f_j as a 1-dimensional compact and connected piecewise C^2-smooth manifold, i.e., a *creased manifold*. Moreover, each max-type function $f_{j,\kappa}$ can itself also be treated as a creased (piecewise) 1-dimensional manifold. More information on connection to manifolds and differential topology can be found in studies of parametric optimization [40, 51, 52, 94]. Obviously, the active pieces of $f_{j,\kappa}$, i.e., $f^{\zeta}_{j,\kappa}$, are C^2*-smooth manifolds* globally or, when restricted on intervals, *with boundary* (points).

Remark 5.3.2. We note that both the function f_j and the intervals $\mathbb{I}_j$ can also be treated as a 1-dimensional *creased manifolds*. This is related with the fact that any connected 1-dimensional piecewise manifold can be be written as a finite union of closed intervals. In particular, the creases in $\mathbb{I}_j$ meet exactly along the strata of dimension less than 1. Moreover, in constructing the max-type functions $f_{j,\kappa} : \mathbb{R} \to \mathbb{R}$ over the manifolds $\mathbb{I}_{j,\kappa}$, we used the fact that the active functions $f^{\zeta_y}_{j,\kappa}$ $(\zeta_y \in Z|_{j,\kappa}(y))$ are, generically, *transversally intersecting* at the point $(y, f^{\zeta_y}_{j,\kappa})$ where the active function changes for the next ζ. For more information on transversality theory, we refer to [51, 89, 107]. This means that the derivatives $(f^{\zeta}_{j,\kappa})'(y)$ of active functions are affinely independent at any $y \in \mathbb{I}_{j,\kappa}$. Hence, the index set of active functions at any $y \in \mathbb{I}_{j,\kappa}$ will locally be constant. We can use this transversality for a *finite* (piecewise) partition of $\mathbb{I}_{j,\kappa}$ into subintervals $\mathbb{I}^{\zeta}_{j,\kappa}$. This finite strucutre by pieces is topologically stable under arbitrarily small perturbations. □

We show the effect of transversality on the structural stability in Figure 5.4. In (a), we see that stability is protected with respect to the C^2-small perturbations. In (b), an arbitrarily slight perturbation causes an increase in the number of critical points and combinatorial change of the piecewise structure deteriorates the stability.

From here to the end of this subsection, we continue with a simplification in our notation. To this aim, let us for any fixed $j \in J$ and fixed $\kappa \in K := K_j$ put $f(\cdot) := f_{j,\kappa}(\cdot)$, $f^{\zeta}(\cdot) := f^{\zeta}_{j,\kappa}(\cdot)$, $l := l_{j,\kappa}$, $u := u_{j,\kappa}$ and $Z := Z_{j,\kappa}$, preserving our basic smoothness structures and assumptions.

Nondifferentiability of the max-type functions f necessitates that we use a continuous local *coordinate transformation* to understand their local behavior via the notion of *nondegeneracy* of a *critical point* which is a generic property for continuous selection functions [51, 52, 53].

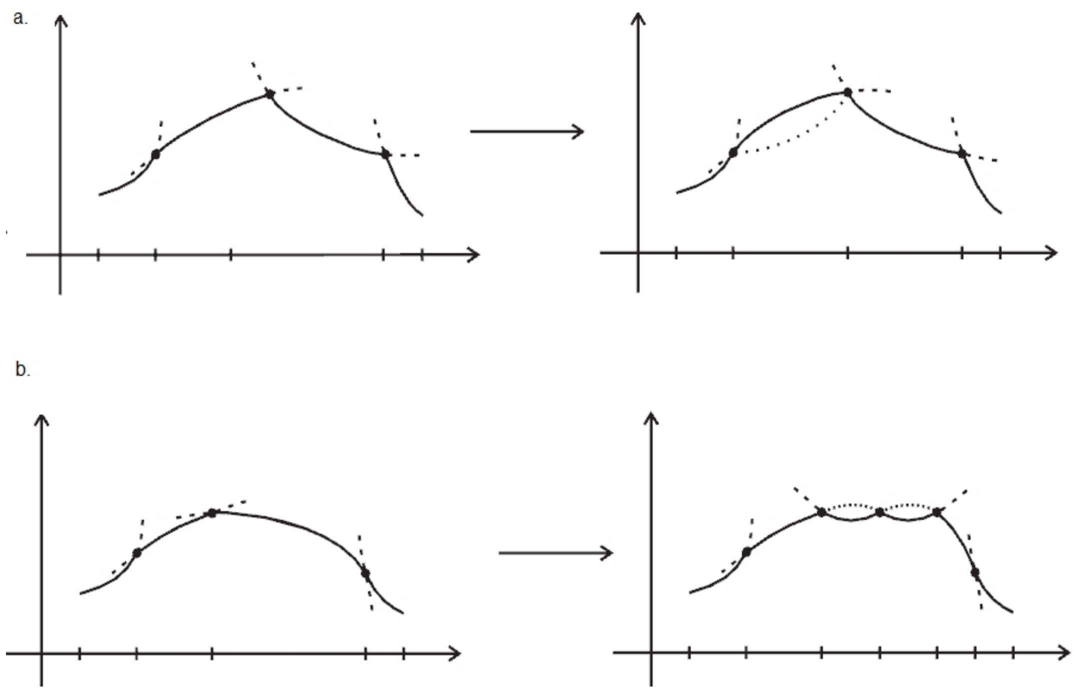

Figure 5.4: (a) Strong and Structural Stability, (b) Instability; in the sense of critical points and optimization theory (Morse theory).

We note that for a detailed background information for this section and especially background for Morse theory we refer to the excellent book of Jongen et al. [51].

5.3.3 Critical Points and Constraint Qualifications

To analyze the critical points and state the constraint qualifications, we proceed with the equivalent smooth problem of (5.5) obtained by a reformulation given in the higher dimension of $\mathbb{R}^2$. In this subsection, at any κ and j, the max-type functions $(f_{j,\kappa}(\cdot)) = f(\cdot)$ have the form:

$$f(y) := \max_{\zeta \in Z} f^{\zeta}(y), \tag{5.14}$$

and their active index sets are globally now, denoted by

$$Z_0(y) := \{\zeta \in Z \mid f(y) = f^{\zeta}(y)\} \quad (y \in [l, u]). \tag{5.15}$$

Remark 5.3.3. We recall that the functions f representing our max-type functions and the functions f^{ζ} are considered to be globally defined functions on $\mathbb{R}$, i.e., $y \in \mathbb{R}$, in this section. However, we could also refer to some space $\mathbb{R}^p$ ($p \in \mathbb{N}$) instead of $\mathbb{R}$ and define $\mathbf{y} \in \mathbb{R}^p$ as a higher-dimensional variable. We may diversify the dimension p_j, for the different vectorial responses $\mathbf{y}_j \in \mathbb{R}^{p_j}$. In case of such kind of generalizations, our main results presented in this subsection and in the following ones will still hold true. □

Now, the constraints of problem (5.5) are $c^l(y) \geq 0$ and $c^u(y) \geq 0$, where $c^l(y) := y - l$ and $c^u(y) =: u - y$. The feasible set $M := M[\mathbf{c}]$ is

$$M[\mathbf{c}] = \{y \in \mathbb{R} \mid \mathbf{c}(y) \geq \mathbf{0}\} \tag{5.16}$$

with $\mathbf{c}(y) := (c^l, c^u)^T(y)$, where $\mathbf{c}(y) = (c_1(y), c_2(y))^T$. Let us define the set of active indices for our feasible set M: $\mathcal{J}_0(y) := \{\jmath \in \mathcal{J} \mid c_\jmath(y) = 0\}$ $(y \in M)$, where $\mathcal{J} := \{1, 2\}$. Hence, the restricted $f|_M$ stands for the optimization problem (5.5).

We know that the max-type function $f : \mathbb{R} \to \mathbb{R}$ contains nondifferentiable points, where the function is lacking of being C^2-differentiable. However, by a reformulation of f and its optimization problem given in (5.5) in the by 1 higher-dimensional space, i.e., $\mathbb{R}^2$, the problem becomes C^2-differentiable. We use a "ˇ" symbol over the notations of vectors, functions, etc., that are then defined in $\mathbb{R}^2$ in correspondence to our usual notations.

In $\mathbb{R}^2$, the equivalent optimization problem of (5.5) can be written as follows:

$$\begin{aligned} \underset{\check{\mathbf{y}}}{\text{minimize}} \quad & \check{f}(\check{\mathbf{y}}) \\ \text{subject to} \quad & \check{\mathbf{c}}(y_1) \geq 0, \end{aligned} \tag{5.17}$$

where $\check{\mathbf{y}} := (y, y_2)^T = (y_1, y_2)^T$ is our vector in $\mathbb{R}^2$ with $y = (y_1)$, and

$$\check{f}(\check{\mathbf{y}}) = \check{f}(y, y_2) := y_2 \tag{5.18}$$

is the corresponding *height function* minimized on the epigraph of $f|_M$:

$$E(f|_M) := \{(y, y_2) \in \mathbb{R}^2 \mid y \in M[\mathbf{c}],\ f|_M(y) \leq y_2\}. \tag{5.19}$$

The constraint function of (5.17) is $\check{\mathbf{c}}(y) := (c^l, c^u, y_2 - f^\zeta)^T(y)$ $\quad (\zeta \in Z)$, where $\check{\mathbf{c}}(y) = (\check{c}_1(y), \check{c}_2(y), \check{c}_3(y))^T$. Now, the corresponding feasible set $\check{M} := \check{M}[\check{\mathbf{c}}] := \{\check{\mathbf{y}} \in \mathbb{R}^2 \mid c_\jmath(y_1) \geq 0\ (\jmath \in \mathcal{J}),\ y_2 - f^\zeta(y_1) \geq 0\ (\zeta \in Z)\}$ can be written as:

$$\check{M}[\check{\mathbf{c}}] := \{\check{\mathbf{y}} \in \mathbb{R}^2 \mid \check{\mathbf{c}}(y) \geq 0\}. \tag{5.20}$$

We note that $\check{f} : \mathbb{R}^2 \to \mathbb{R}$ is a linear function and our max-type function f appears now as a set of additional inequalities in $\check{M}$, i.e., $\check{c}_3(y) = y_2 - f^\zeta(y)$. Here, instead of being concerned with the optimization problem $f|_M$, we consider the minimization of the height function $\check{f}$ on the epigraph $E(f|_M)$ of $f|_M$.

For our further analysis, we need the regularity of $\check{M} \subset \mathbb{R}^2$ *regular* [51, 52, 107]. This is satisfied since the feasible M itself by definition fulfills this regularity condition of *linear independence constraint qualification (LICQ)*, i.e., the following family of the gradient vectors:

$$(c_J'(y), 0)^T \ (J \in (\mathcal{J}_0)(y)) \quad \text{and} \quad (-(f^\zeta)'(y), 1)^T \ (\zeta \in Z_0(y)), \tag{5.21}$$

are *linearly independent* at every point $\check{\mathbf{y}} = (y, y_2)^T \in \check{M}$ with $y_2 = f(y)$. For the regularity of $\check{M}$ at the points $\check{\mathbf{y}}$ with $y_2 \neq f(y)$, the feasible set M of the problem in $\mathbb{R}$ has to be regular necessarily.

Definition 5.3.4. *[51]* An element $\bar{y} \in M = M[\mathbf{c}]$ is called a *(nondegenerate) critical point* for the problem $f|_M$, if $(\bar{y}, f(\bar{y}))$ is a *(nondegenerate) critical point* for the problem $\check{f}|_{\check{M}}$. □

Remark 5.3.5. We note that if $\bar{\check{\mathbf{y}}} := (\bar{y}, \bar{y}_2)^T = (\bar{y}_1, \bar{y}_2)^T \in \check{M}$ is a critical point for $\check{f}|_{\check{M}}$, then necessarily we have $\bar{y}_2 = f(\bar{y})$. □

Definition 5.3.6. *[51]* The *Lagrange function* $L : \mathbb{R} \to \mathbb{R}$ of problem $f|_M$ is given by

$$L(y) := \sum_{\zeta \in Z_0(\bar{y})} \lambda^\zeta f^\zeta(y) - \sum_{J \in \mathcal{J}_0(\bar{y})} \mu_J c_J(y), \tag{5.22}$$

with the *Lagrange multipliers* $\mu_J \in \mathbb{R}$ $(J \in \mathcal{J}_0(\bar{y}))$ and $\lambda^\zeta \in \mathbb{R}$ $(\zeta \in Z_0(\bar{y}))$. □

Theorem 5.3.7. *[51]* We state a *necessary optimality condition* that $\bar{y} \in M$ is a *critical point* for $f|_M$, i.e., there exist $\mu_J \geq 0$ $(J \in \mathcal{J}_0(\bar{y}))$ and $\lambda^\zeta \geq 0$ $(\zeta \in Z_0(\bar{y}))$ such that

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \sum_{J \in \mathcal{J}_0(\bar{y})} \mu_J \begin{pmatrix} c_J'(\bar{y}) \\ 0 \end{pmatrix} + \sum_{\zeta \in Z_0(\bar{y})} \lambda^\zeta \begin{pmatrix} -(f^\zeta)'(\bar{y}) \\ 1 \end{pmatrix}. \tag{5.23}$$

Definition 5.3.8. *[51]* A critical point $\bar{y}$ for $f|_M$ is called a *Karush-Kuhn-Tucker* point if $\mu_J \geq 0$ and $\lambda^\zeta \geq 0$ $(\zeta \in Z_0(\bar{y}), J \in \mathcal{J}_0(\bar{y}))$. □

Definition 5.3.9. *[51]*A critical point $\bar{y}$ for $f|_M$ is called a *nondegenerate critical point* (*nondegenerate Karush-Kuhn-Tucker*), if and only if the following conditions hold (respectively):
(ND1): $\mu_J \neq (>)0 \quad \text{and} \quad \lambda^\zeta \neq (>)0 \quad (\zeta \in Z_0(\bar{y}), J \in \mathcal{J}_0(\bar{y}))$,
(ND2): $V^T \nabla^2 L(\bar{y}) V$ is *nonsingular*, where L is the Lagrange function given in (5.22) and V is a matrix whose columns form a basis for tangent space $T \subseteq \mathbb{R}$, defined by

$$T := \bigcap_{J \in \mathcal{J}_0(\bar{y})} \ker c_J'(\bar{y}) \ \cap \bigcap_{\zeta \in Z_0(\bar{y})} \ker (f^\zeta)'(\bar{y}).$$

In order to obtain (ND1) and (ND2), we first write down the usual nondegeneracy conditions at the critical point $(\bar{y}, f(\bar{y}))$ of the problem $\check{f}|_{\check{M}}$. We note that $\check{M} \subset \mathbb{R}^2$. Then we take into account that $\check{f}$ is a linear function and that the tangent space of $\check{\sum}$ at $(\bar{y}, f(\bar{y}))$ equals $T \times \{0\}$, $0 \in \mathbb{R}$, where $\check{\sum}$ is the *stratum* of $\check{M}$ through $(\bar{y}, f(\bar{y}))$.

The *quadratic index* at a nondegenerate critical point is defined as the (Morse) index, the number of negative eigenvalues, of $\nabla^2 L(\bar{y})|_T$. It is easily seen that $\bar{y} \in M$ is a local minimum for $f|_M$ if and only if $(\bar{y}, f(\bar{y}))$ is a local minimum for $\check{f}|_{\check{M}}$. Consequently, a nondegenerate critical point $\bar{y}$ for $f|_M$ is a local minimum for $f|_M$ if and only if in (ND1) and (ND2), we have $\mu_J > 0$ and $\lambda^\zeta > 0$ ($\zeta \in Z_0(\bar{y}), J \in \mathcal{J}_0(\bar{y})$) and $V^T \nabla^2 L(\bar{y}) V$ is positive definite (meaning that the quadratic index is zero).

5.3.4 Structural Stability

We present the global structural stability properties for the nonsmooth minimax problem (5.5) by perturbation analysis. We call this problem as $P(\mathcal{F}, \mathbf{c})$ in this subsection:

$$P(\mathcal{F}, \mathbf{c}): \quad \text{minimize } f \text{ on } M[\mathbf{c}], \tag{5.24}$$

where $\mathcal{F} := (f^1, f^2, \ldots, f^\ell)^T$, and the max-type objective function $f(\cdot)$ is:

$$f(y) = \max_{\zeta \in Z} f^\zeta(y).$$

The feasible set is $M[\mathbf{c}] = \{y \in \mathbb{R} \mid \mathbf{c}(y) \geq \mathbf{0}\}$, with $\mathbf{c}(y) = (c^l, c^u)^T(y)$, i.e., $(c_1(y), c_2(y))^T = (c^l(y), c^u(y))^T$, where $c^l(y) = y - l$ and $c^u(y) = u - y$, and "$\geq$" is understood coordinatewise. As we did before, again we assume that the defining functions of our problem (5.24), i.e., f^ζ ($\zeta = 1, 2, \ldots, \ell$) and c_J ($J = 1, 2$) are of class C^2.

For the lower level set due to any functional value $a \in \mathbb{R}$, we shall use the notation

$$\mathcal{L}^a(\mathcal{F}, \mathbf{c}) := \{y \in M[\mathbf{c}] \mid f(y) \leq a\}. \tag{5.25}$$

It is very natural that two optimization problems are topologically equivalent whenever globally all the descent flows in one problem are carried over into the corresponding descent flows in the other one. By using this idea, we introduce the following concept which actually gives an equivalance relation.

Definition 5.3.10. The optimization problems $P(\mathcal{F}^1, \mathbf{c}^1)$ and $P(\mathcal{F}^2, \mathbf{c}^2)$ with $f^1(y) := \max_{\zeta \in Z} f^{1,\zeta}(y)$ and $f^2(y) := \max_{\zeta \in Z} f^{2,\zeta}(y)$ are *equivalent* if there exist continuous mappings $\rho : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ and $\sigma : \mathbb{R} \to \mathbb{R}$ with the properties P1, P2, and P3:

P1. For every $t \in \mathbb{R}$, the mapping $\rho_t : \mathbb{R} \to \mathbb{R}$ is a homeomorphism from $\mathbb{R}$ onto itself, where $\rho_t(y) := \rho(t, y)$.

P2. The mapping σ is a homeomorphism from $\mathbb{R}$ onto itself and σ is monotonically increasing.

P3. $\rho_t[\mathcal{L}^t(\mathcal{F}^1, \mathbf{c}^1)] = \mathcal{L}^{\sigma(t)}(\mathcal{F}^2, \mathbf{c}^2)$ for all $t \in \mathbb{R}$. □

Referring to the concept of equivalence, we give the condition on structural stability of an optimization problem as follows:

Definition 5.3.11. The optimization problem $P(\mathcal{F}, \mathbf{c})$ is called *structurally stable* if there exists a C^2_S-neighborhood O of $(\mathcal{F}, \mathbf{c})$ with the property that $P(\mathcal{F}, \mathbf{c})$ and $P(\tilde{\mathcal{F}}, \tilde{\mathbf{c}})$, with $f(y) := \max_{\zeta \in Z} f^\zeta(y)$ and $\tilde{f}(y) := \max_{\zeta \in Z} \tilde{f}^\zeta(y)$, are equivalent for all $(\tilde{\mathcal{F}}, \tilde{\mathbf{c}}) \in O$ with $\tilde{\mathcal{F}} := (\tilde{f}^1, \tilde{f}^2, \ldots, \tilde{f}^\ell)^T$. □

The C^2_S*-topology* for the product $(C^2(\mathbb{R}, \mathbb{R}))^{\ell+2}$ mentioned above is defined as the *product topology* generated by the *strong* (or *Whitney-*) C^2*-topology* C^2_S on each factor $C^2(\mathbb{R}, \mathbb{R})$ [46, 51]. A typical base-neighborhood of a function $\eta \in C^2(\mathbb{R}, \mathbb{R})$ is the set $\eta + W_\epsilon$, where W_ϵ is defined as follows with the aid of a continuous $\epsilon : \mathbb{R} \to \mathbb{R}$ with $\epsilon(y) > 0$ $(y \in \mathbb{R})$:

$$W_\epsilon := \left\{ \vartheta \in C^2(\mathbb{R}, \mathbb{R}) \;\middle|\; |\vartheta(y)| + |\vartheta'(y)| < \epsilon(y) \quad \forall y \in \mathbb{R} \right\}. \tag{5.26}$$

Since structural stability turns out to be a very natural concept, our next result emphasizes again the importance of the constraint qualification of Mangasarian and Fromovitz [41, 51, 104, 105] on the one hand, and the concept of strong stability according to Kojima [61] on the other hand.

Theorem 5.3.12. The optimization problem $P(\mathcal{F}, \mathbf{c})$ with compact feasible set $M[\mathbf{c}]$ is structurally stable if and only if the following three conditions C1, C2 and C3 are satisfied:

C1. The *Mangasarian-Fromovitz constraint qualification* (*MFCQ*) is satisfied at every point of $M[\mathbf{c}]$.

C2. Every Kuhn-Tucker point of $P(\mathcal{F}, \mathbf{c})$ is *strongly stable* in the sense of Kojima.

C3. Different Kuhn-Tucker points have different ($f-$) values.

Remark 5.3.13. Fortunately, the $c^l(y)$ and $c^u(y)$ of our problem (5.24) as being the linear bound constraints for y are always linearly independent vectors satisfying LICQ, and hence, MFCQ. □

Remark 5.3.14. We note that similar to our Remark 5.3.3, the structural stability analysis presented here in y for the optimization problem (5.24) could be generalized to $\mathbf{y}_j \in \mathbb{R}^{p_j}$ ($j = 1, 2, \ldots, m$) and in the presence of $M[\bar{\mathbf{h}}, \bar{\mathbf{g}}]$ instead of $M[\bar{\mathbf{g}}]$ (= $M[\mathbf{c}]$), $\bar{\mathbf{h}}$ representing finitely many equality constraint functions. □

In Chapter 4, we reformulated the optimization problem of overall desirability functions, defined as the geometric mean of the individual desirability functions. What this has yielded is the additive overall function (4.7), which is the weighted sum of the individual functions introduced as the negative logarithm of the individual desirability functions.

The additive separability structure of this objective function makes it possible to find an approximative, in fact, a compromised solution for the multi-objective optimization problem. Let us remember that we represented individual desirability functions by $f^g(\cdot) := f(Y(\cdot))$. By defining $y = Y(\mathbf{x})$ we wrote individual desirability functions f as a function of y and showed that under which conditions they are members of a class of (finite) piecewise smooth functions, namely, piecewise max-type functions.

5.4 A New Approach for Multi-objective Optimization: Two-Stage (Bilevel) Method

If we consider the optimization problem (5.1) (in $\mathbf{y}$ only), its solution will be the ideal solution $\mathbf{t} := (t_1, t_2, \ldots, t_m)^T$. We suggest as one of various approaches of this thesis: (i) First to find the factor levels $\mathbf{x}_j^t := ((x_j^t)_1, (x_j^t)_2, \ldots, (x_j^t)_n)^T$ ($j = 1, 2, \ldots, m$) corresponding to the ideal solutions t_j, i.e., $t_j := Y_j(\mathbf{x}_j^t)$ for each individual function f. (ii) Then to compute the convex hull of these optimal solutions $\mathbf{x}_j^t$ ($j = 1, 2, \ldots, m$) and determine some compromised solution $\bar{\mathbf{x}} := (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)^T$ which may not be the global one for the overall problem given in the previous chapter but a close one.

In other words, we firstly solve a representation problem of searching for an $m \times n$ *design matrix*

$$\mathbf{X}^t := (\mathbf{x}_1^t, \mathbf{x}_2^t, \ldots, \mathbf{x}_m^t)^T \tag{5.27}$$

by finding the zero of the system of $\mathbf{Y}(\mathbf{X}^t) - \mathbf{t}$, where $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_m)^T$. Then we take the convex hull to obtain a compromised factor level $\bar{\mathbf{x}} := (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)^T$, i.e., the solution of $\bar{\mathbf{y}} := \mathbf{Y}(\bar{\mathbf{x}})$, where $\bar{\mathbf{y}} := (\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_m)^T$ is a compromised solution in $\mathbf{y}$-space. We call this approach a *two-stage method*, because it is similar to the other *bilevel* approaches [20]: First, we consider the *optimization problem* only in $\mathbf{y}$ as the lower level problem stated in previous chapter; then, by introducing $\mathbf{x}$ into our analysis, we pass to the upper level of this problem, which contains a *representation problem*.

Let us recall that per y_j, we are in a compact interval $\mathbb{I}_j = [l_j, u_j]$ $(j = 1, 2, \ldots, m)$, i.e., feasible sets of the lower level problem and the individual functions $f_j(y_j)$ are continuous and nonsmooth. By the following assumption, we may think that the space $\mathbb{X} \subset \mathbb{R}^n$ of the factor variable $\mathbf{x}$ is compact, in fact, of the Cartesian product form $\mathbb{X} = [\mathbf{l}_x, \mathbf{u}_x] = \bigtimes_{i=1}^{n} \mathbb{X}_i$ with $\mathbb{X}_i := [l_{x_i}, u_{x_i}]$ $(i = 1, 2, \ldots, n)$ being compact intervals. In this case, $\mathbb{X}$ is a *parallelepiped* and, hence, for each $j = 1, 2, \ldots, m$, the image $Y_j(\mathbb{X})$ is again an interval which can be defined as our interval $\mathbb{I}_j$, i.e., $Y_j(\mathbb{X}) := \mathbb{I}$. We introduce

$$\mathbb{X}^{appr} := \mathrm{co}\{\mathbf{x}_1^t, \mathbf{x}_2^t, \ldots, \mathbf{x}_m^t\}, \tag{5.28}$$

where the points $\mathbf{x}_j^t$ $(j = 1, 2, \ldots, m)$ are solutions of the zero problems $Y_j(\mathbf{x}) - t_j = 0$ $(j = 1, 2, \ldots, m)$ together with the vector-valued condition $\mathbf{x} \in \mathbb{X}$, which can be represented further by 2^n linear inequality constraints. Altogether, we arrive at $2^n + m$ scalar-valued constraints. We note that $\mathbb{X}^{appr}$ in convex, in fact, a *polytope* and, hence, because of the convexity of $\mathbb{X}$, it holds $\mathbb{X}^{appr} \subseteq \mathbb{X}$. Here, we have a discrete structure in the entire $\mathbf{x}$-space, given by the vertices of $\mathbb{X}^{appr}$, and could further optimize (select) over the full polytope $\mathbb{X}^{appr}$ in that space. The weights may, e.g., come from the exponents given in the conventional desirability function. Indeed, we could choose $\bar{\mathbf{x}} = \sum_{j=1}^{m} w_j \mathbf{x}_j^t$. The main advantage of this coupling is that we would get an optimizer in that polytope within the full dimensions of $\mathbb{R}^n$. However, since still the variables are treated in a separated way, this new approach is just an approximation to our original problem. This approximation can be simplifying very much, because of the *joint* dependence of all the $y_j = Y_j(\mathbf{x})$ $(j = 1, 2, \ldots, m)$ on $\mathbf{x}$ and because of the *nonlinearit*y and *nonconvexity* of the function f_j and Y_j $(j = 1, 2, \ldots, m)$. It can be motivated by *game theory* and introduces $\mathbb{X}^{appr}$ as a set of *compromise solutions*.

Another new opportunity is to further look for conditions to apply versions of the *Intermediate Value Theorem* directly in the *full* dimensions of the vector variable $\mathbf{y}$, rather than in each dimension with the difficulty of selecting the suitable optimizer in the $\mathbf{x}$-space then. In more general terms, we may also speak of the *Implicit Function Theorem*. Here, the structure of the functions Y_j, e.g., the relations between the x_i ($i = 1, 2, \ldots, n$) and the y_j ($j = 1, 2, \ldots, m$), is an important issue. We must have an (arcwise) connected domain of the vector-valued function $\mathbf{Y}(\mathbf{x})$ $(= (Y_1(\mathbf{x}), Y_2(\mathbf{x}), \ldots, Y_m(\mathbf{x}))^T)$, which we equate with $(\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_m)^T$, and hence, of each of its components $Y_j(\mathbf{x})$ ($j = 1, 2, \ldots, m$).

Let us summarize that this initial, pioneering and approximative approach has consisted of a separate consideration of the components y_j, combined with an enumeration (minimizing in a set of finitely many indices) along the pieces in each of these components, of a possible application of the Intermediate Value Theorem on the corresponding $Y_j(\mathbf{x})$ and, finally, of a polytope and selection argument in $\mathbb{X}^{appr}$, in order to find a compromise solution $\bar{\mathbf{x}}$ of the given problem.

In any case, what can be done is:

i. We define a weighed sum of the components $Y_j(\mathbf{x})$, e.g., by the exponents that we can take from the desirability function as the weights, and to apply the Intermediate Value Theorem on corresponding real-valued function, then our zero problem of finding $\mathbf{x} = \bar{\mathbf{x}}$ looks, e.g., as follows:

$$(\sum_{j=1}^{m} w_j Y_j)(\mathbf{x}) \; = \; \sum_{j=1}^{m} w_j \bar{y}_j. \tag{5.29}$$

ii. We approach the system of $2^n + m$ equations: $Y_j(\mathbf{x}) - \bar{y}_j = 0$ ($j = 1, 2, \ldots, m$) and $\mathbf{x} \in \mathbb{X}$, and treat it with the help of the theory of Inverse Problems, e.g., by the *Inverse Function Theorem* or the *Implicit Function Theorem*. We select

$$\bar{\mathbf{x}} = \sum_{j=1}^{m} \hat{w}_j \mathbf{x}_j^t \quad \text{(where } \hat{w}_j \geq 0 \ (j = 1, 2, \ldots, m) \text{ and } \sum_{j=1}^{m} \hat{w}_j = 1), \tag{5.30}$$

e.g.,

$$\begin{aligned} \bar{\mathbf{x}} &= \sum_{j=1}^{m} w_j \mathbf{x}_j^t, \quad \text{(where } \hat{w}_j = w_j \ (j = 1, 2, \ldots, m)) \quad \text{or, especially} \\ \bar{\mathbf{x}} &= \tfrac{1}{m} \sum_{j=1}^{m} \mathbf{x}_j^t, \quad \text{(where } \hat{w}_j = 1 \text{ for all } (j = 1, 2, \ldots, m)). \end{aligned} \tag{5.31}$$

Remark 5.4.1. We note that global optimums of our problems from Chapter 3 are not in the convex hull of the set of compromised solutions in both cases. As a future work, we will use some well known metrics from the literature instead of the convex hull operation in our two-stage method to increase the efficiency of the method. □

CHAPTER 6

EXTENSIONS TO OPTIMIZATION OF GDFs

6.1 Introduction

In Chapter 5, we partitioned the interval of the individual logarithmic desirability function $f_j(y)$ into finitely many subintervals and employed max-type functions at each subintervals to obtain the generalized individual desirability functions. We considered the minimization problem of the max-type function at each subinterval, a finitely constrained minimax problem. In this chapter, we extend this idea by employing semi-infinite max-type functions at each subinterval. By doing this, we have the theoretical advantage of using notions of *generalized semi-infinite programming* (GSIP) [107, 105] and *disjunctive optimization* [12, 39, 45, 51, 110] in our attempt of robustification the optimization problem of generalized overall desirability functions. Robust case of this optimization is needed because regression may be done under lack of knowledge about the underlying model and scenarios or there can be noise in the data, and hence, the responses would be *uncertain*. We conclude this chapter by a discussion on robustness in terms of critical point theory and its usage in [26].

6.2 Partitioning by Semi-infinite Max-type Functions

To obtain the generalized individual desirability functions, we partitioned the interval $\mathbb{I}_j = [l_j, u_j]$ of the individual logarithmic desirability function $f_j(y)$ into finitely many subintervals κ, where at each pair (j, κ) $(\kappa \in K_j, j \in J)$ the function $f_{j,\kappa}(y)$ is a creased manifold with compact and connected parts of C^2-smooth submanifolds $f^{\zeta}_{j,\kappa}$ (i.e., graph $(f^{\zeta}_{j,\kappa})$), indexed by ζ from a finite index set $Z_{j,\kappa}$. Hence, the minimization problem (5.5) of the max-type functions $f_{j,\kappa}(y) = \max_{\zeta \in Z_{j,\kappa}} f^{\zeta}_{j,\kappa}(y)$ for a fixed $\kappa \in K_j$ and for a fixed $j \in J$ was considered as a finitely constrained minimax problem for $y \in \mathbb{I}_{j,\kappa}$.

Here, again for a given pair (j, κ) ($\kappa \in K_j$, $j \in J$), we regard the creased manifold with an *infinite* (usually, uncountable) number of competitors ζ for the "max" over each subinterval κ:

$$f_{j,\kappa}(y) := \max_{\zeta \in Z_{j,\kappa}} \mathtt{f}_{j,\kappa}(y, \zeta). \tag{6.1}$$

We note that based on all the functions $\mathtt{f}_{j,\kappa}(\cdot, \zeta)$ ($\zeta \in Z_{j,\kappa}$), the entire function $f_{j,\kappa}(y)$ will be a "more smooth" piecewise function. That smoothing is some kind of *envelope effect* of the piecewise maximum with infinitely many (usually, a continuum of) pieces as in (6.1). The optimization problem of this *semi-infinite* max-type objective function $f_{j,\kappa}$ is:

$$\begin{aligned} &\underset{y}{\text{minimize}} && f_{j,\kappa}(y) \\ &\text{subject to} && y \in \mathbb{I}_{j,\kappa}, \end{aligned} \tag{6.2}$$

which is a general minimax problem with ζ ranging over an infinite compact set $Z_{j,\kappa}$:

$$\underset{y \in \mathbb{I}_{j,\kappa}}{\text{minimize}} \quad \underset{\zeta \in Z_{j,\kappa}}{\text{maximize}} \ \mathtt{f}_{j,\kappa}(y, \zeta). \tag{6.3}$$

We can describe the feasible set of this problem implicitly by finitely many constraints:

$$Z_{j,\kappa} := M[\underline{\mathbf{h}}_{j,\kappa}, \underline{\mathbf{g}}_{j,\kappa}] \subseteq \mathbb{R}.$$

Let us underline that these index manifolds (with boundary) can also be placed in $\mathbb{R}^{p_{j,\kappa}}$ ($p_{j,\kappa} \in \mathbb{N}$), i.e.,

$$Z_{j,\kappa} := M[\underline{\mathbf{h}}_{j,\kappa}, \underline{\mathbf{g}}_{j,\kappa}] \subseteq \mathbb{R}^{p_{j,\kappa}}.$$

Now, let solutions of (6.3) be called $t_{j,\kappa}$ ($\kappa \in K_j$) for each $j \in J$. Similarly to the finite case explained above, the minimization of $f_j(y)$ is a *discrete* optimization problem, actually, an *enumeration problem*, over all κ, for each regarded j. By solving these problems to find the global minimum of $f_j(y)$ per given $j \in J$, we will obtain a set of solutions, say t_j ($j = 1, 2 \ldots, m$), which are, in fact, $t_j := t_{j,\bar{\kappa}_j}$ for a certain $\bar{\kappa}_j \in K_j$. Hence, the solution of the full dimensional problem ((5.1)) in the variable $\mathbf{y}$ is $\mathbf{t} := (t_1, t_2, \ldots, t_m)^T$.

6.3 Robustness in the Optimization of Desirability Functions

For the cases when the regression is done under lack of knowledge about the underlying model and scenarios or if there is noise in the data, etc., the responses will be *uncertain*. In fact, it is quite natural to think uncertainty together with the notion of response since a response is an estimated value, i.e., the mean of several response values obtained during the experimental design. This uncertainty about parameters $y_j \in \mathbb{I}_j$ $(j = 1, 2, \ldots, m)$ can be represented by allowing the inclusion $\mathbf{y} \in \mathbf{Y}(\mathbf{x})$, rather than the equation $\mathbf{y} = \mathbf{Y}(\mathbf{x})$, where $\mathbf{y} = (y_1, y_2, \ldots, y_m)^T$ and $\mathbf{Y}(\mathbf{x}) = (Y_1, Y_2, \ldots, Y_m)^T(\mathbf{x})$. Hence, $\mathbf{Y}(\mathbf{x})$ becomes a *set-valued* x-dependent mapping for $\mathbf{y}$ meaning that each $Y_j(\mathbf{x})$ $(j = 1, 2, \ldots, m)$ is allowed to be a multi-valued index set for y_j rather than a single-valued (vectorial) function.

To handle all these uncertainties in the responses, we introduce the *robust* (i.e., *worst-case*) formulation of the inequality constraints giving rise in an equivalent form of our optimization problem ((5.1)). This robust optimization of the generalized overall desirability function $F(\mathbf{y}) = \sum_{j=1} w_j f_j(y_j)$ becomes a refined (*disjunctive*) *generalized semi-infinite program* (*GSIP*). For more information on robust optimization, we refer to [11, 33] and for disjunctive optimization to [12, 39, 45, 51, 110].

Remark 6.3.1. We define the function $G(\mathbf{x}) := \inf\{F(\mathbf{y}) \mid \mathbf{y} = \mathbf{Y}(\mathbf{x})\ (\mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x])\}$, which may be considered as a special case of *marginal function* [51, 78]. □

The optimization problem of the generalized desirability functions depending on both $\mathbf{x}$ and $\mathbf{y}$ can be written as follows:

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & F(\mathbf{y}) \\ \text{subject to} \quad & \mathbf{y} = \mathbf{Y}(\mathbf{x}) \cap \mathbb{I}, \\ & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x]. \end{aligned} \tag{6.4}$$

Now, we reformulate our optimization problem (6.4) with an uncertainty set of responses $\mathbf{Y}(\mathbf{x})$ as the minimization of the *height variable* φ:

$$\begin{aligned} \underset{\varphi, \mathbf{x}}{\text{minimize}} \quad & \varphi \\ \text{subject to} \quad & F(\mathbf{y}) \leq \varphi \qquad \forall \mathbf{y} \in \mathbf{Y}(\mathbf{x}) \cap \mathbb{I}, \\ & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x]. \end{aligned} \tag{6.5}$$

This problem can be refined componentwise by using the additive definition of $F(\mathbf{y})$ and referring to the termwise *height vector* $\boldsymbol{\varphi} := (\varphi_1, \varphi_2, \ldots, \varphi_m)^T$ as follows:

$$\begin{aligned} \underset{\boldsymbol{\varphi}, \mathbf{x}}{\text{minimize}} \quad & \varphi_1 + \varphi_2 + \ldots + \varphi_m \\ \text{subject to} \quad & f_j(y) \leq \varphi_j \qquad \forall\, y \in Y_j(\mathbf{x}) \cap \mathbb{I}_j, \\ & \qquad\qquad\quad\ \forall\, j \in J, \\ & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x], \end{aligned} \tag{6.6}$$

where $f_j(y)$ are the generalized individual desirability functions having a piecewise max-type structure. This problem is equivalent to

$$\begin{aligned} \underset{\varphi,\mathbf{x}}{\text{minimize}} \quad & \varphi_1 + \varphi_2 + \ldots + \varphi_m \\ \text{subject to} \quad & \min_{\kappa \in K_j} \max_{y \in Y_j(\mathbf{x}) \cap \mathbb{I}_{j,\kappa}} f_{j,\kappa}(y) \le \varphi_j \quad \forall\, j \in J, \\ & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x]. \end{aligned} \tag{6.7}$$

Because of the min-terms, problem (6.7) can be represented as a *nonsmooth GSIP problem*. Using the definition (6.1), we may write this nonsmooth GSIP program as a *smooth GSIP problem* by a *disjunctive*, i.e., "∃" connected model component:

$$\begin{aligned} \underset{\varphi,\mathbf{x}}{\text{minimize}} \quad & \varphi_1 + \varphi_2 + \ldots + \varphi_m \\ \text{subject to} \quad & \mathtt{f}_{j,\kappa}(y,\zeta) \le \varphi_j \qquad \exists\, \kappa \in K_j, \\ & \qquad\qquad\qquad\qquad \forall\, y \in Y_j(\mathbf{x}) \cap \mathbb{I}^{\zeta}_{j,\kappa}, \\ & \qquad\qquad\qquad\qquad \forall\, \zeta \in Z_{j,\kappa}, \\ & \qquad\qquad\qquad\qquad \forall\, j \in J, \\ & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x]. \end{aligned} \tag{6.8}$$

We note that this problem (6.8) is equivalent to

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & \sum_{j \in J} \underset{\kappa \in K_j}{\text{minimize}} \max_{\substack{\zeta \in Z_{j,\kappa} \\ y \in Y_j(\mathbf{x}) \cap \mathbb{I}^{\zeta}_{j,\kappa}}} \mathtt{f}_{j,\kappa}(y,\zeta) \\ \text{subject to} \quad & \mathbf{x} \in [\mathbf{l}_x, \mathbf{u}_x]. \end{aligned} \tag{6.9}$$

This means that up to the choice represented by κ, for all feasible $y_j \in Y_j(\mathbf{x})$ and all feasible $\zeta \in Z_{j,\kappa}$, the inequality constraints in (6.8) have to hold. By minimizing the $\max_{y,\zeta} \mathtt{f}_{j,\kappa}(y,\zeta)$ over $\mathbf{x}$ and ζ like this, we encounter the "worst-case" [62, 108], and hence, we perform robust optimization as in (6.9). We are uncertain about the responses $Y_j(\mathbf{x})$, which is the case when the vector of the y_j lies in a set rather than being a vector. We can consider two cases for the structure of the set $\mathbf{Y}(\mathbf{x})$ of uncertain response vectors:

Special Case: The Cartesian product of the sets of real numbers $Y_j(\mathbf{x})$: $\mathbf{Y}(\mathbf{x}) := \bigtimes_{j=1}^{m} Y_j(\mathbf{x})$, where $Y_j(\mathbf{x})$ usually are intervals. Then, $Y_j(\mathbf{x})$ is a parallelepiped. In this special case, $Y_j(\mathbf{x})$ is parallel to the coordinate axes.

General Case: Polyhedral or ellipsoidal (where we can take into account the correlations of the Y_j), or any other compact manifolds with a generalized boundary. We note that, e.g., ellipsoids can also be assigned to clusters of variables y_j [62]. In this general case, $Y_j(\mathbf{x})$ does not need to be, and typically is not, parallel to the coordinate axes.

For closer discussion on configurations of such kinds of uncertain set and confidence regions, we refer to [51, 62].

6.4 Robustness vs. Stability of the Desirability Functions

In the previous section, we robustify the overall desirability optimization problem when uncertainty in responses is suspected. Also, we remember that, in the previous chapter, we checked the stability conditions of generalized individual desirability functions by considering perturbations in factors. However, in [26], we find the usage of the robustness notion having a rather opposite meaning to what we call strong stability (in the sense of Kojima [61]) or structural stability (in the sense of Jongen et al. [41, 51, 52]). In that study, by looking at the steepness of figure of the overall desirability function with respect to the factor variables, the robustness of the product is decided. When the figure of the overall desirability is more flat the product is considered to be *robust* (see Figure 6.1 a.), when it is steep, then it is called *nonrobust* (see Figure 6.1 b.).

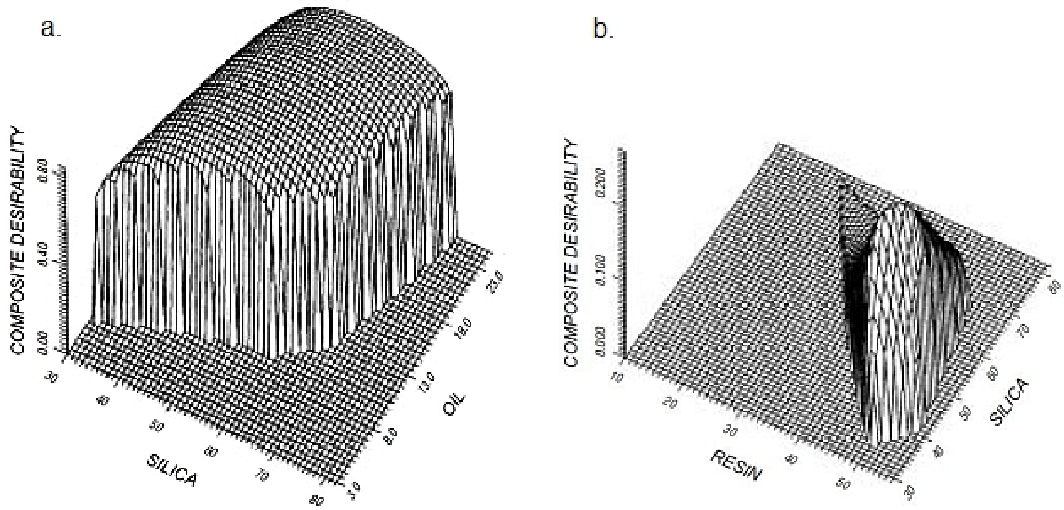

Figure 6.1: Overall desirability of a a. robust and b. nonrobust product in terms of Derringer [26].

However, in the sense of critical point theory, a rapid (steep) hill basically means stability. A relatively flat hill is nonstable in terms of perturbations as seen in Figure (5.4) from Chapter 5 for our case of piecewise defined functions.

CHAPTER 7

CONCLUSION

Desirability functions approach is one of the most common methods of multi-response optimization. There are many different types of desirability functions used in practice; and optimization of these functions continues to be an important research area. In this thesis, we deal with many aspects of optimization of Derringer and Suich's type desirability functions, we both analyze the structure of the functions themselves and propose alternative solution strategies to their optimization problem with nonsmooth and nonlinear optimization techniques. Moreover, we introduce a new multi-objective optimization method motivated by desirability functions.

Firstly, we show that the maximization of an overall desirability function is a nonsmooth composite constrained optimization problem. By a reformulation of individual desirability functions, we obtain adjusted individual and overall desirability functions. Optimization of these functions is performed with two nonsmooth methods: (*i*) modified subgradient algorithm together with CONOPT solver of GAMS, and (*ii*) BARON solver of GAMS. We show that application of modified subgradient algorithm needs some mathematical background in computing the dual problem with respect to sharp augmented Lagrangians; application together with BARON is a strong alternative to the existing desirability maximization methods. Applied on two well-known examples, BARON finds the global optimal efficiently, and the related solution processes turn out to be user-friendly and successful in terms of computation time.

Secondly, we reveal that the mechanism behind desirability functions which give rise to a variation and extension of the piecewise structure of the functions used in practice, can be explained by an abstract class of functions, i.e., continuous selection functions and especially, max-type functions. We show that, component-wise and generically, piecewise max-type functions have such structural and topological properties that enable us to characterize the desirability functions and to scientifically establish our generalized desirability functions.

Thirdly, we propose a new solution strategy called the two-stage (bilevel) approach for multi-objective optimization problems, based on a separation of the parameters: in **y**-space (optimization) and in **x**-space (representation). It is possible to find a compromised solution to the problem via this approach. For the optimization problem in the variable **y**, we characterized its structural stability. The overall problem in both **x** and **y** is extended to a new refined (disjunctive) generalized semi-infinite problem, herewith analyzing the stability and robustness properties of the objective function. In this course, we introduce the so-called robust optimization of desirability functions for the cases where response models contain uncertainty.

For future studies, we suggest to apply smoothing techniques on the optimization of desirability functions, especially, when the individual desirability functions include more than one nondifferentiable point. Further aspects of Morse theory for piecewise max-type functions and a characterization of structural stability of the optimization problem in the variable **x** may proceed. It will be interesting to analyze the reformulated and extended desirability functions which we present throughout this thesis, through a multi-objective optimization research. Another interesting study would be the relation between the functions of MARS, CMARS and desirability functions.

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APPENDIX A

Wire Bonding Process Problem

A pre-molded plastic package with leads and silicon chips adhered on it, is taken into consideration. The aim is to bond leads and silicon chips with wires. This bonding is performed at elevated temperatures to obtain high quality bonds. The elevation of temperature is allowed until the melting point of the plastic mold compound used in the package. We have a heater that blows heated nitrogen on top of the package. We denote the position of leads with A and the position of silicon chips with B on the plastic package. The package is passed under the manifold by gradually increasing the temperature at positions A and B. After the units at A and B exit the manifold, they are placed on the heater block where the wire bonding is performed. This heater block applies heat from the back side of the package which helps to reduce the amount of heat loss at the bonding positions. However, the temperatures at positions A and B decrease after leaving the manifold. Because of this, the temperature is recorded at the following times:

- at the beginning of the bonding process A and B,

- at the end of the bonding process A and B, and

- during the heating cycle for both positions A and B when it is maximal.

The variables which affect the temperature at the wire bond are:

- the N_2 flow rate (x_1),

- the N_2 temperature (x_2), and

- the heater block temperature (x_3).

The goal is to find operating conditions that achieve optimal temperatures during actual wire bonding while not exceeding the melting temperature of the plastic package. The responses are

- the maximum temperature at position A: $Y_1(\mathbf{x})$,

- beginning bond temperature at position A: $Y_2(\mathbf{x})$,

- finish bond temperature at position A: $Y_3(\mathbf{x})$,

- the maximum temperature at position B: $Y_4(\mathbf{x})$,

- beginning bond temperature at position B: $Y_5(\mathbf{x})$, and

- finish bond temperature at position B: $Y_6(\mathbf{x})$,

Corresponding bounds for the factors of this problem are given in Table A.1

Table A.1: Bounds for the factors of wire bonding problem [19].

	l_{x_i}	u_{x_i}
x_1	40	120
x_2	200	450
x_3	150	350

The models for the responses are used as given in Castillo et al. [19]. Their upper, lower and target values are given in Table A.2.

Table A.2: Desirability Parameters of the responses for the Wire Bonding Problem [19].

	l_j	t_j	u_j	$d_j(l_j)$	$d_j(t_j)$	$d_j(u_j)$
y_1	185	190	195	0	1	0
y_2	170	185	195	0	1	0
y_3	170	185	195	0	1	0
y_4	185	190	195	0	1	0
y_5	170	185	195	0	1	0
y_6	170	185	195	0	1	0

Ordinary least-squares estimation techniques were first applied to the data to develop models for the factors. The models $y_j = Y_j(\mathbf{x})$ $(j = 1, 2, \ldots, m)$ generated are as follows:

$$\begin{aligned}
Y_1(\mathbf{x}) &= 174.93 + 23.38x_2 + 3.62x_3 - 19.00x_2x_3,\\
Y_2(\mathbf{x}) &= 141.00 + 6.00x_1 + 21.02x_2 + 14.12x_3,\\
Y_3(\mathbf{x}) &= 139.53 + 7.25x_1 + 16.00x_2 + 19.75x_3,\\
Y_4(\mathbf{x}) &= 154.00 + 10.10x_1 + 30.60x_2 + 6.30x_3 - 11.20x_1^2 + 11.30x_1x_2,\\
Y_5(\mathbf{x}) &= 139.29 + 4.63x_1 + 19.75x_2 + 16.13x_3 - 5.41x_1^2 + 7.00x_1x_2,\\
Y_6(\mathbf{x}) &= 146.86 + 4.87x_1 + 15.62x_2 + 27.00x_3 - 3.98x_1^2 + 4.75x_1x_2.
\end{aligned} \tag{A.1}$$

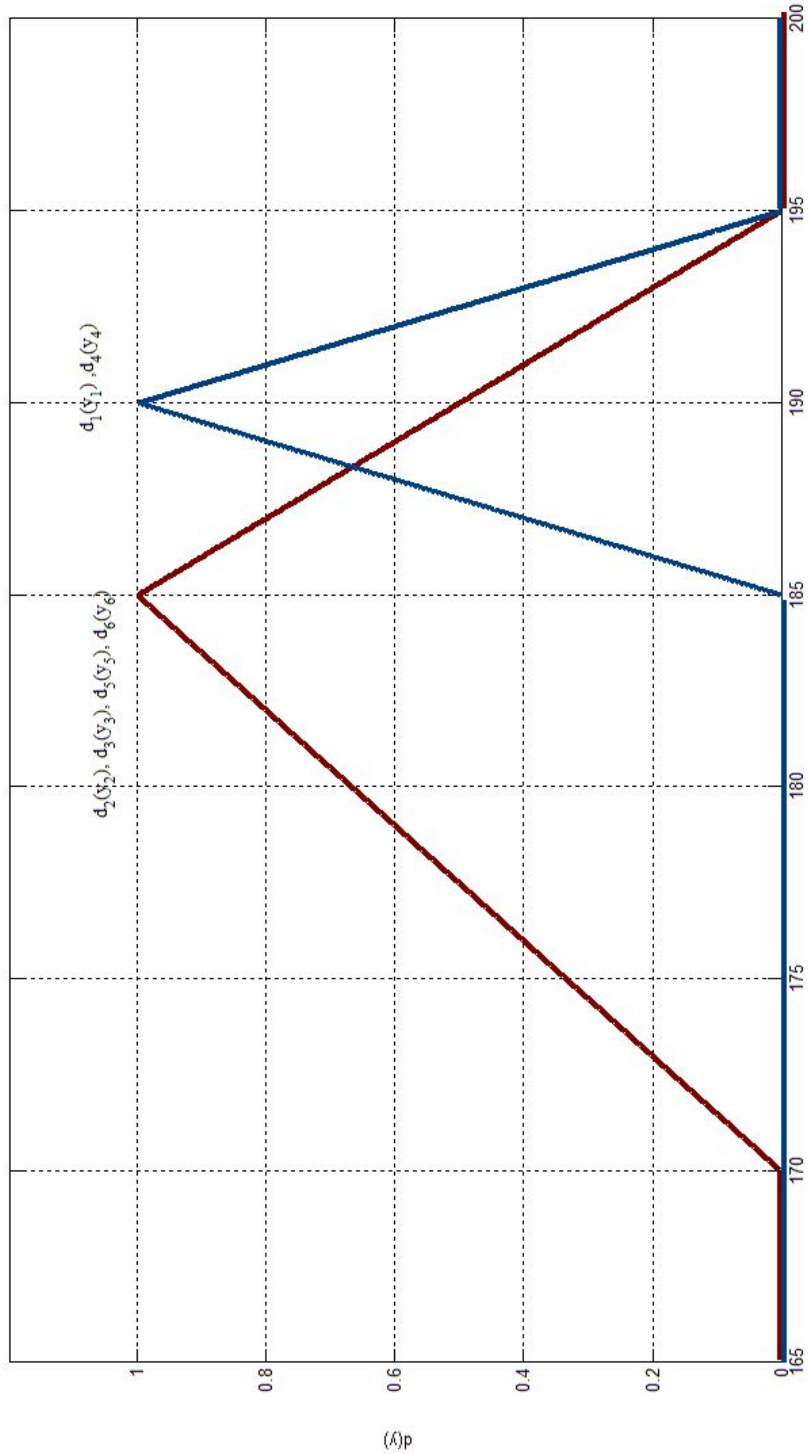

Figure A.1: Individual desirability functions $d_j(y_j)$ $(j = 1, 2, \ldots, 6)$ with $y_j = Y_j(\mathbf{x})$ of the wire bonding process optimization problem.

APPENDIX B

Tire Tread Compound Problem

In the development of a tire tread compound, a problem from rubber industry occurs. There are three variables:

- Hydrated silica level (x_1),
- Silane coupling level (x_2), and
- Sulfur level (x_3).

The goal is the attainment of the best balance among several different response variables:

- PICO Abrasion Index: $Y_1(\mathbf{x})$,
- 200 percent modulus: $Y_2(\mathbf{x})$,
- elongation at break: $Y_3(\mathbf{x})$, and
- elongation at hardness: $Y_4(\mathbf{x})$.

With a three-variable, rotatable, central composite design including six center points, the data are generated and, then, second degree polynomials are fit to obtain the response models in Derringer and Suich's work [25]:

$$
\begin{aligned}
&Y_1(\mathbf{x}) = 139.12 + 16.49x_1 + 17.88x_2 + 10.91x_3 - 4.01x_1x_1 - 3.45x_2x_2 \\
&-1.57x_3x_3 + 5.13x_1x_2 + 7.13x_1x_3 + 7.88x_2x_3, \\
&Y_2(\mathbf{x}) = 1261.11 + 268.15x_1 + 246.5x_2 + 139.48x_3 - 83.55x_1x_1 - 124.79x_2x_2 \\
&+199.17x_3x_3 + 69.38x_1x_2 + 94.13x_1x_3 + 104.38x_2x_3, \\
&Y_3(\mathbf{x}) = 400.38 - 99.67x_1 - 31.4x_2 - 73.92x_3 + 7.93x_1x_1 + 17.31x_2x_2 \\
&+0.43x_3x_3 + 8.75x_1x_2 + 6.25x_1x_3 + 1.25x_2x_3, \\
&Y_4(\mathbf{x}) = 68.91 - 1.41x_1 + 4.32x_2 + 1.63x_3 + 1.56x_1x_1 + 0.06x_2x_2 \\
&-0.32x_3x_3 - 1.63x_1x_2 + 0.13x_1x_3 - 0.25x_2x_3.
\end{aligned}
\tag{B.1}
$$

The first two responses $Y_1(\mathbf{x})$ and $Y_2(\mathbf{x})$ are the upper-the-best type, i.e., they have one-sided desirabilities, the last two responses, $Y_3(\mathbf{x})$ and $Y_4(\mathbf{x})$ are the target-is-the-best type, i.e., they have two-sided desirabilities. For the lower, upper and target values, see Table B.1.

Table B.1: Parameters of the responses for the Tire Tread Compound Problem [25].

	l_j	t_j	u_j	$d_j(l_j)$	$d_j(t_j)$	$d_j(u_j)$
y_1	120	–	170	0	–	1
y_2	1000	–	1300	0	–	1
y_3	400	500	600	0	1	0
y_4	60	67.5	75	0	1	0

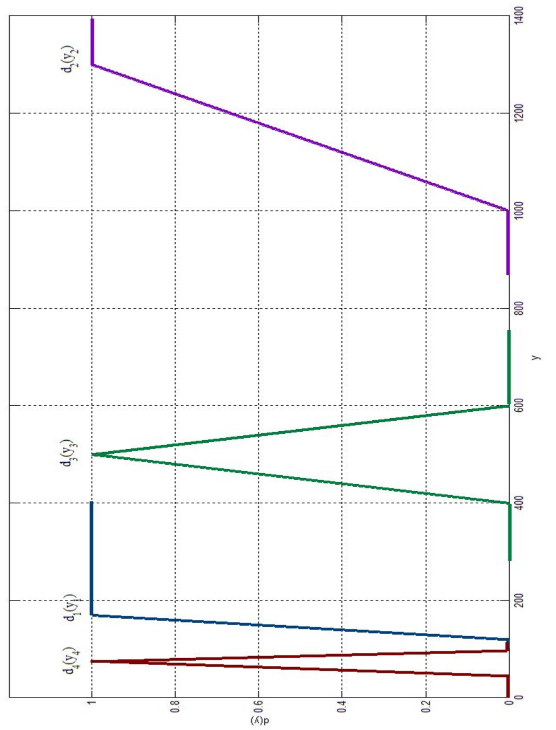

Figure B.1: Individual desirability functions $d_j(y_j)$ ($j = 1, 2, \ldots, 4$) with $y_j = Y_j(\mathbf{x})$ of the tire tread compound optimization problem.

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EDUCATION

B.Sc., Mathematics Department, METU, 2003,

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RESEARCH INTEREST

- Optimization in Operational Research
- Data Mining
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- Aspects of Semi-Infinite and Robust Optimization
- Multi-Objective Optimization
- Algorithms
- e-Learning

QUALIFICATIONS

- MATLAB, GAMS (BARON, CONOPT, DICOPT), SPSS Clementine, LATEX
- C/C++, JAVA, HTML, ASP, PHP, SQL, MySQL, PostgreSQL, Ms SQL 2000 Server,
- Windows Series Administration: XP, 2000 (Advanced) Server, 2003 Server, Vista
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LANGUAGES

- Advanced in English (Exemption from the Basic English Program, METU), KPDS: 90 (A)
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EMPLOYMENT

A. InterMedia A.S., System and e-Learning Tools Administration, Website and Database Programming, **Software Developer**, METU Technopolis, 2003 - 2005.

B. METU Presidency, Instructional Technologies Support Office,
Research Assistant (Instructional Technologist), 2005 - 2008.

C. METU Presidency, Career Planning Center and Alumni Office,
Research Assistant (System, Website and Database Administrator), 2008 - 2010.

D. TÜBİTAK Project 105M138: Use and Development of Data Mining in Quality Improvement (principal investigator Prof. Dr. Gülser Köksal, IE, METU),
Research Assistant, METU, 2006 - 2009.

ACTIVITIES

- EUROPT (The Continuous Optimization Working Group of EURO) Web Page,
http://www.iam.metu.edu.tr/EUROPT,
Web Master and Content Administrator, METU, July 2003 - Ongoing.

- **Stream Organizer:** (http://www.mii.lt/europt-2008/index.php?page,streams.en),
EURO Mini Conference - Continuous Optimization and Knowledge-Based Technologies, Neringa, Lithuania, May 20-23, 2008,
Name of the Stream: Clustering and Its Modern Optimization methods.

- **Session Organizer:** (http://www.euro-2009.de/final_programme.pdf), EURO Conference XXII - OR Creating Competitve Advantage, Bonn, Germany, July 5 – 8, 2009, Name of the Session: Various New Achievements in Mathematical Programming in the Stream of Mathematical Programming.
- **Invited Lecturer:** (http://summerschool.ssa.org.ua/en/courses/tutors/basak-akteke-ozturk), AACIMP 2009 - The Summer School, Achievements and Applications of Contemporary, Informatics, Mathematics and Physics, Kiev Polytechnic Institute, Kiev, Ukraine, August 5 – 16, 2009, Course Title: Modern Operational Research and Its Mathematical Methods.
- **Session Organizer:** (http://or2010.informatik.unibw-muenchen.de), International Conference on Operations Research 2010, Munich, Germany, September 1 – 2, 2010, Name of the Session: Applications of Nonsmooth, Conic and Robust Optimization, in the OR in Life Sciences and Education - Trends, History and Ethics.

PUBLICATIONS

A. International Conference Proceeding Papers

1. **Akteke-Öztürk, B.**, Weber, G.-W., Kropat, E., Continuous Optimization Approaches for Clustering via Minimum Sum of Squares, ISI Proceedings of *EURO Mini Conference - Continuous Optimization and Knowledge-Based Technologies*, 253-258, Neringa, Litvanya, May 20-23, 2008. (refereed)
2. Barzily, Z., Volkovich, Z., **Akteke-Öztürk, B.**, Weber, G.-W., Cluster Stability Using Minimal Spanning Trees, ISI Proceedings of *EURO Mini Conference - Continuous Optimization and Knowledge-Based Technologies*, 248-252, Neringa, Litvanya, May 20-23, 2008. (refereed)
3. Gürbüz, T., Arı, F., **Akteke-Öztürk, B.**, Kubuş, O., Çağıltay, K., METU Instructional Technology Support Office: Accelerating Return on Investment Through e-learning Faculty Development, *2nd International Conference on Innovations In Learning for the Future: e-learning (Future-learning 2008)*, Istanbul, Turkey, 107-114, March 27-29, 2008.

4. Kubuş, O., Arı, F., Çağıltay, K., Gürbüz, T., **Akteke-Öztürk, B.**, METU Open Courseware Project, *2nd International Computer and Instructional Technologies Symposium (ICITS 2008)*, Kuşadası, Turkey, 700-705, April 16-18, 2008.

5. Kropat, E., Weber, G.-W., **Akteke-Öztürk, B.**, Eco-Finance Networks Under Uncertainty, Proceedings of *EngOpt 2008 - International Conference on Engineering Optimization*, Rio de Janeiro, Brazil, June 1-5, 2008, at CD. (refereed)

6. Özögür-Akyüz, S., **Akteke-Öztürk, B.**, Tchemisova, T., Weber, G.-W., New Optimization Methods in Data Mining, *Operations Research Proceedings 2008*, 527-532, 2009, DOI:10.1007/978-3-642-00142-0.

7. **Akteke-Öztürk, B.**, Köksal, G., Weber, G.-W., Optimization of Desirability Functions as a DNLP Model by GAMS/BARON, AIP Conference Proceedings of *PCO 2010 - 3rd Global Conference on Power Control and Optimization*, 1239, 305-310, February 2-4, 2010, Gold Coast, Queensland, Australia. (refereed)

B. National Conference Proceeding Papers

1. **Akteke-Öztürk, B.**, Weber, G.-W., Kayalıgil, S., Kalite İyileştirmede Veri Kümeleme: Döküm Endüstrisinde Bir Uygulama, *Yöneylem Araştırması ve Endüstri Mühendisliği 27. Ulusal Kongresi (YA/EM 2007) Bildiriler Kitabı*, 1207-1212, İzmir, Türkiye, Temmuz 02-04, 2007.

2. **Akteke-Öztürk, B.**, Arı, F., Kubuş, O., Gürbüz, T., Çağıltay, K., Öğretim Teknolojileri Destek Ofisleri ve Üniversitedeki Rolleri, Bildiri Kitapçığı, No: 101, *Akademik Bilişim 2008*, Çanakkale, Türkiye, 30 Ocak - 1 Şubat 2008.

3. **Akteke-Öztürk, B.**, Weber, G.-W., Köksal, G., Çekicilik Fonksiyonlarının Bileşke Fonksiyonlar Olarak Çözümlenmesi, *Yöneylem Araştırması ve Endüstri Mühendisliği 29. Ulusal Kongresi (YA/EM 2009)* Bildiriler Kitabı (CD), Ankara, Türkiye, Haziran 22-24, 2009.

C. Journal Papers

1. Weber, G.-W., Taylan, P., **Akteke-Öztürk, B.**, and Uğur, Ö., Mathematical and Data Mining Contributions to Dynamics and Optimization of Gene-Environment Networks,

Electronic Journal of Theoretical Physics (EJTP), 4, 16 (II), 115-146, (December 2007). (Refereed)

2. Weber, G.-W., Taylan, P., Alparslan-Gök, S. Z, Özöğür, S., and **Akteke-Öztürk, B.**, Optimization of Gene-environment Networks in the Presence of Errors and Uncertainty with Chebychev Approximation, *TOP (the Operational Research journal of SEIO (Spanish Statistics and Operations Research Society))*, 16(2), 284-318, (December 2008). (SCI Expanded)

3. Barzily, Z., Volkovich, Z., **Akteke-Öztürk, B.**, and Weber, G.-W., On a minimal spanning tree approach in the cluster validation problem, *INFORMATICA*, 20 (2), 187-202, (April 2009). (C Grubu)

4. Weber, G.-W., Kropat, E., **Akteke-Öztürk, B.**, and Görgülü, Z. K., A survey on OR and mathematical methods applied on gene-environment networks, *Central European Journal of Operations Research (CEJOR)*, 17(3), 315-341, (September 2009). (SCI Expanded)

5. **Akteke-Öztürk, B.**, Köksal, G., and Weber, G.-W., Optimization of Desirability Functions by Nonlinear and Nonsmooth Methods (to be submitted)

6. **Akteke-Öztürk, B.**, Weber, G.-W., and Köksal, G., Generalized Desirability Functions: A Topological and Structural Analysis of Desirability Functions (to be submitted)

D. Book Chapters

1. Weber, G.-W., Taylan, P., Özöğür, S., and **Akteke-Öztürk B**., Statistical Learning and Optimization Methods in Data Mining, in: *Recent Advances in Statistics*, Ayhan, H. Ö., and Batmaz, I., (eds.), Turkish Statistical Institute Press, Ankara, at the occasion of Graduate Summer School on New Advances in Statistics, 181-195, (August 2007).

2. Weber, G.-W., Taylan, P., **Akteke-Öztürk, B.**, and Uğur, Ö., Mathematical and Data Mining Contributions to Dynamics and Optimization of Gene-Environment Networks, Chapter in the Book *Crossing in Complexity: Interdisciplinary Application of Physics in Biological and Social Systems*, eds.: I. Licata and A. Sakaji, Nova Publisher, May 2010.

E. Posters

1. Tchemisova, T., **Akteke-Öztürk, B.**, and Weber, G.-W., On Continuous Optimization Methods in Data Mining - Cluster Analysis, Classification and Regression - Provided for Decision Support and Other Applications, in proceedings Collaborative Decision Making: Perspectives and Challenges of *IFIP TC8/WG8.3 Working Conference: International Conference on Collaborative Decision Making (CDM'08)*, Toulouse, France, July 1-4, 2008.

F. Conference Presentations/Abstracts

1. Akteke-Öztürk, B., and Weber, G.-W., Semidefinite Programming Approach for Support Vector Clustering, EURO XXI - European Conference on Operational Research, Reykjavik, Iceland, July 02-05, 2006.

2. Akteke-Öztürk, B., and Weber, G.-W., Data Mining for Quality Improvement Data with Nonsmooth Optimization vs. PAM and k-Means, EURO XXII - European Conference on Operational Research, Prague, Czech Republic, July 8-11, 2007.

3. Akteke-Öztürk, B., Weber, G.-W., and Kayalıgil, S., Kalite İyileştirmede Veri Kümeleme: Döküm Endüstrisinde Bir Uygulama, Yöneylem Araştırması ve Endüstri Mühendisliği 27. Ulusal Kongresi (YA/EM 2007), İzmir, Türkiye, Temmuz 02-04, 2007.

4. Akteke-Öztürk, B., Arı, F., Kubuş, O., Gürbüz, T., Çağıltay, K., Öğretim Teknolojileri Destek Ofisleri ve Üniversitedeki Rolleri, Akademik Bilişim 2008, Çanakkale, Türkiye, 30 Ocak - 1 Şubat 2008.

5. Gürbüz, T., Arı, F., Akteke-Öztürk, B., Kubuş, O., Çağıltay, K., METU Instructional Technology Support Office: Accelerating Return on Investment Through e-learning Faculty Development, 2. Uluslararası Gelecek İçin Öğrenme Alanında Yenilikler Konferansı 2008: e-Öğrenme, İstanbul, Türkiye, 27-29 Mart 2008.

6. Kubuş, O., Arı, F., Çağıltay, K., Gürbüz, T., Akteke-Öztürk, B. ODTÜ Açık Ders Malzemeleri Projesi, II. Uluslararası BÖTE Sempozyumu 2008, Kuşadası, Türkiye, 16-18 Nisan 2008.

7. Akteke-Öztürk, B., Weber, G.-W., and Kropat, E., Continuous Optimization Approaches for Clustering via Minimum Sum of Squares, EURO Mini Conference, Neringa, Lithuania, May 20-23, 2008.

8. Akteke-Öztürk, B., Köksal, G., and Weber, G.-W., Çekicilik Fonksiyonları: Pürüzlü Optimizasyon ile Yeni Yaklaşımlar, Yöneylem Araştırması ve Endüstri Mühendisliği 28. Ulusal Kongresi (YA/EM 2008), İstanbul, Türkiye, Haziran 30-Temmuz 02, 2008.

9. Akteke-Öztürk, B., Weber, G.-W., and Köksal, G., Çekicilik Fonksiyonlarının Bileşke Fonksiyonları Olarak Çözümlenmesi, Yöneylem Araştırması ve Endüstri Mühendisliği 29. Ulusal Kongresi (YA/EM 2009), Ankara, Türkiye, Haziran 22-24, 2009.

10. Akteke-Öztürk, B., Köksal, G., and Weber, G.-W., Nonsmooth Optimization of Desirability Functions by MSG Algorithm, EURO XXIII- European Conference on Operational Research, Bonn, Germany, July 5-8, 2009.

11. Akteke-Öztürk, B., and Weber, G.-W., Modern Operational Research and Its Mathematical Methods, AACIMP 2009 - The Summer School, Achievements and Applications of Contemporary Informatics, Mathematics and Physics, Kiev Polytechnic Institute, Kiev, Ukraine, August 5-16, 2009 (Invited lecturer).

12. Akteke-Öztürk, B., Weber, G.-W., and Köksal, G., A Class of Piecewise-smooth Functions Motivated by Desirability Functions, 24th MEC-EurOPT 2010 - Continuous Optimization and Information-Based Technologies in the Financial Sector, Izmir, Turkey, June 23-26, 2010.

G. Talks

1. Akteke-Öztürk, B., Optimization of Stirrer Configurations by Numerical Simulation - Derivative Free Optimization, Students' Seminar, Institute of Applied Mathematics, Middle East Technical University, Ankara, Turkey, December 13, 2003.

2. Akteke-Öztürk, B., Semidefinite and Nonsmooth Optimization for Minimum Sum of Squared Distances Problem, Computational Biology and Medicine Group Seminars, Institute of Applied Mathematics, Middle East Technical University, Ankara, Turkey, December, 08, 2006.

3. Akteke-Öztürk, B., Taylan, P., and Özöğür, S., Tikhonov Regularization for Learning as an Inverse Problem, Computational Biology and Medicine Group Seminars, Institute of Applied Mathematics, Middle East Technical University, Ankara, Turkey, April, 27, 2007.