Ensuring an Efficient Turning Process by Means of Desirability Index Optimization for Correlated Quality Criteria

by

Kris Wonggasem

A dissertation submitted in partial fulfilment of the requirements

for the degree of Doctor rerum naturalium in Statistics

Faculty of *Statistics*

Technische Universität Dortmund

July 2012

Tag der mündlichen Prüfung: 30. August 2012

1. Vorsitzender:	Prof. Dr. Jörg Rahnenführer
2. Gutachter:	Prof. Dr. Claus Weihs
3. Gutachter:	Prof. Dr.-Ing. Dirk Biermann
4. Gutachter:	JProf. Dr. Uwe Ligges
5. Beisitzer:	Dr. Oliver Melsheimer

Abstract

The desirability index (DI) is a method for multi-criteria optimization accepted widely in industrial quality management. The DI integrates expert knowledge into the optimization process by setting up desirability functions (DFs) of the quality criteria regarding their objective regions and aggregating them into a single performance index. However, the independence assumption of DFs rarely holds true in real turning applications, and a number of studies have been conducted proving the existence of dependencies between tool wear, surface roughness, tool life and cutting forces. As a consequence, the optimal solution obtained might be biased towards the group of performance measures, which have a high level of association (positive correlations).

In this thesis, modifications of DI for handling correlated multi-criteria optimization are developed. By integrating principal component analysis (PCA) into the optimization procedure, the correlations of DFs can be eliminated, and the overall performance index, PCA-based DI, is formulated as a strictly monotonically increasing transformation of DFs; thus, the optimality of solutions can be guaranteed through the research of Legrand [26]. Apart from the PCA-based procedure, the weight-adjustment method provides an attractive alternative approach which is simpler and more flexible, by introducing the weight-adjustment coefficients into the original formulas of DIs.

The proposed procedures are demonstrated by means of case studies of a turning process optimization, and the optimization results are benchmarked with the traditional DIs. It has been shown in results that optimizations should be also subjected to the correlation information of performance measures. In addition, the procedure for determining correlation is found to be the second important key for a successful optimization.

Acknowledgements

I would like to express my utmost gratitude to the following persons for their support and cooperation. First of all, my gratitude goes to Prof. Dr. Claus Weihs and Prof. Dr.-Ing. Dirk Biermann, my Ph.D. thesis supervisors at the Technical University, Dortmund, for sparing their precious time and providing valuable comments on my research. Their guidance have been essential to the completion of this thesis. Secondly, I would like to express my appreciation to two of my supportive colleagues, Dr. Heike Trautmann and Dipl.-Inf. Tobias Wagner, whom I constantly cooperated with. Their suggestions were really important milestones for my thesis, without their supports, the completion of this research would not be possible. Thirdly, I would like to acknowledge all of members of the research group Computergestützte Statistik whom I interacted with and earned valuable knowledge and experience from. Last but not the least, my deep gratitude goes to my family members for their unconditional support throughout the years. My parents, Anont and Bunchua Wonggasem who have guided me through my education and have been always cheerful. My special thanks also go to my beloved wife, Sutthiruk Boonmaneewong, who always believed in me, encouraged me and has been always patient. My PhD Journey would not have been possible without their supports.

Wonggasem, Kris

Contents

List of Tables

List of Figures

Chapter 1

Introduction

1.1 Overview

The turning process, one of the most popular material removal processes in industry, has several performance measures, which are usually found to be correlated, such as tool wear, cutting force and surface finish. A number of studies have been conducted proving the effects of the cutting tool wear on surface roughness, tool life and cutting forces [5, 38, 55]. Optimization of turning usually deals with a multi-objective optimization problem (MOP) in which conflict between objectives is inevitable and necessitates the acceptance of the trade-off between objectives. The most practical approaches to solving MOP are either to convert all objectives into a single objective function, e.g., a cost function or to combine them into an overall performance index and thus in most cases, one particular trade-off solution is possible to be obtained.

The desirability index (DI) is a method for solving MOP introduced by Harrington [17] which transforms MOP into a single-objective optimization problem (SOP) and is applied frequently in industrial applications. The DI integrates expert knowledge into the optimization process by setting up desirability functions (DFs) of performance measures, which express experts' preferences regarding to the values of performance measures. However, in these investigations, DFs of performance measures are assumed to be independent, which will not hold true in practice, and the existence of correlation between of the performance measures may cause biased optimization results.

Though the DI is an optimization method which has been developed for a long time, the main contribution of the theoretical research was the derivation of the statistical distribution of DI for different kinds of DFs to allow DI to account for uncertainties in MOP. In contrast with other well-estabilished optimization methods such as Taguchi method, there have been only few researches concerned with the correlated performance and quality characteristics.

1.2 Objective and Outline

The primary objective of this research is to develop a multi-objective optimization method, using the concept of the desirability approach in which the correlations among the responses are accounted in the optimization. The aimed result is expected to obtain an alternative optimization procedure in which the assumption of independence of desirability functions can be eliminated; thus biased optimization results could be prevented. On the other hand, the expected drawbacks of the elimination of this assumption are that the optimization procedure may become even more complicated and less flexible.

Chapter 2 consists of state of the art and basic knowledge. In state of the art, the important literature and their results are summarized. Basic knowledge begins with the fundamental knowledge of the turning process, its important operating conditions and performance measures. Followed by the concept of the desirability approach which consists of desirability functions (DFs) and desirability indices (DIs). Then, a mathematical dimension reduction method, principal component analysis (PCA), and its applications in Taguchi method are described. At the end of the chapter, correlations are classified for the purpose of utilizing them in the correlated multi-objective optimization problems.

In chapter 3, the important properties of the different types of principal components (PCs) are investigated in order to explore the possibility of individual interpretation. Then the formulation of PCA-based DI is introduced and its properties such as monotonicity, upper bound and lower bound are derived and proven. At the end of the chapter, the procedure for applying the PCA in the desirability approach is explained step by step.

In chapter 4 an alternative methodology, the weight adjusted desirability approach, which is more simple and flexible than the method in chapter 3 is introduced. Then, some investigations follow according to the effects of available parameters on the results, and some disadvantages are described by mean of Venn diagrams at the end of the chapter.

Chapter 5 demonstrates an implementation of the PCA-based desirability approach for the optimization of cutting conditions in a turning process. With the initial cutting conditions of the experiment set, the global correlation between responses are firstly involved in the computation of the PCA-based DI. However, in the global correlation matrix plot, multiple correlation patterns can be found which might be caused by the change of cutting status due to the wide range variation in cutting conditions. Since the PCA-based approach is influenced by the correlation information given, errors in the estimation of correlations could lead to unintended results. Then, the optimal results which are obtained from different correlations are compared, and the optimal results obtained from the traditional desirability approach are generally different from the proposed methods due to the effect of correlations.

In the last chapter of this thesis, summary and conclusion of this research can be found and some open issues in the development of desirability approach which would extend the outcome of the research are mentioned.

Chapter 2

State of the Art and Basic Knowledge

The aim of this chapter is to present theories related to this research and the available basic knowledge. In the first section, the relevant literature which are the important pathways to the essential developments in this research are summarized. Basic knowledge begins with the fundamentals of the turning process of which important aspects such as common controllable parameters and performance characteristics are described. This is followed by the desirability approach which is an optimization method widely applied in optimization applications. After that the principal component analysis (PCA) which is a conventional method used to handle correlated data and its applications in Taguchi's method are introduced. At the end of this chapter, correlations are classified according to their applications in correlated multi-objective optimization problems.

2.1 State of the Art

Chou and Evans (1997) [5] investigated tool wear in finish hard turning. There were 3 different Cubic boron nitride (CBN) tools used in their investigation. Their results demonstrated that both of tool wears and surface roughness tend to increase as cutting distance becomes longer.

Scheffer (1999) [38] inspected the feasibility of identifying tool wear through vibration monitoring. As an outcome of the research, a robust tool wear monitoring system was invented and a wide range of usage is guaranteed and it was found that force signal is even more sensitive to tool wear than vibration signal.

A method for solving multi-objective optimization problems (MOPs), the desirability approach, was proposed by Harrington [17] in 1965. Harrington uses desirability functions (DFs) to transform performance and quality characteristics in the different scales into the dimensionless desirability scores which have a range between zero and one. The overall desirability is used to indicate the performance of the operation and is calculated by the geometric mean of DFs.

Subsequently, in 1980, Derringer and Suich [11] proposed a new class of DFs which is simpler, offer more flexibility and becomes more popular in desirability approach than Harrington's DFs. Derringer [10] also suggested the use of the weighted geometric mean of DFs as the overall desirability which is referred desirability index (DI), since each performance characteristic may has a different degree of importance.

In the next era, contributions of researches had been made on investigating the distribution of DFs and DI, in order to derive an analytical solution for robust optimizations. The attempt to investigate the distribution of DI has been made by Steuer [43] in 2005, however there was still no analytical expression available at that moment. In 2006, Trautmann and Weihs [54] succeed to derive the distribution of DFs for different types of Harrington's DFs, whereas the distribution of Derringer's DFs can be found in the study of Henkenjohann [18].

In 2004, Wu [60] introduced a desirability approach which allows variations and correlations of quality characteristics to be integrated into the optimization process. The idea was based on loss functions, and the modified double exponential DFs which were invented by Wu and Hamada [59]. Even though the effectiveness of the

Wu's method has been demonstrated in his work, there is no guideline available for the assignment of the loss coefficients and the correlated loss coefficients which are subjective.

There is a common technique, Principal component analysis (PCA), which is used to handle correlated high-dimensional data. The fundamental concept of PCA was invented in 1901 by Pearson [34] with the target to represent a system of points in three or higher dimension by the best-fitting straight line or plane. In 1933, Hotelling [19] introduced PCA with the aim to find a smaller set of variables for representing the high-dimensional variables. The smaller set of variables had been called "factors" in the psychological literature and in order to avoid confusion with other uses of the word "factor" in mathematics, the alternative term "components" was used instead. Hotelling's "components" are chosen to maximize their contributions to the total of the variances of the original variables, and they are generally referred as "principal components" (PCs). The concept of PCA has been applied in various fields, including data mining, pattern recognition and optimization.

In 1997, Su et al. [44] applied PCA to the Taguchi method, in order to solve correlated MOP. It has been demonstrated by Su et al. that PCA not only reduce the number of dimensions but also decrease the complexity of MOP. However, there are two shortcomings of Su's method which were stated by Liao [27]; First, if more than one PC is selected, the required trade-off for a feasible solution is unknown. Second, when the original variables can only be explained by total variances, i.e., by using all PCs, they cannot be replaced by a single PC. To overcome these shortcomings, Liao (2005) introduced the weighted-PCA in the Taguchi method, and eigenvalues are used as the weight for each PC, since eigenvalues can be used to describe the proportion of variances explained by each PC. The most important improvement of Liao's method is that all PCs can be integrated into the multi-response performance index (MPI) which represents the overall performance. In 2010, Datta et al. [6, 36] introduced an alternative for MPI, the combined quality loss (CQL) which is defined as the absolute deviation of MPI from the ideal situation. The concept of CQL overcomes the problem arising on computation of S/N ratio in Taguchi's method when MPI becomes negative. It has been noted by the authors that the main disadvantage of CQL is the lack of physical interpretation of individual PCs.

Parallel to the development of weighted-PCA in Taguchi method, Tong and Wang (2002) [52] proposed an alternative for MPI by applying grey relational analysis (GRA) in Taguchi method, and later in 2004, Tong et al. [53] introduced an another alternative method the technique for order preference by similarity to ideal solution (TOPSIS) based Taguchi method. The advantage of using GRA or TOPSIS over CQL is that not only the distance from the ideal solution but also the distance from the negative ideal solution are considered by the overall performance index. Both of GRA-based and TOPSIS-based Taguchi method are applied popularly in many researches. In 2009, Bashiri and Salmasnia [3] proposed a method which combines PCA transformation, DFs and TOPSIS. The main disadvantage of their method is obviously that there are so many transformations and variables involved in optimization.

An important research regarding to index optimization has been introduced by Legrand and Touati (2007) [26]. The relation between optimality of results and monotonicity of the index optimization has been proven in their research. As the outcome of their research, they recommended that the index optimization should be strict monotone to guarantee the optimality of optimization results.

2.2 Turning Process

Turning is a metal cutting process in which a single-point tool removes material from the surface of a rotating cylindrical workpiece. It is traditionally operated on a machine tool called a lathe where the tool is fed linearly in a direction parallel to the axis of rotation. Many contributions were made to the study of the effects of cutting conditions on the process and in optimization of cutting parameters.

2.2.1 Cutting Conditions

Cutting conditions in turning process consist of process parameters such as cutting speed, feed, and depth of cut and also other influence factors such as the cutting fluid which are controllable. The selection of these conditions depends on many factors and is very influential on determining the success of turning operation.

2.2.1.1 Cutting Speed

Cutting speed v_c is the primary cutting motion, which denotes the velocity of the cutting tool relative to the workpiece in m/min. Higher v_c results in a higher material removal rate and better surface quality but it produces higher cutting temperatures which reduces the hardness of tool and results in more tool wear. For example, Adesta et. al. [1], Kilickap et. al. [23], and Thamizhmanii [48] found in their studies that tool wear increased with increasing v_c whereas surface roughness decreased. Selection of v_c is based on making the best use of the particular cutting tool, which means choosing a speed that provides a good surface finishing, a high material removal rate and suitably long tool life [15].

2.2.1.2 Feed

Feed f is the amount of material removed per revolution or per pass of the tool over the workpiece in mm. In order to maximize material removal rate, f should be set as high as possible where upper limits on f are imposed by cutting forces, setup rigidity and the machine power. However, the larger f the separation between feed marks increases, leading to an increase in the value of surface roughness [15]. Increasing f increases also cutting temperature and flank wear, but effects on the tool life is known to be small when compared to effects from v_c. The typical setting for f as stated in [15] is 0.5 - 1.25 mm for roughing operations and 0.125 - 0.4 mm for finishing operations.

2.2.1.3 Depth of Cut

Depth of cut a_{p} is the penetration of the cutting tool below the original work surface in mm. It is known as the primary cause and control of chatter and usually predetermined by workpiece geometry and operation sequence. There are some studies in which a_{p} is found to have influence on the surface roughness, e.g., Ting [51] found a_{p} as a significant parameter influencing the surface roughness, and Kandananond [22] minimized surface roughness by setting the depth of cut to the lowest level. There are some studies in which a_{p} is found not to have a significant impact on the surface roughness, Feng [13] and Thomas et al. [49]. In roughing operations, a_{p} is usually set as large as possible within the limitations of machine power, machine tool and setup rigidity, and strength of the cutting tool. In finishing operations, a_{p} is set to achieve the final dimension for the part. However, it is also known that small a_{p} results in friction; thus, tool life will be shortened. The typical setting for a_{p} are 2.5 - 20 mm and 0.75 - 2.0 mm for roughing and finishing operations respectively [15].

2.2.1.4 Cutting Fluid

Cutting fluid acts primarily as a coolant and secondly as a lubricant, reducing the friction effects at the tool-chip interface and the flank. It also carries away the chips and provides friction and force reductions on the contact surfaces between tool and workpiece. The reduction in temperature assists in retaining the hardness of the tool, thereby extending the tool life or permitting increased cutting speed with equal tool life. In addition, the removal of heat from the cutting zone reduces thermal distortion of the work and permits better dimensional control. The efficiency of coolant depends mainly on its thermal capacity and conductivity. In practice, it has to be decided whether a cutting fluid is to be used and, if so, the type of cutting fluid.

2.2.2 Performance and Quality Characteristics

In turning processes there are several performance and quality characteristics which determine the successfulness of the operation. The most often considered performance characteristics are surface finish, tool wear or tool life, and material removal rate. Such characteristics are generally fit into the broader areas of product quality, process productivity, and operating costs. In a robust engineering process, a balance among these characteristics should be considered while the requirements must be met for all critical aspects.

2.2.2.1 Surface Roughness

Surface roughness is the major indication of the surface quality of a turning process which has been considered as an objective in many researches [1, 13, 22, 25, 29, 37, 42, 45, 49, 51, 56]. The typical roughness parameters are the arithmetical mean roughness Ra, the average depth of roughness Rz and the maximum height $Rmax$.

As illustrated in figure 2.1, Ra can be determined by dividing the sum of filled areas that are enclosed by the surface profile $y(x)$ and the center line by the evaluation length L. The value of Ra corresponds to the arithmetic mean deviation from the center line, since the center line is constructed from the average surface profile. For this reason, Ra is also referred as center line average (CLA) or arithmetic average (AA). The computational formula for Ra can be written as the equation 2.1.

$$Ra = \frac{1}{L} \int_0^L |y(x)| \, dx \tag{2.1}$$

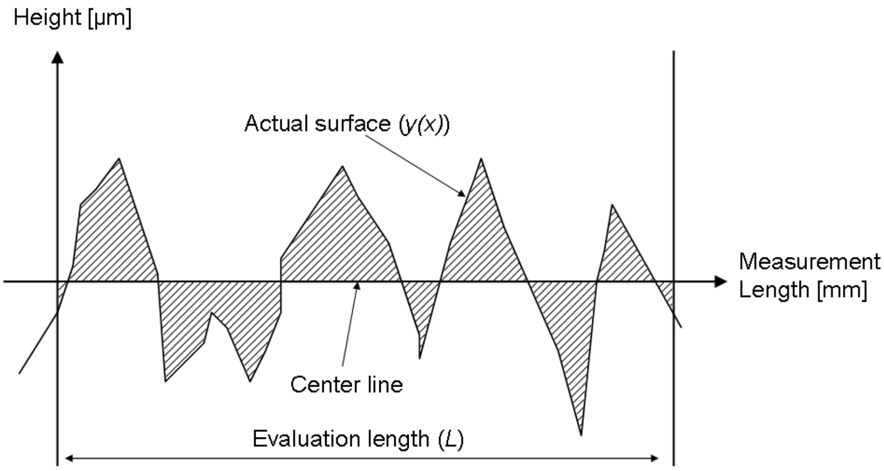


Figure 2.1: The arithmetical mean roughness Ra

According to DIN standard [12], Rz is defined as the arithmetic mean of the distance Z_i between global maximum and minimum in five successive single measuring sections of the total evaluation length, as shown in figure 2.2. Rz can be calculated from equation 2.2.

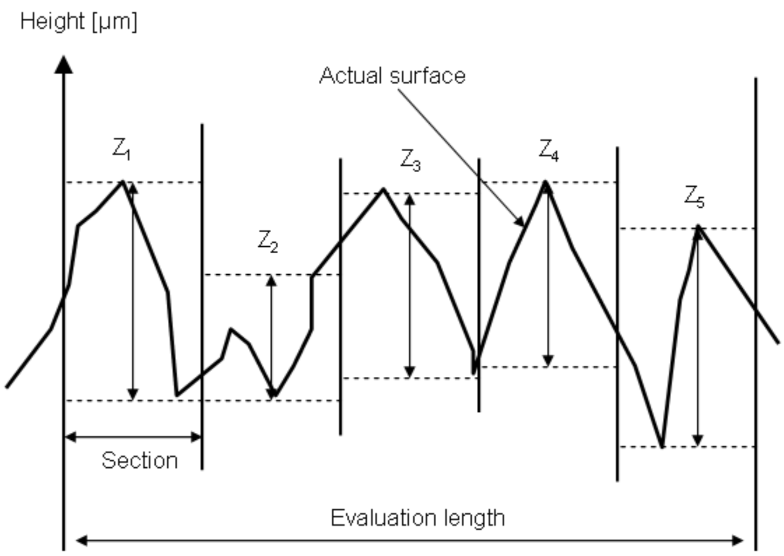


Figure 2.2: The average depth of roughness Rz

$$Rz = \frac{1}{5} \cdot \left(\sum_{i=1}^{5} Z_i \right) \tag{2.2}$$

Rmax is the highest vertical distance between two lines parallel to the center line indicating the highest peak to the lowest valley distance within the evaluation length. One advantage of *Rmax* is the possibility to measure without determining the center line.

2.2.2.2 Tool Wear and Tool Life

Tool wear in machining is defined as the amount of volume loss of the tool material. It occurs principally at two locations on a cutting tool: the top rake face and the flank. Crater wear is tool wear which occurs on the rake face of the tool. It is formed by the action of the chip sliding against the surface and can be measured either by its depth or its area. Flank wear occurs on the flank or relief face of the tool and is measured by the width of the wear band which is sometimes called the flank wear band. Crater wear and flank wear are illustrated in figure 2.3.

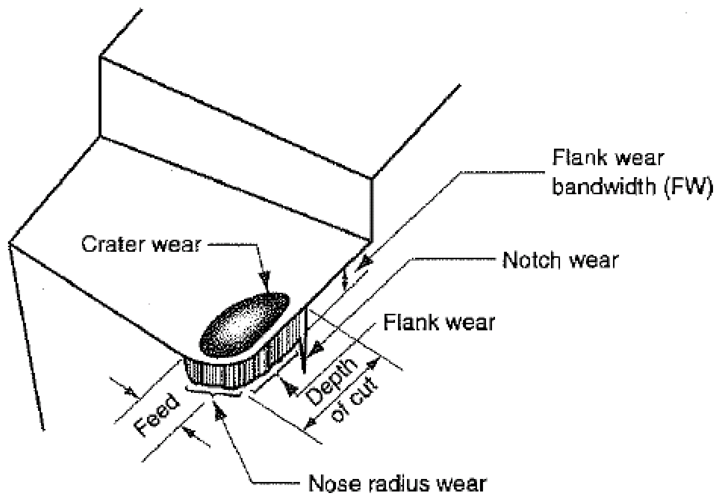


Figure 2.3: Worn of cutting tool and types of wear that occur [15]

These tool wear modes are generated from rubbing between the newly generated work surface and the flank face adjacent to the cutting edge. As the tool wears, its geometry changes and this change will influence the cutting force, the power being consumed, the surface finish obtained, the dimensional accuracy, and even the dynamic stability of the process [8].

Tool life is defined as the length of cutting time that the tool can be used. One way of defining tool life is to operate the tool until the final catastrophic failure occurs. However, in production, it is often a disadvantage to use the tool until this failure occurs because of difficulties in resharpening the tool and problems with surface quality. As an alternative, a level of tool wear is selected as a criterion of tool life and the tool is replaced when wear reaches that level. A convenient tool life criterion is a certain flank wear value, such as 0.5 mm [15]. Taylor's tool life equation is commonly referred as the mathematical model for tool wear [35].

$$v_c T^n = C \tag{2.3}$$

The equation 2.3 provides relationship between v_c, tool life T, and two constants n and C, depending on tool and workpiece material. It was found from experiments that a Taylor equation could yield estimates within ±35 percent of the actual tool life [38]. An expanded version of equation 2.3 can be formulated to include the effects of f, a_p, and even work material hardness. [15]:

$$v_c T^n f^m a_p^p H^q = K T_{ref}^n f_{ref}^m a_{p,ref}^p H_{ref}^q \tag{2.4}$$

where H denotes the hardness, expressed in an appropriate hardness scale; m, p, and q are exponents whose values are experimentally determined for the conditions of the operation; K is a constant analogous to C in equation 2.3; and T_{ref}, f_{ref}, $a_{p,ref}$, and H_{ref} are reference values for T, f, a_p, and H. In addition, the value of m, p and q in equation 2.4 are less than 1.0. Since the exponent of v_c is equal to 1.0, it indicates that v_c has the greater effect on T than a_p.

2.2.2.3 Material Removal Rate

The material removal rate (MRR) is the volume of the workpiece material that is removed per time unit in $\mathrm{mm}^3/\mathrm{min}$. It can be conveniently determined from cutting conditions using equation 2.5. In a turning process, a higher removal rate means shorter machining time and therefore, the higher productivity.

$$\mathrm{MRR} = 1000 \cdot v_\mathrm{c} f a_\mathrm{p} \tag{2.5}$$

2.3 Multi-Objective Optimization Problem

A multi-objection optimization problem (MOP) is a process of optimizing two or more objectives, subjecting to a set of constraints. A common MOP can be written as follows:

$$\min_{\vec{x}} \vec{F}(\vec{x}) = [F_1(\vec{x}), \ldots, F_m(\vec{x})]^\mathrm{T} \tag{2.6}$$

$$\begin{aligned} &\text{subject to} \quad \forall h \in I_1 : g_h(\vec{x}) \leq 0 \\ &\qquad\qquad\quad\ \forall h \in I_2 : g_h(\vec{x}) = 0 \\ &\text{with } I_1, I_2 \subset \mathbb{N}, I_1 \cap I_2 = \emptyset \end{aligned}$$

where m is the number of objectives, I_1 is the set of indices h so that $g_h(\vec{x})$ represents inequality constraints, I_2 is the set of indices h so that $g_h(\vec{x})$ represents equality constraints, $\vec{x} \in \mathbb{R}^q$ is the vector of decision variables, q is the number of decision variables, and $\vec{F}(\vec{x}) \in \mathbb{R}^m$ is the vector of objective functions $F_j(\vec{x}) : \mathbb{R}^q \to \mathbb{R}$.

The goal of MOPs is to find the $\vec{x}$ which satisfies $g_h(\vec{x}) : \forall h$ and best incorporates the decision maker's preferences. It is recommended by Steuer [43] that the decision space for the final solution should be restricted to the set of non-dominated or Pareto-optimal solutions. The non-dominated and Pareto-optimal solutions can be defined as:

Definition 2.3.1. *A vector* $\vec{x}^* \in \mathbb{F}$ *dominates* $\vec{x}$ *if and only if* $F_j(\vec{x}^*) \leq F_j(\vec{x})$ *for all* $j = 1, \ldots, m$ *and* $F_j(\vec{x}^*) < F_j(\vec{x})$ *for at least one* j*, where* $\mathbb{F} \subseteq \mathbb{R}^q$ *denotes the set of all feasible* $\vec{x}$ *that satisfy all constraints of the problem.*

Definition 2.3.2. *A vector* $\vec{x}^* \in \mathbb{F}$ *is non-dominated if and only if there does not exist any vector in* $\mathbb{F}$ *that dominates* $\vec{x}^*$*.*

Definition 2.3.3. *A vector* $\vec{x}^* \in \mathbb{F}$ *is Pareto-optimal if there does not exist* $\vec{x} \in \mathbb{F}$ *such that* $\forall j : F_j(\vec{x}) \leq F_j(\vec{x}^*)$ *and* $F_j(\vec{x}) < F_j(\vec{x}^*)$ *for at least one* j*.*

Furthermore, the relation of the strict monotonicity of index optimization and the pareto-optimality of the obtained solutions has been proven in [26].

2.4 The Desirability Approach

One of the most popular approaches to multi-criteria decision making problems is to aggregate the multiple performance characteristics into a single performance index. The desirability approach is one of those approaches that is widely used in industry for the optimization of multi-response processes. It consists of two transformations, desirability functions (DFs) and desirability index (DI).

2.4.1 Desirability Function

Desirability functions (DFs) are functions that transform each the m response variables $Y_j,\ j = 1, \ldots, m$ into a dimensionless desirability value $d_j(Y_j)$ which is also denoted as d_j. The possible range of values for $d_j(Y_j)$ is between 0 and 1. The value $d_j(Y_j) = 0$ corresponds to a completely undesirable, $d_j(Y_j) = 1$ corresponds to a completely acceptable level of quality, and the value of the DF increases as the desirability of the corresponding response increases. The choice of DFs is subjective and depends on the decision maker (DM) or engineer's judgment. The most widely known DFs used in optimization problems are Harrington's DFs and Derringer's DFs.

2.4.1.1 Harrington's Desirability Functions

Harrington's two-sided DF is defined as

$$d_j(Y_j') = \mathrm{e}^{-\left|Y_j'\right|^{r_j}}, \qquad j = 1, \ldots, m;\ 0 < r_j < \infty. \quad (2.7)$$

where the parameter r_j is to be chosen so that the resulting kurtosis of the function adequately meets the expert's preferences and Y_j' is an appropriate transformation of Y_j. An upper (USL_j) and a lower specification limit (LSL_j) of Y_j are required for the Y_j' transformation in equation 2.8.

$$Y_j' = \frac{2Y_j - (\mathrm{USL}_j + \mathrm{LSL}_j)}{\mathrm{USL}_j - \mathrm{LSL}_j}. \quad (2.8)$$

In case of a one-sided specification, a special form of the Gompertz-Curve shown in equation 2.9 and 2.10 is used.

$$d_j(Y_j') = \mathrm{e}^{-(\mathrm{e}^{-Y_j'})} \quad (2.9)$$

$$Y_j' = -\left[\ln(-\ln(d_j(Y_j')))\right] = b_{0j} + b_{1j}Y_j. \quad (2.10)$$

The constants b_{0j} and b_{1j} in equation 2.10 can be determined by the solution of a system of two linear equations with two values of Y_j and their corresponging values of $d_j(Y_j')$.

2.4.1.2 Derringer's Desirability Functions

Derringer's DF for a two-sided transformation is defined as

$$d_j(Y_j) = \begin{cases} \left[\frac{Y_j - \mathrm{LSL}_j}{T_j - \mathrm{LSL}_j}\right]^{s_j} & \text{for } \mathrm{LSL}_j \leq Y_j \leq T_j \\ \left[\frac{Y_j - \mathrm{USL}_j}{T_j - \mathrm{USL}_j}\right]^{t_j} & \text{for } T_j < Y_j \leq \mathrm{USL}_j \\ 0 & \text{for } Y_j < \mathrm{LSL}_j \text{ or } Y_j > \mathrm{USL}_j \end{cases} \quad (2.11)$$

where T_j is the target value of the jth response, and the exponent parameters $s_j > 0$ and $t_j > 0$ are to be specified by DM, depending on the contribution or importance of the response towards the improvement of the overall desirability of the process and the product.

For the one-sided transformation, the appropriate DF must be selected corresponding to the type quality characteristic. Quality characteristics can be divided in two types, smaller-the-better (STB) and larger-the-better (LTB).

The one-sided transformation for LTB response can be defined as

$$d_j(Y_j) = \begin{cases} 0 & \text{for} \quad Y_j \leq \text{LSL}_j \\ \left[\frac{Y_j - \text{LSL}_j}{Y_{\text{U}j} - \text{LSL}_j}\right]^{r_j} & \text{for} \quad \text{LSL}_j < Y_j < Y_{\text{U}j} \\ 1 & \text{for} \quad Y_j \geq Y_{\text{U}j} \end{cases} \tag{2.12}$$

where $Y_{\text{U}j}$ is the maximum value of the LTB response above which there is no further performance improvement.

The one-sided transformation for STB response can be defined as

$$d_j(Y_j) = \begin{cases} 0 & \text{for} \quad Y_j \geq \text{USL}_j \\ \left[\frac{\text{USL}_j - Y_j}{\text{USL}_j - Y_{\text{L}j}}\right]^{r_j} & \text{for} \quad Y_{\text{L}j} < Y_j < \text{USL}_j \\ 1 & \text{for} \quad Y_j \leq Y_{\text{L}j} \end{cases} \tag{2.13}$$

where $Y_{\text{L}j}$ is the minimum value of the STB-type response below which there is no further performance improvement.

2.4.2 Desirability Index

The desirability index (DI) combines m individual d_j into one overall quality value by either the arithmetic mean or the geometric mean of d_j. The geometric mean of DFs where all d_j contribute equal weight to the objective is given as

$$D_{\text{g}} = \left[\prod_{j=1}^{m} d_j\right]^{\frac{1}{m}} \tag{2.14}$$

where $D_{\text{g}} \in [0, 1]$ is the geometric mean of DFs which is referred as DI. Since the importance of some products' characteristics or responses can be especially higher than others, it makes sense to weight each d_j according to its importance to the intended application. The formulation of the overall desirability which using the weighted geometric mean is given as

$$D_{\mathrm{g}} = \left[\prod_{j=1}^{m} d_j^{w_j}\right]^{\frac{1}{\sum_{j=1}^{m} w_j}} \qquad \text{with} \quad w_j > 0 : \forall j \in \{1, \ldots, m\} \quad (2.15)$$

where w_j, the exponent of each individual d_j, is the weight of the jth response assigned corresponding to the importance of d_j. The geometric mean of DFs given in equation 2.14 is a special case of the weighted geometric mean in which all w_j are equal to one. Let W_j be the normalized weight of d_j with $\sum_{j=1}^{m} W_j = 1$, then equation 2.15 can be simplified as

$$D_{\mathrm{g}} = \prod_{j=1}^{m} d_j^{W_j} \qquad \text{with} \quad W_j > 0 : \forall j \in \{1, \ldots, m\}\,. \quad (2.16)$$

The advantage of using the geometric mean over arithmetic mean in the formulation of DI is obvious. Whenever any Y_j fails to meet the characteristic requirements and the value of $d_j(Y_j)$ is zero, the value of D_{g} becomes zero as well. Additionally, D_{g} is strongly weighted by the small $d_j(Y_j)$ [17], and therefore D_{g} increases as the balance of the $d_j(Y_j)$ is more favorable. For these reasons, the geometric mean is preferred over the arithmetic mean in the formulation of DI.

As an alternative for DI, the arithmetic mean of DFs was used in Fuller's study [14] as an evaluation function. The weighted arithmetic mean of DFs is defined as

$$D_{\mathrm{a}} = \frac{\sum_{j=1}^{m} w_j d_j}{\sum_{j=1}^{m} w_j} \qquad \text{with} \quad w_j > 0 : \forall j \in \{1, \ldots, m\}\,. \quad (2.17)$$

With W_j, it can be defined as

$$D_{\mathrm{a}} = \sum_{j=1}^{m} W_j d_j \qquad \text{with} \quad W_j > 0 : \forall j \in \{1, \ldots, m\}\,. \quad (2.18)$$

The value of DIs, as noted by Kim [24], does not allow a clear physical interpretation, except for the principle that the higher value is preferred. The reason is obvious, since DIs are composed of multiple variables and expert's preferences and information losses generally come together with dimension reduction, the information that can be obtained from DIs can be very low-detailed.

2.4.3 Wu's Desirability Approach for Correlated Performance Characteristics

Wu's desirability approach for correlated performance characteristics has been proposed by Wu (2004) [60]. It has been developed based on the double exponential desirability function of Wu and Hamada [59] and quadratic quality losses. Wu's desirability approach can be described as:

Suppose that in total there are m performance measures $\vec{Y} = [Y_1, Y_2, \ldots, Y_m]^{\mathrm{T}}$ with the target vector $\vec{t} = [t_1, t_2, \ldots, t_m]^{\mathrm{T}}$. The asymmetric quality loss function which is expressed as:

$$L(Y_j) = \begin{cases} c_{j(1)}(Y_j - t_j)^2 & \text{for} \quad Y_j \leq t_j \\ c_{j(2)}(Y_j - t_j)^2 & \text{for} \quad Y_j > t_j \end{cases} \tag{2.19}$$

where $L(Y_j)$ is the loss function for Y_j, $c_{j(1)}$ is the loss coefficient for Y_j smaller than t_j, and $c_{j(2)}$ for Y_j larger than t_j. The reason behind using $c_{j(1)}$, $c_{j(2)}$ and the asymmetric quality loss function is that a deviation of Y_j in one direction can be more harmful than in the other direction. Further, suppose that in total there are n observations for Y_j. The expected quality loss can be defined as:

$$\mathrm{E}(L_j) = \frac{1}{n}\left(c_1 \sum_{k:Y_{kj} \leq t_j}^{n} (Y_j - t_j)^2 + c_2 \sum_{k:Y_{kj} > t_j}^{n} (Y_j - t_j)^2 \right) \tag{2.20}$$

An approximate form of equation 2.20 is given as:

$$\mathrm{E}(L_j) \approx \tilde{c_j} \left((\bar{Y_j} - t_j) + \sigma_j^2 \right) \tag{2.21}$$

with

$$\tilde{c_j} = \begin{cases} c_{j(1)} & \text{if} \;\; \bar{Y_j} < t_j - \sigma_j \\ c_{j(2)} & \text{if} \;\; \bar{Y_j} > t_j + \sigma_j \\ \frac{c_{j(1)}+c_{j(2)}}{2} & \text{if} \;\; t_j - \sigma_j \leq \bar{Y_j} \leq t_j + \sigma_j \end{cases} \tag{2.22}$$

$$\bar{Y_j} = \sum_{k=1}^{n} \frac{Y_{kj}}{n} \tag{2.23}$$

$$\sigma_j^2 = \sum_{k=1}^{n} \frac{(Y_{kj} - \bar{Y_j})^2}{n} \tag{2.24}$$

where $\tilde{c_j}$ is a function of loss coefficients, $c_{j(1)}$ and $c_{j(2)}$ are loss coefficients, and Y_{kj} is the value of Y_j at the kth observation. The quality losses can be expanded in a multivariate Taylor series as:

$$\Lambda = \sum_{j=1}^{m} c_j (Y_j - t_j)^2 + \sum_{i=1}^{m} \sum_{i<j}^{m} c_{ij} (Y_i - t_i)(Y_j - t_j) \tag{2.25}$$

where Λ denotes the quality losses, c_j denotes the loss coefficients of Y_j, r_{ij} denotes the correlation coefficient of performance measures Y_i and Y_j. The expected value of Λ can be approximated from the following formula:

$$\begin{aligned} \mathrm{E}(\Lambda) &\approx \sum_{j=1}^{m} \left[\tilde{c}_j (\bar{Y_j} - t_j)^2 + \sigma_j^2 \right] + \sum_{i=1}^{m} \sum_{i<j}^{m} \tilde{c}_{ij} \left[r_{ij} \sigma_i \sigma_j + (\bar{Y_i} - t_i)(\bar{Y_j} - t_j) \right] \\ &= \sum_{j=1}^{m} \hat{\mathrm{E}}(L_i) + \sum_{i=1}^{m} \sum_{i<j}^{m} \hat{\mathrm{E}}(L_{ij}) \end{aligned} \tag{2.26}$$

with $\tilde{c}_j$ and $\tilde{c}_{ij}$ as defined in equation 2.22, and $\hat{\mathrm{E}}(L_i)$ and $\hat{\mathrm{E}}(L_{ij})$ are the estimators for $\mathrm{E}(L_i)$ and $\mathrm{E}(L_{ij})$ correspondingly.

The desirability functions proposed by Wu can be written as:

$$d_{ii} = \mathrm{e}^{-\hat{\mathrm{E}}(L_i)} \tag{2.27}$$

$$d_{ij} = \begin{cases} 1 & \text{for} \;\; \hat{\mathrm{E}}(L_{ij}) < 0 \\ \mathrm{e}^{-\hat{\mathrm{E}}(L_{ij})} & \text{for} \;\; \hat{\mathrm{E}}(L_{ij}) \geq 0 \end{cases} \tag{2.28}$$

The value of Wu's DF becomes 1 when $\mathrm{E}(L_{ij})$ equals zero (no loss) or $\mathrm{E}(L_{ij})$ is negative (profit). The total desirability D_{wu} is defined as:

$$D_{\mathrm{wu}} = \left[\prod_{i=1}^{m} \prod_{i<j}^{m} d_{ii} \cdot d_{ij} \right]^{\frac{1}{m}} \tag{2.29}$$

It can be seen from equations 2.26, 2.28 and 2.29 that Wu's desirability index does not only integrate the correlation information of performance measures into the overall performance index but also the deviations of performance measures. However, Wu's desirability approach has some drawbacks which are the difficulties of selecting loss coefficients $c_{j(1)}$, $c_{j(2)}$, $c_{ij(1)}$ and $c_{ij(2)}$ as well as the weight factors for each d_{ij}, e.g. in case that the importance of d_i and d_j is not equal.

2.5 Principal Component Analysis

Principal component analysis (PCA) is a common approach used to handle correlated data. The main idea of PCA is to reduce the dimensionality of a data set consisting of a large number of interrelated variables, while retaining as much as possible of the variation present in the data set. This reduction is achieved by transforming those interrelated variables into a new set of variables, the principal components (PCs), which are uncorrelated and are ordered in a way that the first few PCs retain most of the variation present in all of the original variables. PCA has been applied to the Taguchi method in MOPs [7, 31, 44].

2.5.1 The Principal Components

Principal components (PCs) are algebraically particular linear combinations of m random variables $Y_1, Y_2, \ldots, Y_m$. These linear combinations represent geometrically the selection of a new coordinate system obtained by rotating the original axes. The new axes represent the directions with maximum variability and provide a simpler description of the covariance structure. In addition, their development does not require a multivariate normality assumption [16].

Let $\vec{Y} = [Y_1, Y_2, \dots, Y_m]^{\mathrm{T}}$ be the random vector of outputs or performance characteristics which have the covariance matrix $\sum$ with eigenvectors $\vec{a_1}, \vec{a_2}, \dots, \vec{a_m}$ and their corresponding eigenvalues $\lambda_1 \geqq \lambda_2 \geqq \dots \geqq \lambda_m \geqq 0$. Additionally, each Y_i should be standardized or normalized if they are measured on scales with widely differing ranges or if the units of measurement are not commensurate [16, 20]. Then the linear combinations could be written in the following form:

$$\begin{aligned} Z_1 = &\quad \vec{a_1}^{\mathrm{T}}\vec{Y} &= a_{11}Y_1 + a_{12}Y_2 + \cdots + a_{1m}Y_m \\ Z_2 = &\quad \vec{a_2}^{\mathrm{T}}\vec{Y} &= a_{21}Y_1 + a_{22}Y_2 + \cdots + a_{2m}Y_m \\ \vdots &\quad \vdots & \vdots \\ Z_m = &\quad \vec{a_m}^{\mathrm{T}}\vec{Y} &= a_{m1}Y_1 + a_{m2}Y_2 + \cdots + a_{mm}Y_m \end{aligned} \tag{2.30}$$

where Z_i denotes the ith PC, and a_{ij} denotes the jth component of ith eigenvector. Equation 2.30 can be expressed in short form as

$$Z_i = \vec{a_i}^{\mathrm{T}}\vec{Y}. \tag{2.31}$$

In Kaiser's [21] and Antony's [2] studies, PCs with eigenvalue greater than 1 are chosen to replace the original responses.

2.5.2 Weighted Principal Component Analysis

Weighted principal component analysis (WPCA) is a recently proposed generalization of PCA by assigning different weights to data objects based on their estimated importance. The reduction of variables can be achieved by converting PCs into a single response called multi-response performance index (MPI). The formula for computing MPI is given as equation 2.32.

$$\mathrm{MPI} = \sum_{i=1}^{m} W_i Z_i \tag{2.32}$$

$$W_i = \frac{\lambda_i}{\sum_{i=1}^{m} \lambda_i} \tag{2.33}$$

with Z_i as defined in equation 2.30 and W_i is the weight of ith PC which can be estimated using formula 2.33. Since the value of λ_i is determined proportionally to the portion of the variance, the value of W_i is depending on the amount of variance explained by Z_i. It has been proven by Liao [27] that the WPCA method offers significant improvements in quality, since all PCs are involved in the interpretation.

2.5.3 Principal Component Analysis based Taguchi Method

The procedure of the PCA-based Taguchi method proposed by Su [44] is illustrated as a flowchart in figure 2.4. Firstly, the quality loss for each response is computed on the basis of Taguchi's loss function. Secondly, to reduce variability and bias due to different scales, the scale of the quality loss for each response is to be normalized. This is followed by the PCA transformation in which normalized quality losses are transformed into uncorrelated PCs. Finally, PCs with eigenvalue greater than 1 are chosen to replace the original responses.

The flowchart of the method proposed by Liao [27] is illustrated in figure 2.5. As it is mentioned in section 2.5.2, instead of replacing the original responses by PCs, MPI calculated by using equation 2.32 is used to represent the set of original responses

The combined quality loss (CQL) which was proposed by Datta et al. [6, 36] is defined as the absolute deviation of MPI from the ideal situation. It can be expressed as in equation 2.34.

$$\mathrm{CQL} = |\mathrm{MPI} - \mathrm{MPI}_{\mathrm{ideal}}| \tag{2.34}$$

The positive value of CQL overcomes the problem arising in the computation of S/N ratio in Taguchi method when MPI becomes negative.

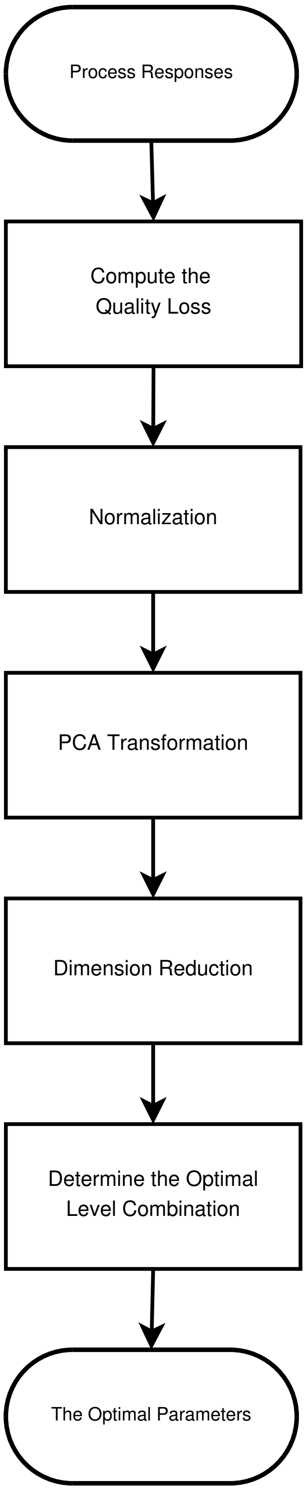


Figure 2.4: Implementation of PCA in Taguchi method

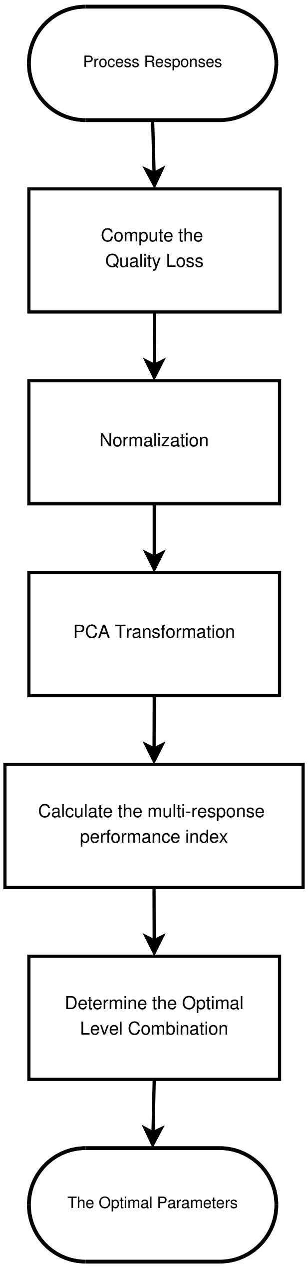


Figure 2.5: Implementation of WPCA in Taguchi method

2.6 Types of Correlation

In common statistical literature, correlations are usually classified either according to their values, i.e., positive, negative and zero, or according to the mathematical formula, i.e., Pearson, Spearman, and Kendall's correlations. In this research, only Pearson's correlation coefficient which is the most common measure for correlation, will be used. In optimizations with correlated performance measures, the importance of understanding the purpose of correlations determined from different experiments would be raised and there is a necessity to reclassify and consider correlations according to their applications and meanings. The usable correlations are classified into two groups according to their methods of determination and applications, namely correlations in the parameter space and conditional correlations.

2.6.1 Correlations in the Parameter Space

Correlations in the parameter space are correlations which are determined with changes in operating parameters, i.e., correlations of performance measures which resulted from the experimental plan. This type of correlation is popularly used in optimizations using PCA-based Taguchi methods in which operating parameters are varied according to Taguchi's orthogonal arrays. Correlations in the parameter space explain how the associations between the performance measure A and the performance measure B are when operating parameters are changed. In general, correlations in the parameter space are the only correlations which can be found in optimization studies.

2.6.2 Conditional Correlation

Conditional correlations are correlation coefficients which are determined with a specific condition, e.g., constant operating parameters. These correlations are commonly found from production quality control processes and studies of dependent between performance measures such as cutting force and tool wear.

In general, the information over the conditional correlation is rarely available in optimization applications due to limitation of the experiment costs that are usually very expensive. For this reason, such conditional correlations are rarely used in optimizations.

Definition 2.6.1. *Let Θ be the set of all parameter combinations, $\vec{X} \in \Theta$ be a parameter combination, $\vec{Y} = (Y_1, Y_2, \ldots, Y_m) \in \mathbb{R}^m$, $(m \geq 2)$ be the vector of performance measures and $\vec{Y} \mid \vec{X} = (Y_1 \mid \vec{X}, Y_2 \mid \vec{X}, \ldots, Y_m \mid \vec{X})$ denotes the vector of conditional performance measures with given parameter $\vec{X}$. The conditional covariance of Y_j and $Y_{j'}$ given $\vec{X}$ is written as*

$$\operatorname{cov}(Y_j \mid \vec{X}, Y_{j'} \mid \vec{X}) = \mathrm{E}\left[(Y_j \mid \vec{X} - \mathrm{E}(Y_j \mid \vec{X}))(Y_j' \mid \vec{X} - \mathrm{E}(Y_j' \mid \vec{X}))\right] \tag{2.35}$$

for $j, j' \in (1, 2, \ldots, m)$ and

$$r(Y_j \mid \vec{X}, Y_{j'} \mid \vec{X}) = \frac{\operatorname{cov}(Y_j \mid \vec{X}, Y_{j'} \mid \vec{X})}{\sqrt{\operatorname{cov}(Y_j \mid \vec{X}, Y_j \mid \vec{X})\operatorname{cov}(Y_{j'} \mid \vec{X}, Y_{j'} \mid \vec{X})}} \tag{2.36}$$

for the conditional correlation coefficient of Y_j and $Y_{j'}$.

From the definition 2.6.1, it follows that each operating parameter combination $\vec{X} \in \Theta$ has its own covariance matrix $\Sigma|\vec{X}$ as well as its correlation matrix. In general, it is to be expected that $\Sigma|\vec{X} \neq \Sigma|\vec{X}^*$ for any $\vec{X} \neq \vec{X}^*$ but in an optimization it is inevitable to compare the desirability index based on different given parameters. It is not proper to compare the values of desirability indices which have different preference settings, e.g. to compare $D|\vec{X}_j$ with $D|\vec{X}_{j*}$ such that $\vec{X}_j \neq \vec{X}_{j*}$. Therefore, the average value of the conditional correlations over the parameter space should be used as the representative. If the selected parameter space contains multiple operating conditions which have different conditional correlations of performance measures, an optimization using the conditional correlations would be very complicated.

Chapter 3

PCA-based Desirability Index

In this section, the proposed multivariate optimization method using the desirability approach with principal component analysis (PCA) will be introduced. The paradigms of this method are the implementations of PCA in Taguchi method to solve the correlated multi-response optimization problem (MOP) which are explained in section 2.5.3. Since both the normalized loss function used in [7, 31, 44] and the desirability function (DF) give a dimensionless output in range $[0, 1]$, and share a similar principle that the higher value is the better, the utilization of PCA in the desirability approach can be accomplished in a similar way. The expected advantage of replacing the normalized loss functions with DFs are the reduction in computation steps and the better physical interpretation in PCA due to the fact that the normalization functions require the maximum and the minimum value of the experimental data, therefore the normalized losses depend not only on the set targets but also on the experimental data.

3.1 Properties of the Principal Components of Desirability Functions

The definition of PC used in this study is slightly different from the standard definition stated in section 2.5.1, specifically the random vector of performance characteristics $\vec{Y}$ in equation 2.31 is replaced by the vector of DFs $d(\vec{Y})$ as shown in equation 3.1.

$$Z_i = \vec{a_i}^{\mathrm{T}} d(\vec{Y}) \tag{3.1}$$

where $\vec{a_i}^{\mathrm{T}}$ is the transpose of the ith eigenvector $\vec{a_i}$. In order to explore the potential to overcome the main disadvantage mentioned in section 2.5.3, the lack of physical interpretation of individual principal components (PCs), some characteristics of PCs have to be explored. Since eigenvectors and eigenvalues are involved in PCA, their properties of should be firstly explored.

3.1.1 Properties of Eigenvalues and Eigenvectors

Let

$$\Sigma = (c_{i,j}) = \begin{bmatrix} c_{1,1} & c_{1,2} & \cdots & c_{1,m} \\ c_{2,1} & c_{2,2} & \cdots & c_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ c_{m,1} & c_{m,2} & \cdots & c_{m,m} \end{bmatrix}$$

be the m x m covariance matrix of the desirability scores d_1, d_2, …, d_m, where $c_{i,j}$ is the covariance of d_i and d_j, and λ_i is the ith eigenvalue of Σ with the corresponding eigenvector $\vec{a_i}$ (non-zero vector).

Lemma 3.1.1. *All Eigenvalues $\lambda_i : i \in \{1, 2, \ldots, m\}$ of a non-singular covariance matrix Σ are non-negative and non-zero.*

Proof. From the definition of eigenvalue λ_i and eigenvector $\vec{a_i}$ the following expression can be obtained:

$$\Sigma\vec{a_i} = \lambda_i\vec{a_i}$$

$$\vec{a_i}^{\mathrm{T}}\Sigma\vec{a_i} = \vec{a_i}^{\mathrm{T}}\lambda_i\vec{a_i}$$

$$\vec{a_i}^{\mathrm{T}}\Sigma\vec{a_i} = \lambda_i\vec{a_i}^{\mathrm{T}}\vec{a_i}$$

$$\vec{a_i}^{\mathrm{T}}\Sigma\vec{a_i} = \lambda_i\|\vec{a_i}\|^2.$$

Since covariance matrix is always symmetric and positive semi-definite,

$$\Rightarrow 0 \leq \vec{a_i}^{\mathrm{T}}\Sigma\vec{a_i} = \lambda_i\|\vec{a_i}\|^2$$

and $\|\vec{a_i}\|^2 > 0$ because $\vec{a_i}$ is defined as a non-zero vector, then

$$\Rightarrow 0 \leq \lambda_i.$$

If $\exists\lambda_{i^*}$ at least one $i^* \in \{1, 2, \ldots, m\}$, then $\det(\Sigma) = 0$ which cannot be true since Σ is a non-singular covariance matrix. Therefore, $\nexists i^* : \lambda_{i^*} = 0$ and the following statement can be obtained:

$$\Rightarrow 0 < \lambda_i.$$

□

Definition 3.1.2 (Orthogonal vector). *Vectors $\vec{v_i}$, $\vec{v_j} \in \mathbb{R}^n$ are orthogonal or perpendicular to each other if $\vec{v_i} \cdot \vec{v_j} := \vec{v_i}^{\mathrm{T}}\vec{v_j} = 0$ and a set of vectors $\{\vec{v_1}, \vec{v_2}, \ldots, \vec{v_m}\}$ is an orthogonal set, if $\forall i \wedge j \in \{1, 2, \ldots, m\} : \vec{v_i} \cdot \vec{v_j} = 0$ when $i \neq j$.*

Definition 3.1.3 (Unit vector). *The length or magnitude of a vector $\vec{v}$ in $\mathbb{R}^n$ is defined as $\|\vec{v}\| = \sqrt{\vec{v} \cdot \vec{v}}$ and a unit vector $\vec{u}$ in $\mathbb{R}^n$ is a vector with $\|\vec{u}\| = 1$.*

Definition 3.1.4 (Orthonormal vector). *An orthonormal set $\{\vec{u_1}, \vec{u_2}, \ldots, \vec{u_m}\}$ is a set of orthogonal vectors which are also unit vectors. The product of two orthogonal vectors can be written as:*

$$\vec{u_i} \cdot \vec{u_j} = \begin{cases} 0 & \text{if} \quad i \neq j \\ 1 & \text{if} \quad i = j \end{cases} \tag{3.2}$$

where $i, j \in \{1, 2, \ldots, m\}$

Definition 3.1.5 (Orthogonal matrix). *An orthogonal matrix Q is defined as a square matrix whose columns are made up from orthonormal vectors $\{\vec{u_1}, \vec{u_2}, \ldots, \vec{u_m}\}$.*

Lemma 3.1.6. *If Q is orthogonal matrix then its rows form an orthonormal set of vectors and the columns of Q^{T} form also an orthonormal set of vectors. See proof of Theorem 9.8 in [33, p.285]*

Let a_{ij} be the jth element of the eigenvector $\vec{a_i} \subset \mathbb{R}^m$ which is defined as a normalized vector. The following expressions can be obtained:

$$\forall i : \ \|\vec{a_i}\|^2 = \ a_{i1}^2 + a_{i2}^2 + \cdots + a_{im}^2 = 1 \tag{3.3}$$

$$\Rightarrow \ \forall i, j : \ \ a_{ij}^2 \in [0, 1]$$

$$\Leftrightarrow \ \forall i, j : \ \ a_{ij} \in [-1, 1]. \tag{3.4}$$

Let a matrix A be a matrix whose columns are made up from the eigenvectors $\{\vec{a_1}, \vec{a_2}, \ldots, \vec{a_m}\}$. According to lemma 3.1.6, the rows of A are orthonormal vectors.

$$\forall j : \ \ a_{1j}^2 + a_{2j}^2 + \cdots + a_{mj}^2 = 1 \tag{3.5}$$

3.1.2 Types of Principal Components

In this subsection, principal components (PCs) are divided into 3 types, depending on the value of their corresponding eigenvector. The relations between PCs and desirability scores will be investigated.

Definition 3.1.7 (Type 1 : Principal component with a positive eigenvector). *Any PC with corresponding $\vec{a_i} = [a_{i1}, \ldots, a_{im}]^{\mathrm{T}}$ such that $\forall j : a_{ij} \in [0,1]$ is classified as the type 1 PC.*

Subjecting to section 2.4.1 and equation 2.30, the range of the type 1 Z_i can be given as

$$0 \leq Z_i = \sum_{m}^{j=1} a_{ij} d_j(Y_j) \leq \sum_{m}^{j=1} a_{ij}. \tag{3.6}$$

The most undesirable value of Z_i, denoted by $Z_{i(\text{worst})}$, is given when $\forall j : d_j(Y_j) = 0$, and is zero which is equal to the lower limit $\underline{Z_i}$ while the most desirable value $Z_{i(\text{ideal})}$, is given when $\forall j : d_j(Y_j) = 1$, is equal to $\sum_{m}^{j=1} a_{ij}$ which is the upper limit $\overline{Z_i}$. Hence, equation 3.6 could be extended as

$$0 = \underline{Z_i} = Z_{i(\text{worst})} \leq Z_i \leq Z_{i(\text{ideal})} = \overline{Z_i} = \sum_{m}^{j=1} a_{ij}. \tag{3.7}$$

Theorem 3.1.8. *Every type 1 PC is a positive monotonic transformation of $d_j(Y_j)$, and if $\forall j : a_{ij} \neq 0$, then it is a strictly positive monotonic transformation of $d_j(Y_j)$.*

Proof. Let $\vec{Y_k} = [Y_{k1}, \ldots, Y_{km}]^{\mathrm{T}} \subset \mathbb{R}^m$ be the process outputs of the kth experiment, $d(\vec{Y_k}) = [d_1(Y_{k1}), \ldots, d_m(Y_{km})]^{\mathrm{T}} \subset [0, 1]^m$ the desirability scores of $\vec{Y_k}$ and $\vec{a_i} = [a_{i1}, \ldots, a_{im}]^{\mathrm{T}} \subset [-1, 1]^m$ the ith eigenvector.

Suppose that there exist experiments k_0 and k_1 such that

$$\forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}),$$

subjecting to $\forall j : a_{ij} \in$ [0,1] and $\forall j : d_j(Y_{k_1 j}), d_j(Y_{k_0 j}) \in$ [0,1]:

$$\Rightarrow a_{i1}d_1(Y_{k_1 1}) + \cdots + a_{im}d_m(Y_{k_1 m}) \geq a_{i1}d_1(Y_{k_0 1}) + \cdots + a_{im}d_m(Y_{k_0 m})$$

$$\overset{3.1}{\Leftrightarrow} Z_{k_1 i} \geq Z_{k_0 i}$$

$$\forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}) \Rightarrow Z_{k_1 i} \geq Z_{k_0 i}. \tag{3.8}$$

Therefore, the type 1 PC is a positive monotonic transformation of $d_j(Y_j)$. Furthermore, if it exists at least one $j^* \in \{1, \ldots, m\}$ such that $d_j(Y_{k_1 j^*}) > d_j(Y_{k_0 j^*})$ with $a_{ij^*} > 0$, then

$$a_{i1}d_1(Y_{k_1 1}) + \cdots + a_{ij^*}d_{j^*}(Y_{k_1 j^*}) + \cdots + a_{im}d_m(Y_{k_1 m})$$

$$> a_{i1}d_1(Y_{k_0 1}) + \cdots + a_{ij^*}d_{j^*}(Y_{k_0 j^*}) + \cdots + a_{im}d_m(Y_{k_0 m})$$

$$\overset{3.1}{\Leftrightarrow} Z_{k_1 i} > Z_{k_0 i}. \tag{3.9}$$

Then, the type 1 PC is a strictly positive monotonic transformation of $d_j(Y_j)$. □

Definition 3.1.9 (Type 2 : Principal component with a negative eigenvector). *Any PC with corresponding $\vec{a_i}$ such that $\forall j : a_{ij} \in$ [-1,0] is defined as the type 2 PC.*

Subjecting to section 2.4.1 and equation 2.30, the range of type 2 Z_i is given as

$$\sum_{m}^{j=1} a_{ij} \leq Z_i = \sum_{m}^{j=1} a_{ij} d_j(Y_j) \leq 0. \tag{3.10}$$

The most undesirable value $Z_{i(\text{worst})}$, given when $\forall j : d_j(Y_j) = 0$, is zero which is equal to the upper limit $\overline{Z_i}$ while the most desirable value $Z_{i(\text{ideal})}$, given when $\forall j : d_j(Y_j) = 1$, is equal to $\sum_{m}^{j=1} a_{ij}$, the lower limit of the PC $\underline{Z_i}$. Hence, equation 3.10 could be extended as

$$\sum_{m}^{j=1} a_{ij} = \underline{Z_i} = Z_{i(\text{ideal})} \leq Z_i \leq Z_{i(\text{worst})} = \overline{Z_i} = 0. \tag{3.11}$$

Theorem 3.1.10. *Every type 2 PC is a negative monotonic transformation of $d_j(Y_j)$, and if $\forall j : a_{ij} \neq 0$, then it is a strictly negative monotonic transformation of $d_j(Y_j)$.*

Proof. Let $\vec{Y_k} = [Y_{k1}, \ldots, Y_{km}]^{\text{T}} \subset \mathbb{R}^m$ be the process outputs of the kth experiment, $d(\vec{Y_k}) = [d_1(Y_{k1}), \ldots, d_m(Y_{km})]^{\text{T}} \subset [0,1]^m$ the desirability scores of $\vec{Y_k}$ and $\vec{a_i} = [a_{i1}, \ldots, a_{im}]^{\text{T}} \subset [-1,1]^m$ the ith eigenvector.

Suppose that there exist experiments k_0 and k_1 such that

$$\forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}),$$

and subjecting to $\forall j : a_{ij} \in$ [-1,0] and $\forall j : d_j(Y_{k_1 j}), d_j(Y_{k_0 j}) \in$ [0,1]:

$$\Rightarrow a_{i1}d_1(Y_{k_1 1}) + \cdots + a_{im}d_m(Y_{k_1 m}) \leq a_{i1}d_1(Y_{k_0 1}) + \cdots + a_{im}d_m(Y_{k_0 m})$$

$$\overset{3.1}{\Leftrightarrow} Z_{k_1 i} \leq Z_{k_0 i}$$

$$\therefore\ \forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}) \Rightarrow Z_{k_1 i} \leq Z_{k_0 i}. \tag{3.12}$$

Therefore, the type 2 PC is a negative monotonic transformation of $d_j(Y_j)$. Furthermore, if it exists at least one $j^* \in \{1, \ldots, m\}$ such that $d_j(Y_{k_1 j^*}) > d_j(Y_{k_0 j^*})$ with $a_{ij^*} < 0$, then

$$\begin{aligned}
& a_{i1}d_1(Y_{k_1 1}) + \cdots + a_{ij^*}d_{j^*}(Y_{k_1 j^*}) + \cdots + a_{im}d_m(Y_{k_1 m}) \\
& < a_{i1}d_1(Y_{k_0 1}) + \cdots + a_{ij^*}d_{j^*}(Y_{k_0 j^*}) + \cdots + a_{im}d_m(Y_{k_0 m}) \\
& \overset{3.1}{\Leftrightarrow} Z_{k_1 i} < Z_{k_0 i}. \qquad (3.13)
\end{aligned}$$

Then, the type 2 PC is a strictly negative monotonic transformation of $d_j(Y_j)$. □

Definition 3.1.11 (Type 3 : Principal component with an eigenvector that contains both positive and negative elements). *Any PC with $\vec{a_i}$ such that $\exists j'$: $a_{ij'} \in$ (0,1] $\wedge$ $\exists j''$: $a_{ij''} \in$ [-1,0) is defined as the type 3 PC.*

Subjecting to section 2.4.1 and equation 2.30, the range of the type 3 Z_i can be expressed as

$$\sum_{j=1}^{m} a_{ij}\mathbb{1}_{[-1,0)}(a_{ij}) < Z_i = \sum_{j=1}^{m} a_{ij}d_j(Y_j) < \sum_{j=1}^{m} a_{ij}\mathbb{1}_{[0,1]}(a_{ij}), \qquad (3.14)$$

where $\mathbb{1}_A(x)$ is indicator function and is defined as

$$\mathbb{1}_A(x) = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{if } x \notin A \end{cases} \qquad (3.15)$$

Similar to the first two types, the most undesirable value $Z_{i(\text{worst})}$, is given when $\forall j : d_j(Y_j) = 0$, equals zero. The most desirable value $Z_{i(\text{ideal})}$, is given when $\forall j$: $d_j(Y_j) = 1$, is $\sum_{j=1}^{m} a_{ij}$. However, the lower limit $\underline{Z_i}$ is identical to the summation of the negative elements of $\vec{a_i}$, and the upper limit $\overline{Z_i}$ equals the summation of the positive elements as written correspondingly in equation 3.16 and 3.17.

$$\underline{Z_i} = \sum_{j=1}^{m} a_{ij}\mathbb{1}_{[-1,0)}(a_{ij}) \qquad (3.16)$$

$$\overline{Z_i} = \sum_{j=1}^{m} a_{ij}\mathbb{1}_{[0,1]}(a_{ij}) \qquad (3.17)$$

The interpretation of the type 3 PC is very difficult, since both $Z_{i(\text{ideal})}$ and $Z_{i(\text{worst})}$ lie in an open interval between $\underline{Z_i}$ and $\overline{Z_i}$, and it is not a monotonic transformation of $d_j(Y_j)$.

Based on the idea of the combined quality loss (CQL) [36], a value of Z_i that close to $Z_{i(\text{ideal})}$ is preferred. On the contrary, the distance between Z_i and $Z_{i(\text{worst})}$ will not be taken into account. Whereas the ideal based on the methods such as the technique for order preference by similarity to ideal solution (TOPSIS) [3, 53] or the grey relation analysis (GRA) [7, 39, 40, 46, 57] include the distance between Z_i and $Z_{i(\text{worst})}$ in the result. However, when the value of $\sum_{j=1}^{m} a_{ij}$ is very close to zero, the probability of misinterpretation using these methods can be very high, and as a consequence the dominance relation of the solutions might has been changed during the transformations [32]. Thus, a monotonic transformation of the type 3 PC would be necessitated before integrate such PCs into the overall performance index.

3.2 The PCA-based Desirability Index

Due to the lack of monotonicity of the indices formulated by the weighted-PCA (WPCA), CQL, GRA and TOPSIS, the PCA-based desirability index (DI) [50, 58] is developed and formulated as a monotonic transformation of the desirability scores $d_j(Y_j)$. Further investigations on the properties of the PCA-based DI has been performed by [50], from which the PCA-based DI is proven to be a kind of desirability index. An investigation on the distribution of the PCA-based DI is also attempted by [50] but an analytical formula seems very difficult. With the strict monotonicity of the PCA-based DI, the dominance relation of the solutions will not be changed after the transformations and the optimality of the solutions can be guaranteed as it is proven by Legrand [26].

Let $\vec{Y_k} = [Y_{k1}, \ldots, Y_{km}]^{\mathrm{T}} \subset \mathbb{R}^m$ be the process outputs of the kth experiment, $d(\vec{Y_k})$ $= [d_1(Y_{k1}), \ldots, d_m(Y_{km})]^{\mathrm{T}} \subset [0,1]^m$ the desirability scores of $\vec{Y_k}$, $\vec{a_i} = [a_{i1}, \ldots, a_{im}]^{\mathrm{T}}$

$\subset [-1,1]^m$ the ith eigenvector and Z_{ki} the ith principal component of the kth experiment. In order to formulate the PCA-based DI that is monotonically increasing in $d_j(Y_j)$, the PC scores must increase monotonically in the value of $d_j(Y_j)$. The function f is defined as a function which is used to transform Z_{ki} into the scores $N_{ki} \in$ [0,1].

$$N_{ki} = f(\vec{a_i}, d(\vec{Y_k}), Z_{ki}) = \begin{cases} \frac{Z_{ki}}{Z_{i(\text{ideal})}} & \text{if } \forall j : a_{ij} \in [0,1] \\ & \text{or } \forall j : a_{ij} \in [-1,0) \\ \frac{1}{2}\left(\frac{\Psi_{ki}}{\Psi_{i(\text{ideal})}} + \frac{Z_{ki}-\Psi_{ki}}{Z_{i(\text{ideal})}-\Psi_{i(\text{ideal})}}\right) & \text{else} \end{cases} \tag{3.18}$$

with

$$Z_{ki} = \sum_{j=1}^{m} a_{ij} d_j(Y_{kj})$$

$$Z_{i(\text{ideal})} = \sum_{j=1}^{m} a_{ij}$$

$$\Psi_{ki} = \sum_{j=1}^{m} a_{ij} d_j(Y_{kj}) \mathbb{1}_{[0,1]}(a_{ij})$$

$$\Psi_{i(\text{ideal})} = \sum_{j=1}^{m} a_{ij} \mathbb{1}_{[0,1]}(a_{ij})$$

where Ψ_{ki} denotes the summation of the multiplications of $d_j(Y_{kj})$ and the positive a_{ij}, and is required to be calculated only when Z_{ki} is the type 3 PC. The ideal value of Z_{ki} and Ψ_{ki} are denoted correspondingly by $Z_{i(\text{ideal})}$ and $\Psi_{i(\text{ideal})}$, are valid for all experiments k, and can be obtained when $\forall j : d_j(Y_j) = 1$. Even though the main purpose of f is to transform Z_{ki} into the PC scores N_{ki}, the values of N_{ki} cannot be computed without the values of $\vec{a_i}$ and $d(\vec{Y_k})$ being given.

Based on the concept of weighted principal component analysis (WPCA) which is described in section 2.5.2, the PCA-based DI is defined as

$$D_{\mathrm{PCA}k} = \sum_{i=1}^{m} W_i N_{ki} \tag{3.19}$$

where W_i is a normalized weight of the ith PC ,$\sum_{i=1}^{m} W_i = 1$, and $D_{\mathrm{PCA}k}$ is the PCA-based DI for the kth experiment.

The value of $D_{\mathrm{PCA}k}$ is in the range [0,1] for all k, and the $D_{\mathrm{PCA}k}$ value is monotonically increasing in $d(\vec{Y_k})$; thus, a higher value means the more favorable. The value $D_{\mathrm{PCA}} = 1$ can be referred as the ideal value for the PCA-based DI.

Theorem 3.2.1. *The PCA-based DI which is defined in equation 3.19 is a positive monotonic transformation of $d_j(Y_j)$, if it exists at least one $\lambda_i \neq 0$.*

Proof. Let $\vec{Y_k} = [Y_{k1}, \ldots, Y_{km}]^{\mathrm{T}} \subset \mathbb{R}^m$ be the process outputs of the kth experiment, $d(\vec{Y_k}) = [d_1(Y_{k1}), \ldots, d_m(Y_{km})]^{\mathrm{T}} \subset [0,1]^m$ the desirability scores of $\vec{Y_k}$ and $\vec{a_i} = [a_{i1}, \ldots, a_{im}]^{\mathrm{T}} \subset [-1,1]^m$ the ith eigenvector. Suppose that there exist experiments k_0 and k_1 such that

$$\forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}).$$

For the first type of PC, according to equation 3.7 and 3.8, and subjecting to $\forall j : a_{ij} \in$ [0,1] and $\forall j : d_j(Y_{k_1 j}), d_j(Y_{k_0 j}) \in$ [0,1]:

$$\Rightarrow Z_{i(\mathrm{ideal})} \geq Z_{k_1 i} \geq Z_{k_0 i} \geq 0,$$

since $Z_{i(\mathrm{ideal})} = \sum_{j=1}^{m} a_{ij}$ and $\sum_{j=1}^{m} a_{ij}^2 = 1$, it is obvious that $Z_{i(\mathrm{ideal})} > 0$. Therefore, the following expressions can be obtained:

$$1 \geq \frac{Z_{k_1 i}}{Z_{i(\mathrm{ideal})}} \geq \frac{Z_{k_0 i}}{Z_{i(\mathrm{ideal})}} \geq 0$$

$$\overset{3.18}{\Leftrightarrow} 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0. \tag{i}$$

For the second type of PC, according to equation 3.11 and 3.12, and subjecting to $\forall j : a_{ij} \in$ [-1,0] and $\forall j : d_j(Y_{k_1 j}), d_j(Y_{k_0 j}) \in$ [0,1]:

$$Z_{i(\text{ideal})} \leq Z_{k_1 i} \leq Z_{k_0 i} \leq 0,$$

since $Z_{i(\text{ideal})} = \sum_{j=1}^{m} a_{ij}$ and $\sum_{j=1}^{m} a_{ij}^2 = 1$, it is obvious that $Z_{i(\text{ideal})} < 0$. Therefore, the following expressions can be obtained:

$$1 \geq \frac{Z_{k_1 i}}{Z_{i(\text{ideal})}} \geq \frac{Z_{k_0 i}}{Z_{i(\text{ideal})}} \geq 0$$

$$\overset{3.18}{\Leftrightarrow} 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0 \qquad \text{(ii)}$$

For the third type of PC, the following expressions can be given:

$$\sum_{j=1}^{m} a_{ij} \mathbb{1}_{[0,1]}(a_{ij}) \geq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[0,1]}(a_{ij}) \geq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[0,1]}(a_{ij}) \geq 0$$

$$\overset{3.18}{\Leftrightarrow} \Psi_{i(\text{ideal})} \geq \Psi_{k_1 i} \geq \Psi_{k_0 i} \geq 0.$$

According to the definition of the type 3 PC that $\exists j^* : a_{ij^*} \in$ (0,1], then $\Psi_{i(\text{ideal})} > 0$ and the following expressions can be given:

$$1 \geq \frac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} \geq \frac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} \geq 0, \qquad (*)$$

and again from the definition that $\exists j^{**} : a_{ij^{**}} \in$ [-1,0), the following expression can be derived:

$$\sum_{j=1}^{m} a_{ij} \mathbb{1}_{[-1,0)}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[-1,0)}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[-1,0)}(a_{ij}) \leq 0$$

$$\Leftrightarrow \sum_{j=1}^{m} a_{ij} - \sum_{j=1}^{m} a_{ij} \mathbb{1}_{[0,1]}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) - \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[0,1]}(a_{ij})$$

$$\leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) - \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[0,1]}(a_{ij}) \leq 0$$

$$\overset{3.18}{\Leftrightarrow} Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})} \leq Z_{k_1 i} - \Psi_{k_1 i} \leq Z_{k_0 i} - \Psi_{k_0 i} \leq 0.$$

Since $\exists j^* : a_{ij^*} \in (0,1] \Rightarrow \Psi_{i(\text{ideal})} > 0$ and $\Psi_{i(\text{ideal})} > Z_{i(\text{ideal})}$, then $\sum_{j=1}^{m} a_{ij} \mathbb{1}_{[-1,0)}(a_{ij}) = Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})} < 0$. Thus, the following expression can be derived:

$$\Leftrightarrow 1 \geq \frac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq \frac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq 0. \qquad (**)$$

By summing up (*) with (**), the following expressions can be obtained:

$$2 \geq \frac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq \frac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq 0$$

$$\Leftrightarrow 1 \geq \frac{1}{2}\left[\frac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}}\right] \geq \frac{1}{2}\left[\frac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}}\right] \geq 0$$

$$\overset{3.18}{\Leftrightarrow} 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0 \qquad \text{(iii)}$$

From (i), (ii), and (iii), the following expression can be obtained:

$$\forall i \in \{1, \ldots, m\} : 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0,$$

since only 3 types of PCs exist and therefore,

$$\forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}) \Rightarrow \forall i : N_{k_1 i} \geq N_{k_0 i}. \qquad (3.20)$$

The monotonicity of N_{ki} has been proven and with $\sum_{i=1}^{m} W_i = 1$ and $\forall i \in \{1, \ldots, m\}$: $W_i \in [0, 1]$

$$\Rightarrow 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0.$$

Furthermore $\exists \lambda_i \neq 0$ and that means $\exists W_i \neq 0$. The following expressions can be derived:

$$\overset{3.19}{\Leftrightarrow} 1 \geq D_{\text{PCA}k_1} \geq D_{\text{PCA}k_0} \geq 0$$

$$\therefore \ \forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}) \Rightarrow D_{\text{PCA}k_1} \geq D_{\text{PCA}k_0}. \qquad (3.21)$$

Finally, it has been proven that $D_{\text{PCA}k}$ is a positive monotonic transformation of $d(\vec{Y}_k)$. □

Theorem 3.2.2. *The PCA-based DI is a strictly positive monotonic transformation of $d_j(Y_j)$, if at least one of the following statements is true:*

1. *The covariance matrix Σ of $d_j(Y_j)$ is a full rank matrix.*
2. *The covariance matrix Σ of $d_j(Y_j)$ is a non-singular matrix.*
3. *All eigenvalues λ_i are positive.*
4. *There exists at least one pair of eigenvector $\vec{a_{i^*}}$ and eigenvalue λ_{i^*} such that $\forall j$: $a_{i^*j} \neq 0$ and $\lambda_{i^*} > 0$.*

Proof. The statements 1, 2 and 3 can be proven at the same way, since a full rank covariance matrix is also a non-singular matrix, and it has only positive eigenvalues (Lemma 3.1.1). Let $\vec{Y_k} = [Y_{k1}, \ldots, Y_{km}]^{\mathrm{T}} \subset \mathbb{R}^m$ be the process outputs of the kth experiment, $d(\vec{Y_k}) = [d_1(Y_{k1}), \ldots, d_m(Y_{km})]^{\mathrm{T}} \subset [0,1]^m$ the desirability scores of $\vec{Y_k}$ and $\vec{a_i} = [a_{i1}, \ldots, a_{im}]^{\mathrm{T}} \subset [-1,1]^m$ the ith eigenvector. Suppose that there exist experiments k_0 and k_1 such that

$$\forall j : d_j(Y_{k_1 j}) \geq d_j(Y_{k_0 j}),$$

with at least one $j^* \in \{1, \ldots, m\}$ such that $d_j(Y_{k_1 j^*}) > d_j(Y_{k_0 j^*})$. For the first type of PC, according to equation 3.7 and 3.9, and subjecting to $\forall j : a_{ij} \in$ [0,1] and $\forall j : d_j(Y_{k_1 j}), d_j(Y_{k_0 j}) \in$ [0,1]:

$$\begin{aligned} \Rightarrow \quad & Z_{i(\text{ideal})} \geq Z_{k_1 i} \geq Z_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} = 0 \\ & Z_{i(\text{ideal})} \geq Z_{k_1 i} > Z_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} \neq 0 \end{aligned}$$

and the following expressions can be obtained by the same way as in the proof of theorem 3.2.1:

$$\begin{aligned} \overset{3.18}{\Leftrightarrow} \quad & 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} = 0 \\ & 1 \geq N_{k_1 i} > N_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} \neq 0 \end{aligned} \tag{iv}$$

For the second type of PC, according to equation 3.11 and 3.13, and subjecting to $\forall j : a_{ij} \in$ [-1,0] and $\forall j : d_j(Y_{k_1 j}), d_j(Y_{k_0 j}) \in$ [0,1]:

$$\begin{aligned} \Rightarrow \quad & Z_{i(\text{ideal})} \leq Z_{k_1 i} \leq Z_{k_0 i} \leq 0 \quad \text{, if } a_{ij^*} = 0 \\ & Z_{i(\text{ideal})} \leq Z_{k_1 i} < Z_{k_0 i} \leq 0 \quad \text{, if } a_{ij^*} \neq 0 \end{aligned}$$

and the following expressions can be obtained obtained by the same way as the proof of theorem 3.2.1:

$$\begin{aligned} \overset{3.18}{\Leftrightarrow} \quad & 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} = 0 \\ & 1 \geq N_{k_1 i} > N_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} \neq 0 \end{aligned} \tag{V}$$

For the third type of PC, the following expression can be given:

$$\sum_{j=1}^{m} a_{ij} \mathbb{1}_{[0,1]}(a_{ij}) \geq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[0,1]}(a_{ij}) \geq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[0,1]}(a_{ij}) \geq 0$$

and if $a_{ij^*} \neq 0$, then

$$\Rightarrow \sum_{j=1}^{m} a_{ij} \mathbb{1}_{[0,1]}(a_{ij}) \geq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[0,1]}(a_{ij}) > \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[0,1]}(a_{ij}) \geq 0.$$

$$\begin{aligned} \overset{3.18}{\Leftrightarrow} \quad & \Psi_{i(\text{ideal})} \geq \Psi_{k_1 i} \geq \Psi_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} = 0 \\ & \Psi_{i(\text{ideal})} \geq \Psi_{k_1 i} > \Psi_{k_0 i} \geq 0 \quad \text{, if } a_{ij^*} \neq 0 \end{aligned}$$

According to the definition of the type 3 PC that $\exists j' : a_{ij'} \in$ (0,1], then $\Psi_{i(\text{ideal})} > 0$ and the following expressions can be given:

$$\begin{aligned} \Leftrightarrow \quad & 1 \geq \tfrac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} \geq \tfrac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} \geq 0 \quad \text{, if } a_{ij^*} = 0 \\ & 1 \geq \tfrac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} > \tfrac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} \geq 0 \quad \text{, if } a_{ij^*} \neq 0 \end{aligned} \tag{*}$$

and again from the definition that $\exists j'' : a_{ij''} \in$ [-1,0), the following expressions can be derived, if $a_{ij^*} > 0$ or $a_{ij^*} = 0$:

$$\Rightarrow \sum_{j=1}^{m} a_{ij} \mathbb{1}_{[-1,0)}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[-1,0)}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[-1,0)}(a_{ij}) \leq 0$$

$$\Leftrightarrow \sum_{j=1}^{m} a_{ij} - \sum_{j=1}^{m} a_{ij} \mathbb{1}_{[0,1]}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) - \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[0,1]}(a_{ij})$$

$$\leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) - \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[0,1]}(a_{ij}) \leq 0$$

$$\overset{3.18}{\Leftrightarrow} Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})} \leq Z_{k_1 i} - \Psi_{k_1 i} \leq Z_{k_0 i} - \Psi_{k_0 i} \leq 0.$$

and if $a_{ij^*} < 0$:

$$\Rightarrow \sum_{j=1}^{m} a_{ij} \mathbb{1}_{[-1,0)}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[-1,0)}(a_{ij}) < \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[-1,0)}(a_{ij}) \leq 0$$

$$\Leftrightarrow \sum_{j=1}^{m} a_{ij} - \sum_{j=1}^{m} a_{ij} \mathbb{1}_{[0,1]}(a_{ij}) \leq \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) - \sum_{j=1}^{m} a_{ij} d_j(Y_{k_1 j}) \mathbb{1}_{[0,1]}(a_{ij})$$

$$< \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) - \sum_{j=1}^{m} a_{ij} d_j(Y_{k_0 j}) \mathbb{1}_{[0,1]}(a_{ij}) \leq 0$$

$$\overset{3.18}{\Leftrightarrow} Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})} \leq Z_{k_1 i} - \Psi_{k_1 i} < Z_{k_0 i} - \Psi_{k_0 i} \leq 0.$$

Since $\exists j' : a_{ij'} \in (0,1] \Rightarrow \Psi_{i(\text{ideal})} > 0$ and $\Psi_{i(\text{ideal})} > Z_{i(\text{ideal})}$, then $\sum_{j=1}^{m} a_{ij} \mathbb{1}_{[-1,0)}(a_{ij}) = Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})} < 0$. Thus, the following expression can be derived, if $a_{ij^*} > 0$ or $a_{ij^*} = 0$:

$$\begin{aligned} \Leftrightarrow \quad & 1 \geq \tfrac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq \tfrac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq 0 \quad \text{, if } a_{ij^*} \geq 0 \\ & 1 \geq \tfrac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} > \tfrac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq 0 \quad \text{, if } a_{ij^*} \neq 0. \end{aligned} \qquad (**)$$

By adding (*) with (**), the following expressions can be obtained, if $a_{ij^*} = 0$

$$2 \geq \frac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq \frac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq 0$$

$$\Leftrightarrow 1 \geq \frac{1}{2}\left[\frac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}}\right] \geq \frac{1}{2}\left[\frac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}}\right] \geq 0$$

anf if $a_{ij^*} \neq 0$

$$2 \geq \frac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} > \frac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}} \geq 0$$

$$\Leftrightarrow 1 \geq \frac{1}{2}\left[\frac{\Psi_{k_1 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_1 i} - \Psi_{k_1 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}}\right] > \frac{1}{2}\left[\frac{\Psi_{k_0 i}}{\Psi_{i(\text{ideal})}} + \frac{Z_{k_0 i} - \Psi_{k_0 i}}{Z_{i(\text{ideal})} - \Psi_{i(\text{ideal})}}\right] \geq 0$$

Then, the following statement can be derived:

$$\stackrel{3.18}{\Leftrightarrow} \begin{array}{ll} 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0 & , \text{if } a_{ij^*} = 0 \\ 1 \geq N_{k_1 i} > N_{k_0 i} \geq 0 & , \text{if } a_{ij^*} \neq 0. \end{array} \tag{vi}$$

From (iv), (v), and (vi), it can be concluded that

$$\begin{array}{ll} 1 \geq N_{k_1 i} \geq N_{k_0 i} \geq 0 & , \text{if } a_{ij^*} = 0 \\ 1 \geq N_{k_1 i} > N_{k_0 i} \geq 0 & , \text{if } a_{ij^*} \neq 0. \end{array} \tag{3.22}$$

It is obvious that if and only if $\forall i : a_{ij^*} = 0$ then $D_{\text{PCA}k}$ is not strictly monotonic. According to lemma 3.1.6, the statement $\forall i : a_{ij^*} = 0$ can never be true because it must follow the equation 3.5 for j^* that

$$\sum_{i=1}^{m} a_{ij^*}^2 = a_{1j^*}^2 + a_{2j^*}^2 + \cdots + a_{mj^*}^2 = 1.$$

Therefore,

$$\Rightarrow D_{\text{PCA}k_1} > D_{\text{PCA}k_0},$$

and the statements 1, 2 and 3 have been proven.

The proof of the statement 4 follows from the equation 3.22 in the case that $a_{ij^*} \neq 0$:

$$\exists i^* : 1 \geq N_{k_1 i^*} > N_{k_0 i^*} \geq 0. \tag{3.23}$$

Since $\forall i : \lambda_i \geq 0$ and $\lambda_{i^*} > 0$, it is clear that

$$\Rightarrow D_{\text{PCA}k_1} > D_{\text{PCA}k_0}.$$

Therefore the statement 4 has been proven. □

Now let's have some examples when the conditions in theorem 3.2.2 are satisfied and not satisfied.

Example 3.2.3. *Suppose that there are in total 4 performance measures and d_j denotes the desirability score of the jth performance measure. The variances of d_j are assumed as 0.5 for $j \in \{1, 2, 3, 4\}$ and their correlation coefficients $r_{(j,j*),j*\neq j}$ are assumed to be 1 (perfectly correlated). The covariance matrix of d_j can be formulated as in table 3.1 as well as its eigenvectors and eigenvalues that are derived as shown in table 3.2.*

Table 3.1: Covariance matrix of d_j for example 3.2.3

Variable	d_1	d_2	d_3	d_4
d_1	0.5000	0.5000	0.5000	0.5000
d_2	0.5000	0.5000	0.5000	0.5000
d_3	0.5000	0.5000	0.5000	0.5000
d_4	0.5000	0.5000	0.5000	0.5000

Table 3.2: Eigenvectors and eigenvalues for example 3.2.3

	1st PC	2nd PC	3rd PC	4th PC
Eigenvector	$\begin{bmatrix} 0.5000 \\ 0.5000 \\ 0.5000 \\ 0.5000 \end{bmatrix}$	$\begin{bmatrix} 0.7887 \\ -0.2113 \\ -0.5774 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -0.2113 \\ 0.7887 \\ -0.5774 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0.2887 \\ 0.2887 \\ 0.2887 \\ -0.8660 \end{bmatrix}$
Eigenvalue	2.0000	0.0000	0.0000	0.0000

For this case it is obvious that all of d_1, d_2, d_3 and d_4 can be represented by only a single principal component, since they correlate perfectly. Their covariance matrix is clearly a singular matrix and not a full rank matrix, and furthermore λ_2, λ_3 and λ_4 are equal zero; hence, the 1st-3rd conditions of theorem 3.2.2 are unsatisfied. Anyhow, the 4th is satisfied because $\vec{a_1}$ contains only non-zero elements and $\lambda_1 = 2$. For this case, D_{PCA} is a strictly monotone transformation of d_1, d_2, d_3 and d_4 and each d_j

accounts 25 percent of D_{PCA} *(which means that* $\forall j : W_{d_j} = 0.25$*).*

Example 3.2.4. *Now let's modify an assumption in example 3.2.3 so that* d_1 *is linearly independent from* d_2*,* d_3 *and* d_4*, and for* $\hat{j} \in \{2, 3, 4\} : r_{(1,\hat{j})} = 0$*. The covariance matrix of the* d_j *can be formulated as in table 3.3 as well as its eigenvectors and eigenvalues that are derived as shown in table 3.4.*

Table 3.3: Covariance matrix of d_j for example 3.2.4

Variable	d_1	d_2	d_3	d_4
d_1	0.5000	0.0000	0.0000	0.0000
d_2	0.0000	0.5000	0.5000	0.5000
d_3	0.0000	0.5000	0.5000	0.5000
d_4	0.0000	0.5000	0.5000	0.5000

Table 3.4: Eigenvectors and eigenvalues for example 3.2.4

	1st PC	2nd PC	3rd PC	4th PC
Eigenvector	$\begin{bmatrix} 0.0000 \\ 0.5774 \\ 0.5774 \\ 0.5774 \end{bmatrix}$	$\begin{bmatrix} 1.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \end{bmatrix}$	$\begin{bmatrix} 0.0000 \\ 0.4082 \\ 0.4082 \\ -0.8165 \end{bmatrix}$	$\begin{bmatrix} 0.0000 \\ 0.7071 \\ -0.7071 \\ 0.0000 \end{bmatrix}$
Eigenvalue	1.5000	0.5000	0.0000	0.0000

The covariance matrix in table 3.3 is clearly a singular matrix and none of the conditions in theorem 3.2.2 is valid. Even though theorem 3.2.2 cannot be used, an analytical solution for D_{PCA} *is still available.*

$$\begin{aligned} D_{\text{PCA}} &= W_1 * N_1 + W_2 * N_2 + W_3 * N_3 + W_4 * N_4 \qquad (W_3, W_4 = 0) \\ &= W_1 * N_1 + W_2 * N_2 \\ &= \frac{1.5}{2} * N_1 + \frac{0.5}{2} * N_2 \end{aligned}$$

$$
\begin{aligned}
&= \frac{1.5}{2} * \frac{a_{12} * d_2 + a_{13} * d_3 + a_{14} * d_4}{a_{12} + a_{13} + a_{14}} + \frac{0.5}{2} * \frac{a_{21} * d_1}{a_{21}} \\
&= \frac{1.5}{2} * \frac{0.5774 * d_2 + 0.5774 * d_3 + 0.5774 * d_4}{0.5774 + 0.5774 + 0.5774} + \frac{0.5}{2} * d_1 \\
&= \frac{3}{4} * \left[\frac{1}{3} * d_2 + \frac{1}{3} * d_3 + \frac{1}{3} * d_4\right] + \frac{1}{4} * d_1 \\
&= \frac{1}{4} * d_2 + \frac{1}{4} * d_3 + \frac{1}{4} * d_4 + \frac{1}{4} * d_1
\end{aligned}
$$

As a result, D_{PCA} is an arithmetic mean of d_1, d_2, d_3 and d_4 with equal weights, and it is a strictly monotone transformation of d_1, d_2, d_3 and d_4. However, since d_2, d_3 and d_4 are perfectly correlated while d_1 is uncorrelated, it would be expected that d_1 should be handled more important than d_2, d_3 and d_4. It has been shown in this example that for an optimization problem with a singular covariance matrix such as in table 3.3, an unintentional optimization result might be produced using D_{PCA}.

Example 3.2.5. *Furthermore, let's assume that d_1 in example 3.2.4 has a zero variance. The covariance matrix of d_j can be formulated as in table 3.5 and its eigenvectors and eigenvalues that are derived as shown in table 3.6.*

Table 3.5: Covariance matrix of d_j for example 3.2.5

Variable	d_1	d_2	d_3	d_4
d_1	0.0000	0.0000	0.0000	0.0000
d_2	0.0000	0.5000	0.5000	0.5000
d_3	0.0000	0.5000	0.5000	0.5000
d_4	0.0000	0.5000	0.5000	0.5000

Table 3.6: Eigenvectors and eigenvalues for example 3.2.5

	1st PC	2nd PC	3rd PC	4th PC
Eigenvector	$\begin{bmatrix} 0.0000 \\ 0.5774 \\ 0.5774 \\ 0.5774 \end{bmatrix}$	$\begin{bmatrix} 0.0000 \\ 0.4082 \\ 0.4082 \\ -0.8165 \end{bmatrix}$	$\begin{bmatrix} 1.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \end{bmatrix}$	$\begin{bmatrix} 0.0000 \\ 0.7071 \\ -0.7071 \\ 0.0000 \end{bmatrix}$
Eigenvalue	1.5000	0.0000	0.0000	0.0000

It follows as in the previous case that none of the conditions in theorem 3.2.2 is valid and theorem 3.2.2 cannot be used. Also, the analytical analysis can be performed analog to the previous example.

$$\begin{aligned}
D_{\text{PCA}} &= W_1 * N_1 + W_2 * N_2 + W_3 * N_3 + W_4 * N_4 \qquad (W_2, W_3, W_4 = 0) \\
&= W_1 * N_1 \\
&= 1 * N_1 \\
&= \frac{a_{12} * d_2 + a_{13} * d_3 + a_{14} * d_4}{a_{12} + a_{13} + a_{14}} \\
&= \frac{0.5774 * d_2 + 0.5774 * d_3 + 0.5774 * d_4}{0.5774 + 0.5774 + 0.5774} \\
&= \frac{1}{3} * d_2 + \frac{1}{3} * d_3 + \frac{1}{3} * d_4 \\
&= \frac{1}{3} * d_2 + \frac{1}{3} * d_3 + \frac{1}{3} * d_4 + 0 * d_1
\end{aligned}$$

For this case, d_1 has no contribution on D_{PCA} and D_{PCA} is a strictly monotone transformation of d_2, d_3 and d_4 but it is not a strictly monotone transformation of d_1, d_2, d_3 and d_4. As a consequence, the results of this optimization problem using D_{PCA} may not be Pareto-optimal.

Example 3.2.6. *Now let's vary the value of $r_{(1,\hat{j})}$ in example 3.2.3 from -1 to 1 while $r_{(\hat{j},\hat{j}^*),\hat{j}\neq\hat{j}^*} = 1$ and compute the normalized weight for d_1, d_2, d_3 and d_4. The contributions of d_1, d_2, d_3 and d_4 on D_{PCA} are then computed and illustrated in figure*

3.1 and it shows that the normalized weight for d_1 *becomes larger than 0.25, only when* d_1 *has negative correlations with* d_2, d_3 *and* d_4. *The case* $r_{1,\hat{j}} = 0$ *is identical with example 3.2.4 in which* a_{11}, a_{22}, a_{23}, a_{24}, λ_3 *and* $\lambda_4 = 0$, *so that* $W_{d_1} = \frac{\lambda_2}{\lambda_1+\lambda_2} = 0.25$.

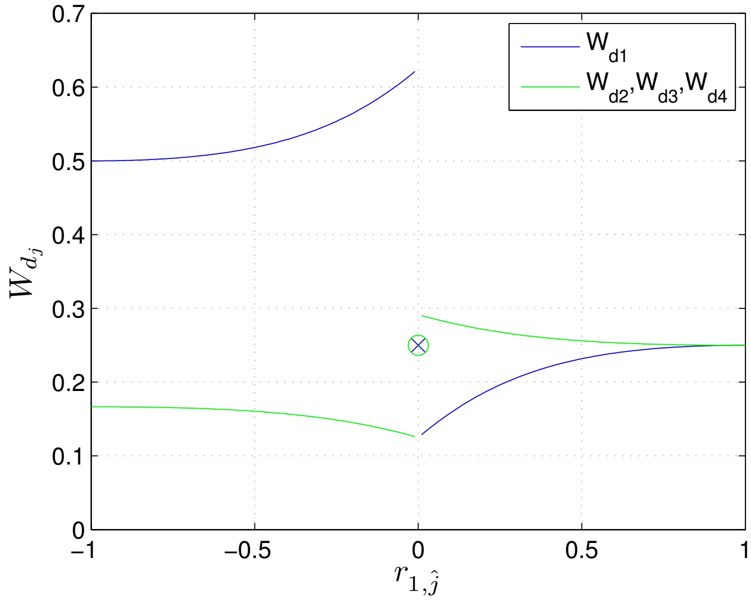


Figure 3.1: Contributions of d_1, d_2, d_3 and d_4 on D_{PCA}

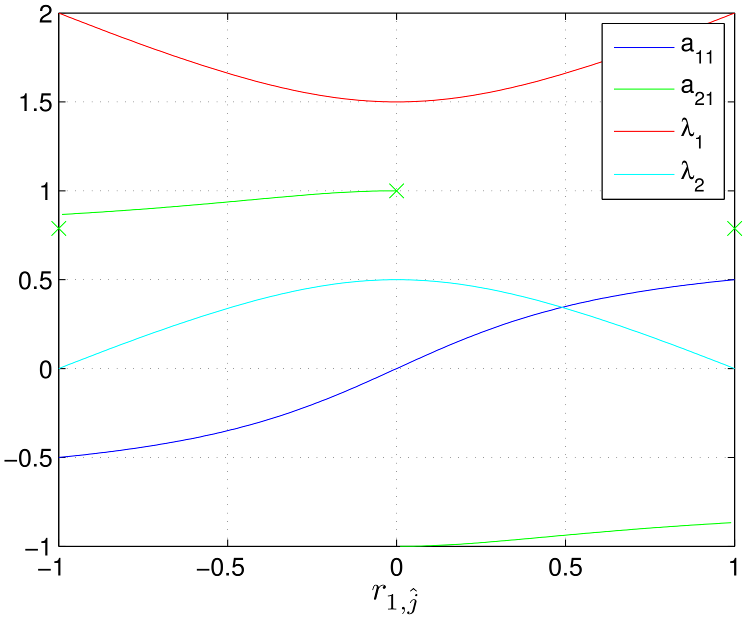


Figure 3.2: Values of a_{11}, a_{21}, λ_1 and λ_2

Figure 3.2 is then used to explain the phenomenon of discrete W_{d_j} in figure 3.1. For negative $r_{1,\hat{j}}$, d_1 is projected in a different direction with d_2, d_3 and d_4 so that a_{11} is negative. As consequences, the first principal component (Z_1) becomes the third type PC, and according the lower case of N_{ki} in equation 3.18, d_1 would possess 50 percent of W_1. Additionally, d_1 also possesses some proportion of W_2; thus, W_{d_1} jumps suddenly when $r_{1,\hat{j}}$ becomes negative. Due to the fact that d_1 also possesses some proportion of W_2, $W_{d_1} \geq 0.5$. The stronger $r_{1,\hat{j}}$ becomes negative, the closer λ_2 to zero and the less W_{d_1} becomes, and when $r_{1,\hat{j}} = -1$, then $\lambda_2 = 0$ and $W_{d_1} = 0.5$.

For positive $r_{1,\hat{j}}$, d_1 is projected in the same direction as d_2, d_3 and d_4 in Z_1 where the value of a_{11} is smaller than a_{12}, a_{13}, a_{14} for $r_{1,\hat{j}} < 1$. For this reason, d_1 possesses only a small proportion of W_1 when compared to d_2, d_3 and d_4. Even though, d_1 may possess 50 percent of W_2 (due to negative a_{21} and positive a_{22}, a_{23} and a_{24}), the value of λ_2 is at least 3 times smaller than λ_1; therefore, W_{d_1} is found to be small, especially when $r_{1,\hat{j}}$ is small. As $r_{1,\hat{j}}$ increases, a_{11} also increases and the contribution *of d_1 in W_1 increases while W_2 approaches zero. As a consequence, W_{d_1} increases and approach 0.25.*

From this and previous examples, it has been found that the contributions of d_1, d_2, d_3 and d_4 on D_{PCA} may depend on the direction of projection for d_1, d_2, d_3 and d_4. It is very difficult to modify for a D_{PCA} such that W_{d_j} are continuous in $r_{1,\hat{j}} \in [-1, 1]$, since elements of eigenvectors can be discrete, i.e., a_{21} jumps suddenly from 1 to -1 when $r_{1,\hat{j}}$ becomes positive as shown in figure 3.2. Finally, it is recommended that uncorrelated or independent desirability scores should be handled separately in PCA-based desirability approach.

3.3 Procedure of PCA-based Desirability Approach

The main concept of this method is to use PCA transformation to decorrelate desirability values $d_1, \ldots, d_m$ by transforming them into PCs $Z_1, \ldots, Z_m$. Then, based on the principle of WPCA which is explained in section 2.5, PCs are combined into the overall performance index D_{PCA}.

Suppose that there are totally m responses and n experiments. The proposed procedure is described in the following:

Step 1 : $Compute\ the\ desirability\ value\ of\ each\ response.$ Let Y_{kj} be the value of the jth response in the kth experiment. As described in section 2.4.1, the type of DFs is to be selected. With the selected DFs Y_{kj} are to be transformed into the desirability values $d_j(Y_{kj})$.

Step 2 : $Perform\ PCA\ transformation.$ To perform PCA transformation, using the procedure described in section 2.5.1, the covariance matrix $\sum$ of $d_j(Y_{kj})$ is to be estimated. For each kth experiment, using eigenvectors $\vec{a_1}, \vec{a_2}, \ldots, \vec{a_m}$ and eigenvalues $\lambda_1 \geqq \lambda_2 \geqq \ldots \geqq \lambda_m \geqq 0$ which are derived from $\sum$, $d_1(Y_{k1}), \ldots, d_m(Y_{km})$

can be transformed into PCs $Z_{k1}, \ldots, Z_{km}$.

$$\begin{aligned}
Z_{k1} = \quad & \vec{a}_1^{\mathrm{T}} d(\vec{Y}_k) \quad & = a_{11}d_1(Y_{k1}) + a_{12}d_2(Y_{k2}) + \cdots + a_{1m}d_m(Y_{km}) \\
Z_{k2} = \quad & \vec{a}_2^{\mathrm{T}} d(\vec{Y}_k) \quad & = a_{21}d_1(Y_{k1}) + a_{22}d_2(Y_{k2}) + \cdots + a_{2m}d_m(Y_{km}) \\
\vdots \quad & \quad \vdots & \vdots \\
Z_{km} = \quad & \vec{a}_m^{\mathrm{T}} d(\vec{Y}_k) \quad & = a_{m1}d_1(Y_{k1}) + a_{m2}d_2(Y_{k2}) + \cdots + a_{mm}d_m(Y_{km})
\end{aligned} \tag{3.24}$$

Step 3 : *Compute the desirability index*. The PCA-based desirability index D_{PCA} is to be computed using equations 3.19 and 3.18 in section 3.2.

Step 4 : *Find the optimal combination of parameters*. Since D_{PCA} is monotone increasing in $d(\vec{Y})$, the value of D_{PCA} is to be maximized in the optimization.

Chapter 4

Desirability Approach and the Adjustment Factors for Correlated Responses

Apart from the principal component analysis (PCA) based desirability approach, there are still other possibilities for developing desirability approach such that the correlation information of desirability scores or performance measures are integrated, i.e., Wu's desirability approach [60] which has been described in section 2.4.3. The purpose of this chapter is to introduce an alternative for the PCA-based desirability approach which is more flexible than the PCA-based desirability approach and simpler than Wu's desirability approach.

4.1 The Weight Adjusted Desirability Approach

Due to the complication and the lack of flexibility of PCA-based desirability approach, in this section, a simpler and more flexible alternative which is called weight adjusted desirability approach will be introduced. The most essential ideal of the weight adjusted desirability approach is the implementation of weight adjustment factors which are used to multiply with the original weights, e.g., w_j in equation 2.15. Then, the product of the adjustment factor and the original weight will be used as the weight of desirability scores.

4.1.1 Adjustment Factors

The adjustment factors α are defined as coefficients which are used to adjust the original weights of the desirability scores. The values of α are derived based on the correlation coefficients of each desirability score. When the correlation of a pair of desirability scores d_i and d_j ($i \neq j$) are positive, their weights w_i and w_j should be reduced to avoid to bias optimization results. In an extreme case, such when there is a $d_i - d_j$ correlation that approaches 1, it is possible either to select a representative from one of them or reduce their weight by approximately half of the original weight. On the other hand, if the $d_i - d_j$ correlation approaches -1 which reflects a conflict between d_i and d_j, an improvement in d_i means generally a deterioration in the another; thus, neither d_i or d_j can be chosen as a representative for this case and their weights w_i and w_j should be either increased or maintained. Handling the negative correlations can be varied depending on the decision of engineer but it is obvious that the negative correlations should not be handled as the positive correlations.

Suppose that there are totally m ($m \geq 2$) performance measures in the optimization, the weight adjustment factor can be defined as:

$$\alpha_j = 1 - \frac{\eta}{m} \sum_{i=1, i \neq j}^{m} r_{ji} \tag{4.1}$$

where α_j denotes the adjustment factor for the jth desirability score, r_{ji} the correlation coefficient of the jth and the ith desirability scores (or performance measures), $\eta \in [0, \frac{m}{m-1})$ is the correlation effect factor. In order to prevent zero values of α_j, e.g., when all r_{ji} equal 1, the number of desirability scores m is chosen as the default denominator instead of $m - 1$. In practice, it is also possible to select $m - 1$ as the denominator. The value of η determines the effects of correlation coefficients on α_j

and a higher η allows correlation coefficients to have a stronger effects on α_j. The choice of $\eta = 0$ will give the same result as in the traditional desirability approach in which the information of correlations are ignored, whereas the choice of $\eta = 1$ will result the range of α_j in $[\frac{1}{m}, \frac{2m-1}{m}]$. The closer η to $\frac{m}{m-1}$ the stronger it effects α_j, but the value of η must be less than $\frac{m}{m-1}$ to prevent $\alpha_j \leq 0$.

Proof. If $\eta = 0$, then there is no adjustment by $\vec{\alpha}$. The value of $r_{ji} \in [-1, 1]$ is given by the definition of correlation coefficient, and it is clear that m is an integer, $m \geq 2$ and is finite. Then the following expressions are valid:

$$-(m-1) \leq \sum_{i=1, i\neq j}^{m} r_{ji} \leq m-1$$

$$\Leftrightarrow -\frac{1}{m}(m-1) \leq \frac{1}{m} \sum_{i=1, i\neq j}^{m} r_{ji} \leq \frac{1}{m}(m-1)$$

$$\Rightarrow \begin{cases} \frac{\eta}{m} \sum_{i=1, i\neq j}^{m} r_{ji} = 0 & \text{for} \quad \eta = 0 \\ -\frac{\eta(m-1)}{m} \leq \frac{\eta}{m} \sum_{i=1, i\neq j}^{m} r_{ji} \leq \frac{\eta(m-1)}{m} & \text{for} \quad \eta \in (0, \frac{m}{m-1}). \end{cases}$$

Recall that $m \geq 2$ and m is finite, then $0.5 \leq \frac{(m-1)}{m} < 1$

$$\Leftrightarrow \begin{cases} 1 - \frac{\eta}{m} \sum_{i=1, i\neq j}^{m} r_{ji} = 1 & \text{for} \quad \eta = 0 \\ 1 - \frac{\eta(m-1)}{m} \leq 1 - \frac{\eta}{m} \sum_{i=1, i\neq j}^{m} r_{ji} \leq 1 + \frac{\eta(m-1)}{m} & \text{for} \quad \eta \in (0, \frac{m}{m-1}) \end{cases} \tag{4.2}$$

So if $\eta = 0$, then $\forall j : \alpha_j = 1$ and $w_j * \alpha_j = w_j$, there is no adjustment. □

Proof. If $\eta = 1$, then $\alpha \in [\frac{1}{m}, \frac{2m-1}{m}]$. The proof follows from equation 4.2, for $\eta = 1$.

$$1 - \frac{m-1}{m} \leq 1 - \frac{\eta}{m} \sum_{i=1, i\neq j}^{m} r_{ji} \leq 1 + \frac{m-1}{m}$$

$$\Leftrightarrow \frac{1}{m} \leq \alpha_j \leq \frac{2m-1}{m}$$

□

Proof. A higher η results in a stronger effect on the weights. Suppose that there are η_1 and η_2 such that $0 < \eta_1 < \eta_2 < \frac{m}{m-1}$ with $\alpha_j|\eta_1$ and $\alpha_j|\eta_2$ which are defined as

$$\alpha_j|\eta_1 = 1 - \frac{\eta_1}{m} \sum_{i=1, i\neq j}^{m} r_{ji},$$

$$\alpha_j|\eta_2 = 1 - \frac{\eta_2}{m} \sum_{i=1, i\neq j}^{m} r_{ji}.$$

According to equation 4.2, the following expressions are derived.

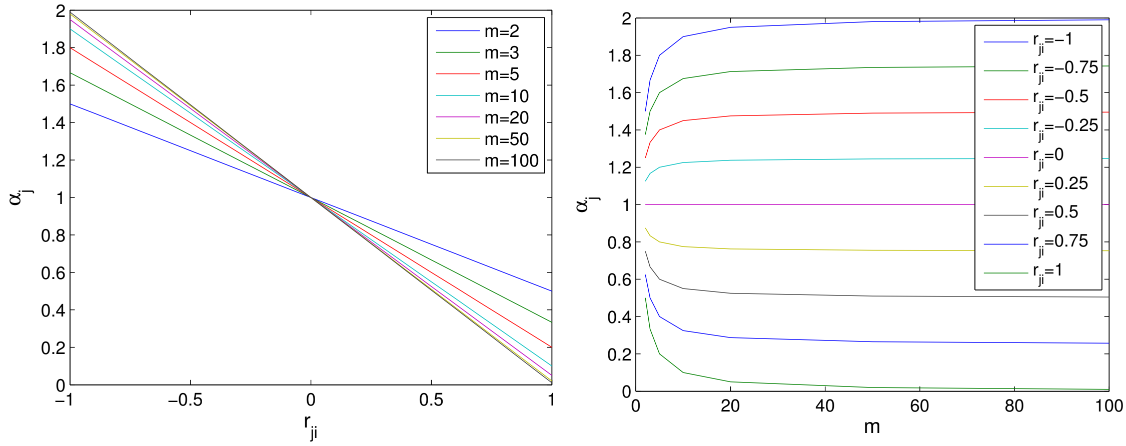
$$\begin{cases} 1 < 1 - \frac{\eta_1}{m} \sum_{i=1, i\neq j}^{m} r_{ji} < 1 - \frac{\eta_2}{m} \sum_{i=1, i\neq j}^{m} r_{ji} & \text{for} \quad \sum_{i=1, i\neq j}^{m} r_{ji} < 0 \\ 1 > 1 - \frac{\eta_1}{m} \sum_{i=1, i\neq j}^{m} r_{ji} > 1 - \frac{\eta_2}{m} \sum_{i=1, i\neq j}^{m} r_{ji} & \text{for} \quad \sum_{i=1, i\neq j}^{m} r_{ji} > 0 \\ 1 = 1 - \frac{\eta_1}{m} \sum_{i=1, i\neq j}^{m} r_{ji} = 1 - \frac{\eta_2}{m} \sum_{i=1, i\neq j}^{m} r_{ji} & \text{for} \quad \sum_{i=1, i\neq j}^{m} r_{ji} = 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} 1 < \alpha_j|\eta_1 < \alpha_j|\eta_2 & \text{for} \quad \sum_{i=1, i\neq j}^{m} r_{ji} < 0 \\ 1 > \alpha_j|\eta_1 > \alpha_j|\eta_2 & \text{for} \quad \sum_{i=1, i\neq j}^{m} r_{ji} > 0 \\ 1 = \alpha_j|\eta_1 = \alpha_j|\eta_2 & \text{for} \quad \sum_{i=1, i\neq j}^{m} r_{ji} = 0 \end{cases}$$

Therefore, $\alpha_j|\eta_2$ has stronger effects than $\alpha_j|\eta_1$ as long as $\sum_{i=1, i\neq j}^{m} r_{ji} \neq 0$. (Because the closer value of α_j to 1, the smaller is the adjustment and vice versa.) □

The weight adjusted desirability approach using α_j as defined in equation 4.1 is limited by the value $\alpha_j \in (0, 2)$ and that means the weight of each desirability score cannot be adjusted, e.g., twice or more than twice of its original weight, unless the formula of α_j would have been modified.

Example 4.1.1. *Now let's assume that $\forall i, j : r_{ji}$ are all equal to a constant. The relations of r_{ji} and m to α_j at $\eta = 1$ can be illustrated as figure 4.1. The effects of r_{ji} are clearly shown in figure 4.1b in that the value of α_j is smaller than 1 when r_{ji} are positive, and larger than 1 when r_{ji} are negative. The effect of m on α_j can be clearly observed in figure 4.1a since as the number of m becomes large the values of α_j change stronger with the values of r_{ji}. This also means that the value of η will* *play a less important role, if the number of m is large. It can be seen using equation 4.1 that m could have much larger scale than η which is divided by m; hence, small changes in η might be negligible for large m.*



(a) Plot of α_j versus r_{ji} (b) Plot of α_j versus m

Figure 4.1: The effects of r_{ji} and m on α_j at $\eta = 1$

Example 4.1.2. *Let's extend the example 4.1.1 by assuming that performance measures Y_1, Y_2, $\ldots$, Y_m are equally important with Y_1 at least linearly independent from Y_2, Y_3, $\ldots$, Y_m so that $\forall i$, $i \neq 1 : r_{1i} = 0$. The normalized weight W_j in traditional desirability approach can be illustrated in figure 4.2 in which the maximum value of $W_j = 0.5$ is given at $m = 2$. It is certain that the value of each W_j decreases as the number of m increases. In the weight adjusted desirability approach, each W_j is to be multiplied with α_j and their product ($W_j * \alpha_j$) must be re-normalized.*

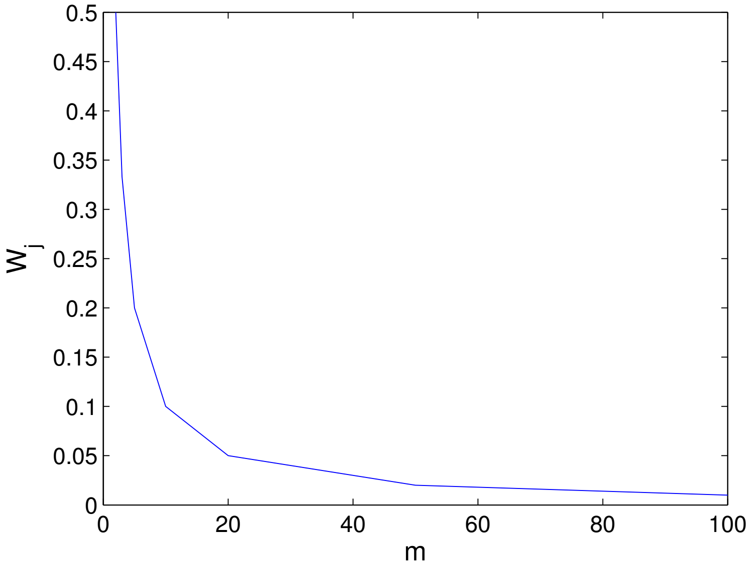
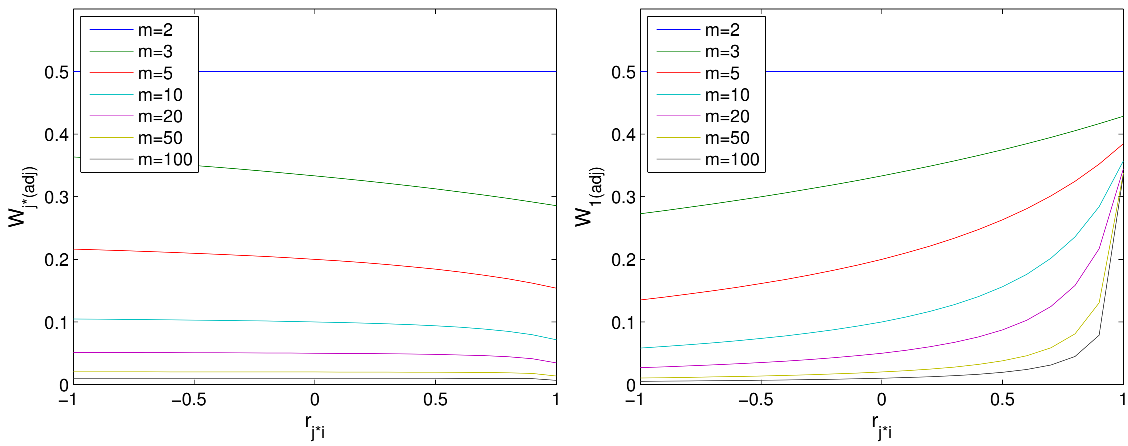


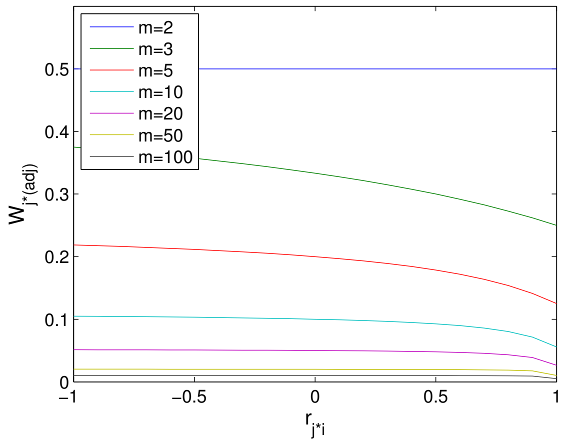
Figure 4.2: The normalized weight W_j in traditional desirability approach



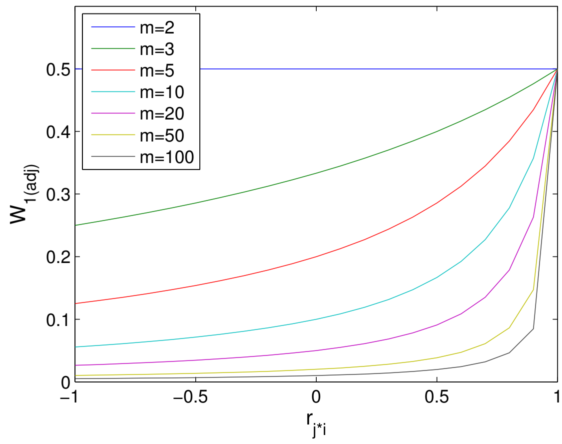
(a) Plot of $W_{j^*(\text{adj})}$ versus r_{j^*i}

(b) Plot of $W_{1(\text{adj})}$ versus r_{j^*i}

Figure 4.3: The plots of $W_{j^*(\text{adj})}$ and $W_{1(\text{adj})}$ versus r_{j^*i} at $\eta = 1$



(a) Plot of $W_{j^*(\text{adj})}$ versus r_{j^*i}



(b) Plot of $W_{1(\text{adj})}$ versus r_{j^*i}

Figure 4.4: The plots of $W_{j^*(\text{adj})}$ and $W_{1(\text{adj})}$ versus r_{j^*i} at $\eta = \frac{m}{m-1}$

In figures 4.3 and 4.4 the values of W_j according to r_{ji} and m are illustrated. The index j^* in figures 4.3a and 4.4a is defined as $j^* = 2, 3, \ldots, m$. The adjusted values of W_{j^*} ($W_{j^*(\text{adj})}$) in figures 4.3a and 4.4a may change not so significantly when r_{j^*i} are changed due to the reason that all W_{j^*} are adjusted in the same way at the same time, i.e., increased or decreased; thus, their proportional values remain nevertheless close to their original values, especially for large m. Only the weight of Y_1 which is multiplied with $\alpha_1 = 1$ remains identical to its initial value. As a result, the re-normalized adjusted weight of Y_1 ($W_{1(\text{adj})}$) is illustrated in figures 4.3b and 4.4b with $\eta = 1$ and $\eta = \frac{m}{m-1}$ correspondingly. It is shown that the effects from $\eta = \frac{m}{m-1}$ are stronger than from $\eta = 1$, and $\eta = \frac{m}{m-1}$ is applicable for this case because Y_1 is linearly independent (so $\forall j : \sum_{i=1,i\neq j}^{m}(r_{ji}) < \frac{m}{m-1} \Rightarrow \alpha_j > 0$). In an extreme case where $\forall j^* : r_{j*i} = 1$ ($i \neq j$ and $i \neq 1$) using $\eta = \frac{m}{m-1}$, the desirability score of Y_1 ($d_1(Y_1)$) would account totally 50 percent of the overall performance index. When $\eta = 1$ and $m = 3$, $d_1(Y_1)$ could account up to 42.86 percent in total.

Additionally, the formula of α_j in equation 4.1 can be varied according to the expert's preferences, e.g., replace r_{ji} with the partial correlation or the semi-partial correlation. For another example, if the negative correlations are to be neglected, then the equation 4.1 can be modified as

$$\alpha_j = 1 - \frac{\eta}{m} \sum_{i=1, i \neq j}^{m} r_{ji} \mathbb{1}_{[0,1]}(r_{ji}) \tag{4.3}$$

where $\mathbb{1}_{[0,1]}(r_{ji})$ is indicator function which is defined in equation 3.15.

4.1.2 Weight Adjusted Desirability Index

The weight adjusted desirability index (DI) is defined based on the formula of DIs that are introduced in section 2.4.2. The weight adjusted geometric mean of DFs ($D_{\mathrm{g(adj)}}$) is defined as:

$$D_{\mathrm{g(adj)}} = \left[\prod_{j=1}^{m} d_j^{\alpha_j w_j} \right]^{\frac{1}{\sum_{j=1}^{m} \alpha_j w_j}}, \tag{4.4}$$

and the weight adjusted arithmetic mean of DFs ($D_{\mathrm{a(adj)}}$) as:

$$D_{\mathrm{a(adj)}} = \frac{1}{\sum_{j=1}^{m} \alpha_j w_j} \sum_{j=1}^{m} \alpha_j w_j d_j \tag{4.5}$$

with w_j the weight of the jth performance measure as defined in section 2.4.2.

The advantage of using the weight adjusted DI over the traditional DI is that correlations information can be taken into account. Compare to the PCA-based desirability approach, the weight adjusted approach has much less computational steps and simpler formulas. It also has a better flexibility, i.e., it is able to handle correlated performance measures which are not equally important and also feasible when negative correlations are to be ignored by using α as defined in equation 4.3. Additionally, since correlation matrix is utilized in place of covariance matrix, weight adjusted DIs are not variance biased.

Due to the limitation of the Pearson's correlation coefficient which is a pairwise relationship and the inexistence of a negative multiple correlation coefficient, multiple correlation coefficients cannot be integrated into α and DI. As a possible consequence, if the number of m becomes so large, the adjusted weights can be biased due to the large number of multiple correlations that are included in Pearson's correlation coefficients, or are ignored when (semi-)partial correlation coefficients are used.

4.1.2.1 Weight Adjusted Desirability Index using Pearson's Correlation Coefficients

The Pearson correlation coefficient is one of the most common correlation coefficients used in statistics. It is defined as a number in [-1,1] used to measure the degree of association between 2 variables. A large magnitude of the number implies a strong association and a number close to zero implies a weak association. If 2 variables are independent, then their correlation coefficient is zero, but the converse is not valid. The Pearson correlation coefficient of desirability scores can be written as:

$$r_{j,i} = \frac{\sum_{k=1}^{n}(d_{kj})(d_{ki})}{(n-1)s_{d_j}s_{d_i}} \tag{4.6}$$

where r_{ji} denotes the Pearson correlation coefficient between the jth and the ith desirability scores, computed from the all n sample data.

One of the most conventional ways to describe correlations is to illustrate them using Venn diagrams. For any a pair of desirability scores which are linearly uncorrelated, the illustration in a Venn diagram can be obtained as figure 4.5, and for a pair desirability scores which are correlated as figure 4.6.

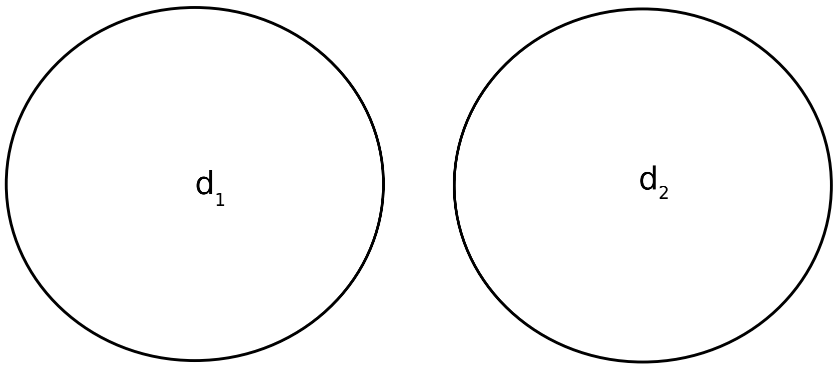


Figure 4.5: The Venn diagram of 2 uncorrelated desirability scores

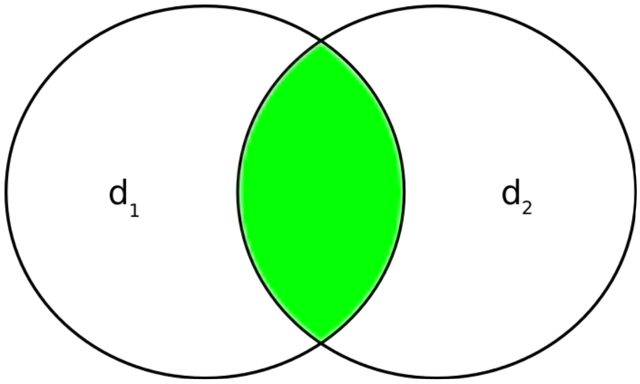


Figure 4.6: The Venn diagram of 2 correlated desirability scores

The green region in figure 4.6 represents the association level between d_1 and d_2. In case that there are more than 3 correlated desirability scores in the optimization, then there might be a presence of a multiple correlation. The Venn diagram of 3 correlated desirability scores and 4 correlated desirability scores are illustrated in figure 4.7 and 4.8 respectively.

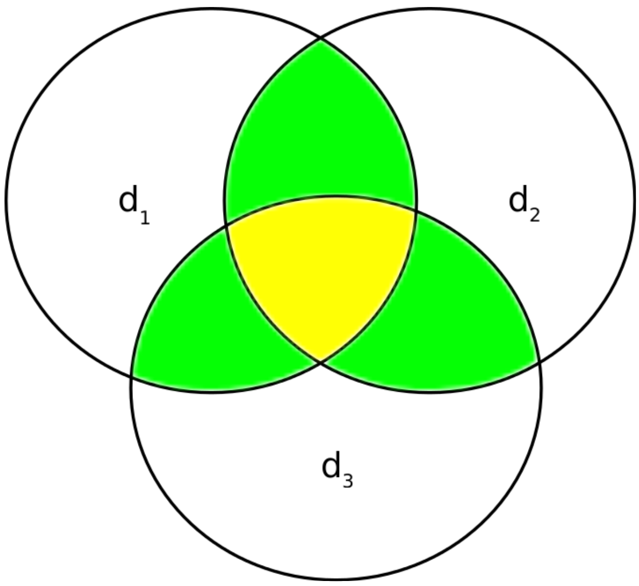


Figure 4.7: The Venn diagram of 3 correlated desirability scores

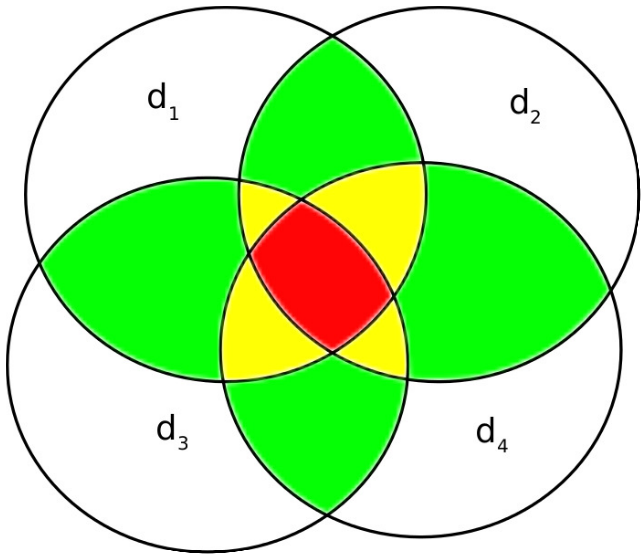


Figure 4.8: The Venn diagram of 4 correlated desirability scores

The yellow areas in figure 4.7 and 4.8 stand for the multiple correlation of 3 desirability scores, and the red area in figure 4.8 stands for the multiple correlation of 4 desirability scores. It has been illustrated through these diagrams that as the number of desirability scores raises, the number of their multiple correlations will raise exponentially. Let m be the number of optimization objectives (desirability scores), then the number of pairwise correlation coefficients $n(r)$ and multiple correlation coefficients $n(R^2)$ can be computed using the following formula:

$$n(r) = \frac{m!}{(m-2)!2!} \qquad \text{with} \quad m \geq 2 \tag{4.7}$$

$$n(R^2) = \sum_{j=3}^{m} \frac{m!}{(m-j)!j!} \qquad \text{with} \quad m \geq 3 \tag{4.8}$$

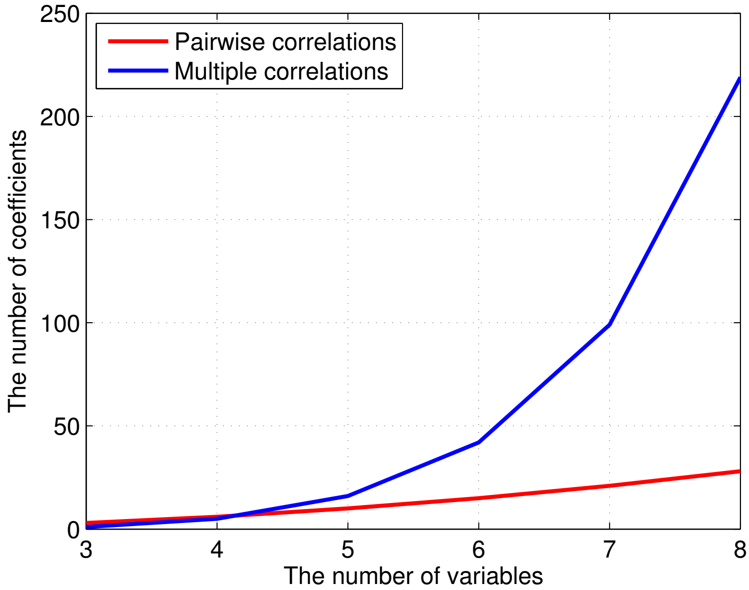


Figure 4.9: The number of correlation coefficients and multiple correlation coefficients

Figure 4.9 illustrates the number of correlation coefficients and multiple correlation coefficients when the number of desirability scores raises. If the number of desirability scores is equal or greater than 5, then the number of multiple correlation coefficients becomes greater than the number of correlation coefficients. Hence, the weight adjusted approach is suitable specifically for optimization problems with a small number of objectives or variables, e.g., less than 5.

4.1.2.2 Weight Adjusted Desirability Index using Partial Correlation Coefficients

The partial correlation is a measure which determines the degree of association of 2 variables when the effect of the other variables are removed. Suppose that there are in total m ($m \geq 3$) performance measures in the optimization and the set of indices $M = \{1, \ldots, m\} \setminus \{j, i\}$, the formula of the partial correlation coefficient can be computed using the recursive formula of Yule and Kendall [61]:

$$r_{ji.M} = \frac{r_{ji.M\backslash\{m_0\}} - r_{jm_0.M\backslash\{m_0\}} r_{m_0 i.M\backslash\{m_0\}}}{\sqrt{1 - r^2_{jm_0.M\backslash\{m_0\}}}\sqrt{1 - r^2_{m_0 i.M\backslash\{m_0\}}}} \tag{4.9}$$

with $m_0 \in M$.

The Venn diagram of partial correlation, e.g., $r_{13.2}$ can be illustrated as in figure 4.10 in which the effects of d_2 are removed from the coefficient r_{ji}. By using only $r_{12.3}$, $r_{13.2}$ and $r_{23.1}$ in the computation of weight adjusted DI, it is clear that the multiple correlation of d_1, d_2 and d_3 will be excluded as it is illustrated in figure 4.11.

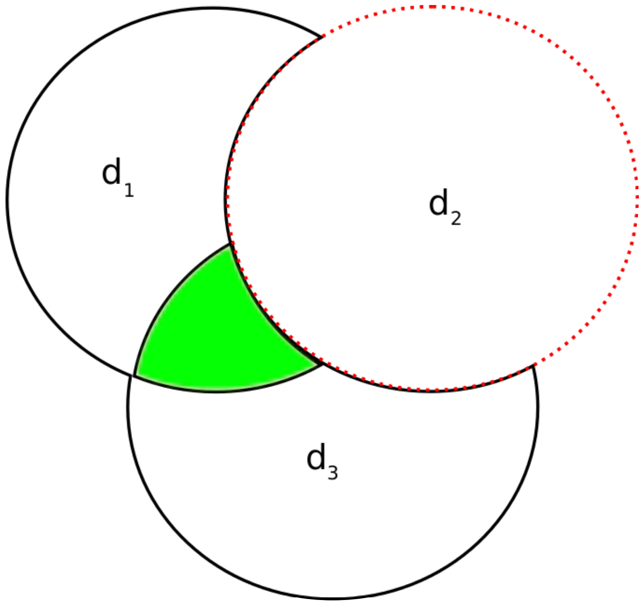


Figure 4.10: The Venn diagram of partial correlation $r_{13.2}$

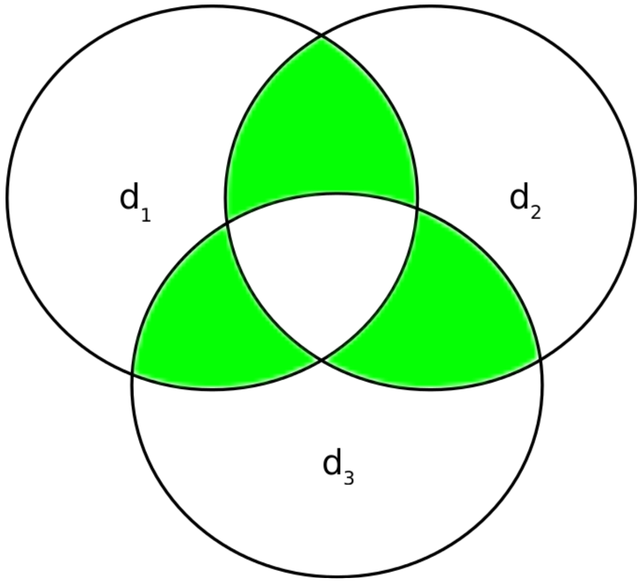


Figure 4.11: The Venn diagram of partial correlations utilized for 3 correlated desirability scores

The advantages of using the (semi-)partial correlations would decline rapidly when the number of desirability scores become so large, not only biases from ignoring multiple correlations can result but also the number of iterations required for computing correlation coefficients raise rapidly.

As an alternative, semi-partial correlation coefficients which are scaled relative to their variances, can be used in place of the partial correlation coefficients. Nevertheless, the bias of ignoring multiple correlations still cannot be avoided.

Chapter 5

Case Study: Multi-objective Optimization of Hard Turning of AISI 6150 Steel

The purpose of this section is to demonstrate the proposed optimization methods as well as their advantages and disadvantages. The results obtained from the proposed methods will be compared with the results from the original desirability approach. For case studies in this chapter, instead of performing experiments, the empirical models developed by Sieben et al. [41] are used due to the limitation of the number of the experiment data. Their experiments were carried out on a Monforts RNC 602 CNC lathe, and the material and properties of the cutting tool which are used, are summarized in table 5.1. The dry turning operation was performed using CNGA-120408 polycrystalline cubic boron nitride (PCBN) tools, where the AISI 6150 heat-treatable steel workpieces turned have an initial diameter of 150 mm with a length of 500 mm. An experiment design of 15 parameter combinations which created from a latin hypercube design was used, in which parameters feed, depth of cut, and cutting speed are involved. Cutting tools were utilized until the width of flank wear of 100 μm was reached.

Table 5.1: Workpiece and properties of cutting tool used by [41]

Workpiece material	AISI 6150 heat-treatable steel
Workpiece diameter	150 mm
Workpiece length	500 mm
Surface hardness of material	62 ± 2 HRc
Cutting tool insert	CNGA 120408
Cutting tool material	Polycrystalline Cubic Boron Nitride

5.1 Optimization Problem

The cutting parameters controlled are feed f, depth of cut a_p, and cutting speed v_c which are shown in table 5.2.

Table 5.2: Cutting parameters used in simulation.

Parameter	Notation	Unit	Values
Feed	f	mm	0.05, 0.06, . . . , 0.15, 0.16
Depth of cut	a_p	mm	0.05, 0.06, . . . , 0.39, 0.4
Cutting speed	v_c	m/min	100,101, . . . , 199, 200

The selection of the optimization objectives is an important process which determines the success in optimization. If the number of responses selected becomes too large, the trade-off among objectives can become very complicated. On the other hand, if the number of objectives is too small, some important characteristics of the turning process might be missing. In this study, the following 3 performance measures are selected as the optimization objectives:

1. The passive force F_p [N]

2. The width of flank wear land on the minor cutting edge VB_m [µm]

3. The cutting time t [s]

The passive force F_p is a measure which is used to determine the mechanical load of the tool-workpiece contact interface. A high F_p is known as a cause for poor surface finish, dynamic instability, high mechanical loads, thermal loads and tool wears. The width of flank wear on minor cutting edges VB_m affects the quality of finished surface, the production costs and lead time, as the cutting tool is required to be changed after a certain tool wear has been generated. The last performance measure, t, is an important measure of productivity where a lower value means a higher productivity. In addition, F_p, VB_m and t are assumed to be equally important.

The quality of surface finish is controlled through the constraint of average depth of roughness Rz that

$$Rz_{95} \leq 3 \quad \mu\mathrm{m}, \tag{5.1}$$

where Rz_{95} denotes the 95th percentile of Rz.

In order to have an optimization model which resembles a real turning process, a constant volume of material removal of 20,000 mm^3 is selected. This is due to the fact that in turning, a certain volume of material removal would be required in order to produce a finished product. On the other hand, if this volume is not fixed as a constant, a biased optimization result could be obtained, since a small tool wear might be generated from a small volume of material removal, e.g., by decreasing depth of cut and feed when the cutting path length is constant, or decreasing cutting speed when the processing time is constant. The optimization of this turning operation is to find the best combination of f, a_p and v_c which minimize F_p, VB_m and t, while satisfying the surface roughness constraint.

5.2 Deterministic Optimization

The deterministic model which has no error terms for F_p, VB_m and t will be used to demonstrate the procedure for the principal component analysis-based desirability index (PCA-based DI). In the deterministic model, the mathematical models for F_p, VB_m, t and Rz are defined as

$$F_\mathrm{p} = \hat{f}_1(f, a_\mathrm{p}, v_\mathrm{c}) \tag{5.2}$$

$$VB_\mathrm{m} = \mathrm{e}^{\hat{f}_2(f, a_\mathrm{p}, v_\mathrm{c})} \tag{5.3}$$

$$t = \mathrm{e}^{\hat{f}_3(f, a_\mathrm{p}, v_\mathrm{c})} \tag{5.4}$$

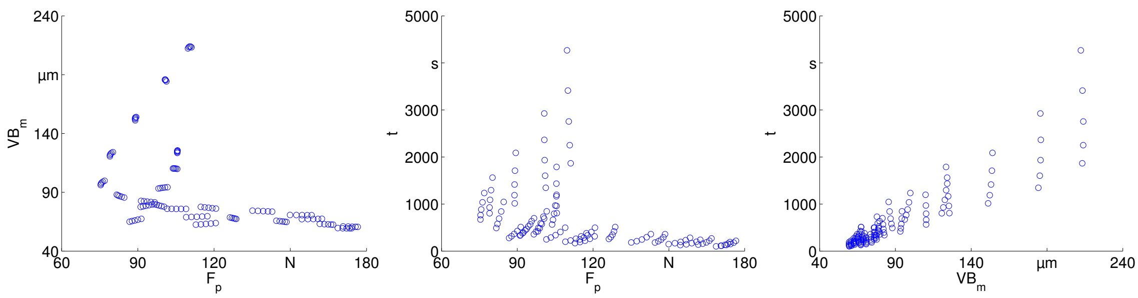
$$Rz = \mathrm{e}^{(\hat{f}_4(f, a_\mathrm{p}, v_\mathrm{c}) + \epsilon_{Rz})} \tag{5.5}$$

where $\hat{f}_1$, $\hat{f}_2$, $\hat{f}_3$ and $\hat{f}_4$ are functions used to predict the values of F_p, VB_m, t and Rz respectively, ϵ_{Rz} is a stochastic error term which is normally distributed and has mean zero. The mathematical models of VB_m, t and Rz utilized the exponential form because $\hat{f}_2$, $\hat{f}_3$ and $\hat{f}_4$ are calculated from a logarithmic scale, in order to obtain a more accurate predictor while avoiding a negative value of the predicted responses. These empirical models are constructed based on a toolbox in MATLAB, Design and analysis of computer experiments (DACE) [28], and are provided by Dipl.-Inf. Wagner who is one of the authors in [41]. The values of $\hat{f}_1$, $\hat{f}_2$, $\hat{f}_3$ and $\hat{f}_4$ can be generated using the predictor function which is featured in [28].

5.2.1 Optimization using Global Correlations

Before the PCA-based desirability approach can be performed, the correlation of F_p, VB_m and t as well as their correlations in desirability scale should be firstly investigated, in case that their correlations are not so strong or they are uncorrelated, there would be no necessity for performing PCA transformation or using PCA-based DI. In order to obtain a non-biased correlation information of F_p, VB_m and t, a full factorial experimental design with 3 factors and 5 levels is used to generate the simulation data of F_p, VB_m and t from the empirical models, so that a uniform coverage of the parameter space can be achieved. Due to the reason that the data used in this case study are generated from empirical models, the number of factor levels can be selected as high as 5 to ensure that the number of data is significant for estimating the correlation information. In real experiments, the number of data can be very limited.

Table 5.3 illustrates the 5^3 full factorial experimental design which has been explained. The lth level of f, a_p and v_c are denoted as f_l, $a_{\mathrm{p}l}$ and $v_{\mathrm{c}l}$, e.g., f_1, $a_{\mathrm{p}1}$ and $v_{\mathrm{c}1}$ for the 1st level. The last 3 columns contain the values of F_p, VB_m and t at each kth trial, e.g., $F_{\mathrm{p}125}$, $VB_{\mathrm{m}125}$ and t_{125} for the 125th trial.



(a) $r_{(F_\mathrm{p},VB_\mathrm{m})}$ = -0.4292 (b) $r_{(F_\mathrm{p},t)}$ = -0.4143 (c) $r_{(VB_\mathrm{m},t)}$ = 0.9190

Figure 5.1: Scatter plots of performance measures

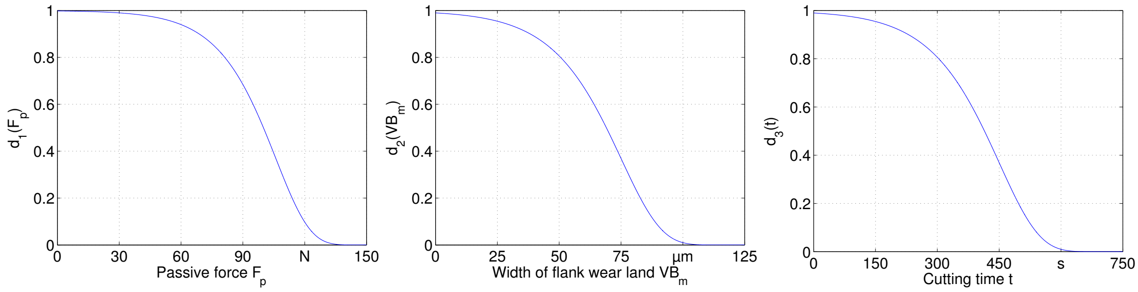
Using the predictor of [28], the values of $F_{\mathrm{p}k}$, $VB_{\mathrm{m}k}$ and t_k are generated as listed in table 5.3 and their correlations are illustrated as the scatter plots in figure 5.1. The correlation coefficients are displayed below the figures of the scatter plots. The correlations between F_p and VB_m ($r_{(F_\mathrm{p},VB_\mathrm{m})}$) and between F_p and t ($r_{(F_\mathrm{p},t)}$) are found to be moderately negative, while the correlation between VB_m and t ($r_{(VB_\mathrm{m},t)}$) is found to be strongly positive. Unexpectedly, $r_{(F_\mathrm{p},VB_\mathrm{m})}$ is found to be negative which contradicts to the correlations found in [9, 41, 62] that are shown to be positive. The possible causes are as following: First, most of the relationship between specific performance

Table 5.3: 5^3 full factorial experimental design

Trial	Cutting parameters			Performance measures		
	f	a_{p}	v_{c}	F_{p}	VB_{m}	t
1	f_1	$a_{\mathrm{p}1}$	$v_{\mathrm{c}1}$	$F_{\mathrm{p}1}$	$VB_{\mathrm{m}1}$	t_1
2	f_1	$a_{\mathrm{p}1}$	$v_{\mathrm{c}2}$	$F_{\mathrm{p}2}$	$VB_{\mathrm{m}2}$	t_2
3	f_1	$a_{\mathrm{p}1}$	$v_{\mathrm{c}3}$	$F_{\mathrm{p}3}$	$VB_{\mathrm{m}3}$	t_3
4	f_1	$a_{\mathrm{p}1}$	$v_{\mathrm{c}4}$	$F_{\mathrm{p}4}$	$VB_{\mathrm{m}4}$	t_4
5	f_1	$a_{\mathrm{p}1}$	$v_{\mathrm{c}5}$	$F_{\mathrm{p}5}$	$VB_{\mathrm{m}5}$	t_5
6	f_1	$a_{\mathrm{p}2}$	$v_{\mathrm{c}1}$	$F_{\mathrm{p}6}$	$VB_{\mathrm{m}6}$	t_6
7	f_1	$a_{\mathrm{p}2}$	$v_{\mathrm{c}2}$	$F_{\mathrm{p}7}$	$VB_{\mathrm{m}7}$	t_7
8	f_1	$a_{\mathrm{p}2}$	$v_{\mathrm{c}3}$	$F_{\mathrm{p}8}$	$VB_{\mathrm{m}8}$	t_8
9	f_1	$a_{\mathrm{p}2}$	$v_{\mathrm{c}4}$	$F_{\mathrm{p}9}$	$VB_{\mathrm{m}9}$	t_9
10	f_1	$a_{\mathrm{p}2}$	$v_{\mathrm{c}5}$	$F_{\mathrm{p}10}$	$VB_{\mathrm{m}10}$	t_{10}
11	f_1	$a_{\mathrm{p}3}$	$v_{\mathrm{c}1}$	$F_{\mathrm{p}11}$	$VB_{\mathrm{m}11}$	t_{11}
12	f_1	$a_{\mathrm{p}3}$	$v_{\mathrm{c}2}$	$F_{\mathrm{p}12}$	$VB_{\mathrm{m}12}$	t_{12}
13	f_1	$a_{\mathrm{p}3}$	$v_{\mathrm{c}3}$	$F_{\mathrm{p}13}$	$VB_{\mathrm{m}13}$	t_{13}
14	f_1	$a_{\mathrm{p}3}$	$v_{\mathrm{c}4}$	$F_{\mathrm{p}14}$	$VB_{\mathrm{m}14}$	t_{14}
15	f_1	$a_{\mathrm{p}3}$	$v_{\mathrm{c}5}$	$F_{\mathrm{p}15}$	$VB_{\mathrm{m}15}$	t_{15}
16	f_1	$a_{\mathrm{p}4}$	$v_{\mathrm{c}1}$	$F_{\mathrm{p}16}$	$VB_{\mathrm{m}16}$	t_{16}
17	f_1	$a_{\mathrm{p}4}$	$v_{\mathrm{c}2}$	$F_{\mathrm{p}17}$	$VB_{\mathrm{m}17}$	t_{17}
18	f_1	$a_{\mathrm{p}4}$	$v_{\mathrm{c}3}$	$F_{\mathrm{p}18}$	$VB_{\mathrm{m}18}$	t_{18}
19	f_1	$a_{\mathrm{p}4}$	$v_{\mathrm{c}4}$	$F_{\mathrm{p}19}$	$VB_{\mathrm{m}19}$	t_{19}
20	f_1	$a_{\mathrm{p}4}$	$v_{\mathrm{c}5}$	$F_{\mathrm{p}20}$	$VB_{\mathrm{m}20}$	t_{20}
21	f_1	$a_{\mathrm{p}5}$	$v_{\mathrm{c}1}$	$F_{\mathrm{p}21}$	$VB_{\mathrm{m}21}$	t_{21}
22	f_1	$a_{\mathrm{p}5}$	$v_{\mathrm{c}2}$	$F_{\mathrm{p}22}$	$VB_{\mathrm{m}22}$	t_{22}
23	f_1	$a_{\mathrm{p}5}$	$v_{\mathrm{c}3}$	$F_{\mathrm{p}23}$	$VB_{\mathrm{m}23}$	t_{23}
24	f_1	$a_{\mathrm{p}5}$	$v_{\mathrm{c}4}$	$F_{\mathrm{p}24}$	$VB_{\mathrm{m}24}$	t_{24}
25	f_1	$a_{\mathrm{p}5}$	$v_{\mathrm{c}5}$	$F_{\mathrm{p}25}$	$VB_{\mathrm{m}25}$	t_{25}
26	f_2	$a_{\mathrm{p}1}$	$v_{\mathrm{c}1}$	$F_{\mathrm{p}26}$	$VB_{\mathrm{m}26}$	t_{26}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
125	f_5	$a_{\mathrm{p}5}$	$v_{\mathrm{c}5}$	$F_{\mathrm{p}125}$	$VB_{\mathrm{m}125}$	t_{125}

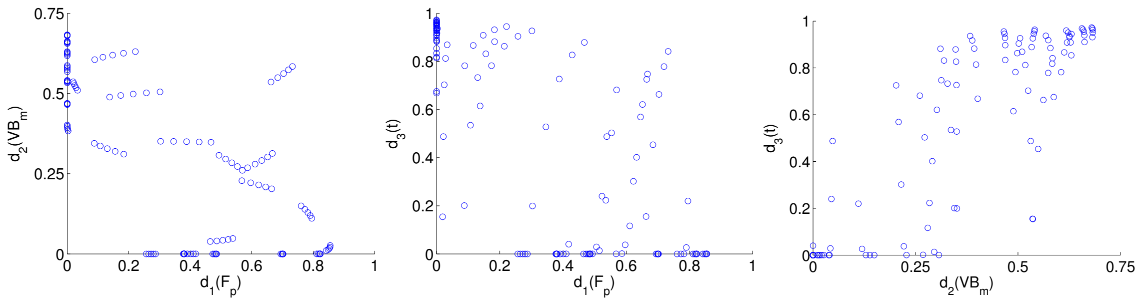
measures are analyzed from experiments in which operating parameters are constants [9, 62] or vary by one parameter at a time, but the correlations shown in figure 5.1 are determined from a factorial experimental design in which various combinations of operating parameters are involved so that effects of cutting parameters may dominate the mechanical dependency between performance measures. Second, the performance measures are interpolated for the operation with a fixed volume of material removal which is different from the studies of [9, 41, 62]. Third, in this case study, VB_{m} is defined as the width of flank wear land on the minor cutting edge which differs from the flank wear found on the major cutting edge VB_{c}; thus, the correlation between F_{p} and VB_{m} may not be comparable to F_{p} and VB_{c} which analyzed by [9, 62]. For this case study, the negative $F_{\mathrm{p}} - VB_{\mathrm{m}}$ correlation is a result of the variations of cutting parameters. An increase in a_{p} or f increases F_{p} and simultaneously decreases VB_{m} while an increase in v_{c} decreases F_{p} slightly and simultaneously increases VB_{m}. In figure 5.1a, there is also a subpattern of $r_{(F_{\mathrm{p}}, VB_{\mathrm{m}})}$ which indicates their positive relationship and is the interference factor for the negative correlation of F_{p} and VB_{c}. This subpattern is confirmed to result from the parameter combinations with small f and a_{p}, especially, those with $a_{\mathrm{p}} \leq 0.15$ mm, because a_{p} has a larger scale than f and parameters with small f and a_{p} would necessitate a long cutting path length. Consequently, VB_{m} increases steeply and appears as the subpattern found in figure 5.1a. The negative $F_{\mathrm{p}} - t$ correlation in figure 5.1b can be explained as follows: increase in f or a_{p} would increase F_{p} due to the larger tool-chip contact surface whereas t becomes shorter due to the higher rate of material removal. However, there is also a subpattern which contradicts the negative correlation of F_{p} and t. This subpattern represents the values of F_{p} and t which are generated from cutting parameters that contain small f, a_{p} and v_{c}. Since t is depending on the material removal rate (MRR), then it is also depending on f, a_{p} and v_{c}, and therefore, t is large for small f, a_{p} and v_{c}. The strong positive $VB_{\mathrm{m}} - t$ correlation can be simply explained by the shorter cutting path length and t trend to produce less VB_{m} which can be achieved by increasing either f or a_p. In addition, the scatter plots in figure 5.1 show significant nonlinear relationships between $F_\mathrm{p} - VB_\mathrm{m}$ and $VB_\mathrm{m} - t$ in the selected parameter range, using correlation coefficients can potentially lead to inaccurate results.

As F_p, VB_m and t are measures which have one-sided specification, the one-sided Harrington's desirability function (DF) is applied to transform these performance measures into the desirability scores $d_1(F_\mathrm{p}), d_2(VB_\mathrm{m})$ and $d_3(t)$. By minimizing F_p, the dynamic stability of the turning operation as well as the surface finish of the product can be enhanced. However, F_p will not cause process instability before a specific threshold is exceeded; hence, F_p will not be strictly minimized ($d_1^{(2)}$=0.5) and any F_p value which is lower than 30 N is assumed to provide no performance improvement ($d_1^{(1)}$=0.99). The values VB_m of 100 µm or above are considered as tool failure [41] ($d_2^{(2)}$=0.01) and the value t of 600 s or above is selected as totally undesirable processing time ($d_3^{(2)}$=0.01); thus, they are to be strictly minimized. According to the preferences, the configurations for Harrington's functions can be defined as following:
$(F_\mathrm{p}^{(1)}, d_1^{(1)})$ =(30, 0.99), $(F_\mathrm{p}^{(2)}, d_1^{(2)})$=(100,0.5),
$(VB_\mathrm{m}^{(1)}, d_2^{(1)})$=(0, 0.99), $(VB_\mathrm{m}^{(2)}, d_2^{(2)})$=(100,0.01) and
$(t^{(1)}, d_3^{(1)})$ =(0, 0.99), $(t^{(2)}, d_3^{(2)})$=(600,0.01),
where $d_j^{(1)}$ denotes the desirability score of the jth performance measure for the first linear equation and $d_j^{(2)}$ for the second linear equation as defined in equation 2.10. After the constants b_{0j} and b_{1j} in equation 2.10 have been solved from the two linear equations, $d_1(F_\mathrm{p}), d_2(VB_\mathrm{m})$ and $d_3(t)$ can be obtained by using equation 2.9. The configured Harrington's one-sided DFs for F_p, VB_m and t can be illustrated as in figure 5.2 and the correlations of desirability scores are illustrated in figure 5.3.



(a) $d_1(F_\mathrm{p})$ (b) $d_2(VB_\mathrm{m})$ (c) $d_3(t)$

Figure 5.2: Configured Harrington's one-sided DFs



(a) $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ = -0.6972 (b) $r_{(d_1(F_\mathrm{p}),d_3(t))}$ = -0.7164 (c) $r_{(d_2(VB_\mathrm{m}),d_3(t))}$ = 0.8846

Figure 5.3: Scatter plots of the desirability scores

After F_p, VB_m and t are converted into $d_1(F_\mathrm{p})$, $d_2(VB_\mathrm{m})$ and $d_3(t)$, changes in their correlation pattern are found. The correlations between $d_1(F_\mathrm{p})$ and $d_2(VB_\mathrm{m})$ ($r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$) and between $d_1(F_\mathrm{p})$ and $d_3(t)$ ($r_{(d_1(F_\mathrm{p}),d_3(t))}$) are found to become stronger after the transformation with DFs. In this case, the zero values of $d_1(F_\mathrm{p})$, $d_2(VB_\mathrm{m})$ and $d_3(t)$ shown in figure 5.3a and 5.3b strengthen the correlations $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ and $r_{(d_1(F_\mathrm{p}),d_3(t))}$. This means that the range of cutting parameters shown in table 5.2 could be too large for this optimization problem. In order to redefine the range of cutting parameters, we might further investigate on the favorable range of each parameter. Note that the traditional desirability approach can be performed without being effected by these correlations, and additionally, it would be interesting to compare the results obtained from PCA-based DI with different covariance matrices.

As it is recommended by [16], the principal component analysis (PCA) transformation should not be performed directly on F_{p}, VB_{m} and t in their original scales, because these measures hold different scales and units. Consequently, the direct PCA transformation from F_{p}, VB_{m} and t would lead to a bias toward t which has the highest numerical value.

The PCA transformation is then performed on $d_1(F_{\mathrm{p}})$, $d_2(VB_{\mathrm{m}})$ and $d_3(t)$, as the procedure described in section 3.3. For the transformation, eigenvalues and eigenvalues are to be derived from the covariance matrix of $d_1(F_{\mathrm{p}})$, $d_2(VB_{\mathrm{m}})$ and $d_3(t)$ which is shown in table 5.4. The Eigenvectors, eigenvalues, and normalized weights W which are necessary for computing PCA-based DI are shown in table 5.5.

Table 5.4: Covariance of the desirability scores

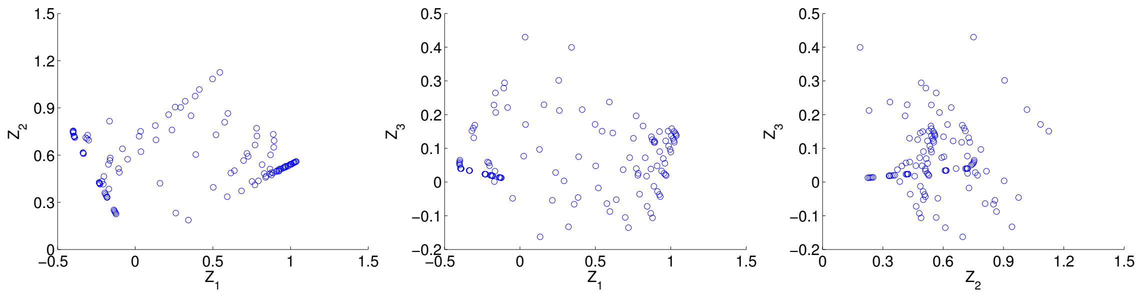
Variable	$d_1(F_{\mathrm{p}})$	$d_2(VB_{\mathrm{m}})$	$d_3(t)$
$d_1(F_{\mathrm{p}})$	0.0894	-0.0518	-0.0881
$d_2(VB_{\mathrm{m}})$	-0.0518	0.0618	0.0905
$d_3(t)$	-0.0881	0.0905	0.1692

Table 5.5: Eigenvectors, eigenvalues, and normalized weights of PCs

	1st PC	2nd PC	3rd PC
Eigenvector	$\begin{bmatrix} -0.4793 \\ 0.4367 \\ 0.7613 \end{bmatrix}$	$\begin{bmatrix} 0.8763 \\ 0.1898 \\ 0.4429 \end{bmatrix}$	$\begin{bmatrix} 0.0489 \\ 0.8794 \\ -0.4736 \end{bmatrix}$
Eigenvalue	0.2765	0.0336	0.0102
W_j	0.8631	0.1050	0.0319

Using equation 3.24, the uncorrelated principal components (PCs) are obtained from the transformation. According to the types of PCs defined in section 3.1, the 1st PC and the 3rd PC which account almost 90 percent of W, are classified as the third type PCs. On the other hand, the 2nd PC which is classified as the first type has a much smaller W than the first PC and that means much less influence on the optimization. It has been shown in this case that the third type PCs play the major role in this optimization problem, since they account for the largest proportion of W. The lack of monotonicity of overall performance indices in Taguchi method may cause misinterpretation of the third type PCs and lead to the erroneous optimization results.

In figure 5.4, the matrix of PCs Z_{k1}, Z_{k2} and Z_{k3} is illustrated to confirm their correlation. Their correlation coefficients are found approximately zero which shows PCA transformation is correctly and successfully performed. From figure 5.4, it can be observed that each PC has a different scale, i.e., Z_1 range between -0.5 and 1.1, Z_2 range between 0.2 and 1.2, and Z_3 range between -0.2 and 0.45, and it is obvious that their values are no longer on the desirability scale.



(a) $r_{(Z_1,Z_2)} = 0.0000$ (b) $r_{(Z_1,Z_3)} = 0.0000$ (c) $r_{(Z_2,Z_3)} = 0.0000$

Figure 5.4: Correlation matrix of PCs

Using equation 3.18 in section 3.2, Z_{k1}, Z_{k2} and Z_{k3} are transformed into the PC scores N_{k1}, N_{k2} and N_{k3}, and the PCA-based DI can be calculated by combining N_{k1},

N_{k2} and N_{k3}. For the turning process, the values of f and a_p are usually rounded to 2 decimal places and v_c is rounded to integer, because they are limited by the machine-precision numbers and in fact, parameters with many decimal places are not used in practice. For this case study, the value of PCA-based DI (D_PCA) can be calculated for every combination of cutting parameters.

The best ten parameter combinations are listed and sorted descendingly according to the value of D_PCA in table 5.6. It can be clearly observed that all of them share a similar favorable range such that f = 0.06-0.09 mm, a_p = 0.23-0.027 mm and v_c = 195-200 m/min, and the combinations with a higher v_c can outperforms the combinations with a lower v_c, e.g. the combination f = 0.07 mm, a_p = 0.25 mm and v_c = 200 m/min (0.07,0.25,200) outperform the combinations (0.07,0.25,199) and (0.07,0.25,198) in terms of D_PCA.

Table 5.6: Best ten cutting parameters evaluated by PCA-based DI

f	a_p	v_c	F_p	VB_m	t	$d_1(F_\mathrm{p})$	$d_2(VB_\mathrm{m})$	$d_3(t)$	D_PCA
0.07	0.25	200	89.3172	82.2197	337.0605	0.6954	0.2124	0.7304	0.6170
0.07	0.25	199	89.3592	82.2033	338.9506	0.6948	0.2128	0.7260	0.6153
0.07	0.26	200	90.9546	81.6625	324.7461	0.6696	0.2238	0.7581	0.6152
0.07	0.26	199	90.9989	81.6456	326.5507	0.6689	0.2241	0.7542	0.6137
0.07	0.25	198	89.4015	82.1868	340.8635	0.6941	0.2131	0.7214	0.6136
0.07	0.26	198	91.0434	81.6287	328.3771	0.6681	0.2245	0.7502	0.6121
0.07	0.25	197	89.4440	82.1703	342.7993	0.6935	0.2134	0.7167	0.6118
0.07	0.24	200	88.4079	82.9011	350.4422	0.7090	0.1988	0.6976	0.6107
0.07	0.26	197	91.0882	81.6118	330.2256	0.6674	0.2248	0.7461	0.6105
0.06	0.27	200	87.8573	82.2774	358.1020	0.7171	0.2113	0.6775	0.6105

In the weight adjusted desirability approach, the vector of adjustment factors $\vec{\alpha} = [\alpha_1\ \alpha_2\ \alpha_3]^\mathrm{T}$ is to be calculated. Using equation 4.1 and the values of correlation shown in figure 5.3 with the value of $\eta = 1$, the values of α_1, α_2 and α_3 can be computed as:

$$\alpha_1 = 1 - \frac{1}{3}(-0.6972 + (-0.7164)) = 1.4712$$

$$\alpha_2 = 1 - \frac{1}{3}(-0.6972 + 0.8846) = 0.9375$$

$$\alpha_3 = 1 - \frac{1}{3}(-0.7164 + 0.8846) = 0.9439.$$

Hence, $\vec{\alpha} = [1.4712\ 0.9375\ 0.9439]^{\mathrm{T}}$ can be obtained and it can be directly implied that the importance of $d_1(F_{\mathrm{p}})$ would be increased while the importance of $d_2(VB_{\mathrm{m}})$ and $d_3(t)$ would be very slightly decreased. The best 10 cutting parameters obtained using the weight adjusted DI using arithmetic mean $D_{\mathrm{a(adj)}}$ and geometric mean of DFs $D_{\mathrm{g(adj)}}$ are listed in table 5.7 and 5.8 correspondingly. The optimal solutions obtained from by weight adjusted arithmetic mean of DFs are similar with the solutions obtained from PCA-based DI although the importance of $d_1(F_{\mathrm{p}})$ has been increased unequally by both indices.

From the weight adjusted geometric mean index, a different set of solutions is obtained. It can be suspected that $D_{\mathrm{g(adj)}}$ is heavily weighted by $d_2(VB_{\mathrm{m}})$ which has the lowest value among the desirability scores, since values of VB_{m} shown in table 5.8 are relatively low when compared to table 5.6 or 5.7.

Table 5.7: Best ten cutting parameters evaluated by weight adjusted arithmetic mean of DFs

f	a_p	v_c	F_p	VB_m	t	$d_1(F_p)$	$d_2(VB_m)$	$d_3(t)$	$D_{a(adj)}$
0.07	0.25	200	89.3172	82.2197	337.0605	0.6954	0.2124	0.7304	0.5702
0.07	0.26	200	90.9546	81.6625	324.7461	0.6696	0.2238	0.7581	0.5698
0.07	0.25	199	89.3592	82.2033	338.9506	0.6948	0.2128	0.7260	0.5688
0.07	0.26	199	90.9989	81.6456	326.5507	0.6689	0.2241	0.7542	0.5685
0.07	0.25	198	89.4015	82.1868	340.8635	0.6941	0.2131	0.7214	0.5673
0.07	0.26	198	91.0434	81.6287	328.3771	0.6681	0.2245	0.7502	0.5672
0.08	0.24	200	93.0247	81.0747	309.1512	0.6347	0.2359	0.7896	0.5668
0.07	0.26	197	91.0882	81.6118	330.2256	0.6674	0.2248	0.7461	0.5658
0.07	0.25	197	89.4440	82.1703	342.7993	0.6935	0.2134	0.7167	0.5658
0.08	0.24	199	93.0753	81.0624	310.8570	0.6338	0.2362	0.7863	0.5656

Table 5.8: Best ten cutting parameters evaluated by weight adjusted geometric mean of DFs

f	a_p	v_c	F_p	VB_m	t	$d_1(F_p)$	$d_2(VB_m)$	$d_3(t)$	$D_{g(adj)}$
0.09	0.23	200	96.4878	79.4782	286.6209	0.5709	0.2699	0.8289	0.5143
0.09	0.23	199	96.5456	79.4703	288.1739	0.5698	0.2701	0.8264	0.5135
0.09	0.23	198	96.6035	79.4625	289.7457	0.5687	0.2703	0.8239	0.5127
0.08	0.25	200	94.4243	80.5931	297.3696	0.6097	0.2461	0.8110	0.5126
0.08	0.25	199	94.4775	80.5800	298.9964	0.6088	0.2463	0.8082	0.5119
0.09	0.23	197	96.6617	79.4547	291.3364	0.5676	0.2704	0.8213	0.5119
0.09	0.24	200	97.7724	79.0608	275.1475	0.5456	0.2790	0.8463	0.5118
0.08	0.24	200	93.0247	81.0747	309.1512	0.6347	0.2359	0.7896	0.5118
0.08	0.25	198	94.5309	80.5670	300.6430	0.6078	0.2466	0.8053	0.5112
0.09	0.24	199	97.8333	79.0520	276.6264	0.5444	0.2792	0.8441	0.5110

Table 5.9: Best ten cutting conditions evaluated by the arithmetic mean of the DFs

f	a_p	v_c	F_p	VB_m	t	$d_1(F_p)$	$d_2(VB_m)$	$d_3(t)$	D_a
0.09	0.24	200	97.7724	79.0608	275.1475	0.5456	0.2790	0.8463	0.5570
0.09	0.23	200	96.4878	79.4782	286.6209	0.5709	0.2699	0.8289	0.5566
0.09	0.24	199	97.8333	79.0520	276.6264	0.5444	0.2792	0.8441	0.5559
0.08	0.25	200	94.4243	80.5931	297.3696	0.6097	0.2461	0.8110	0.5556
0.09	0.23	199	96.5456	79.4703	288.1739	0.5698	0.2701	0.8264	0.5554
0.09	0.24	198	97.8943	79.0432	278.1234	0.5432	0.2794	0.8419	0.5548
0.08	0.25	199	94.4775	80.5800	298.9964	0.6088	0.2463	0.8082	0.5544
0.09	0.23	198	96.6035	79.4625	289.7457	0.5687	0.2703	0.8239	0.5543
0.09	0.24	197	97.9555	79.0344	279.6385	0.5420	0.2796	0.8397	0.5537
0.08	0.24	200	93.0247	81.0747	309.1512	0.6347	0.2359	0.7896	0.5534

Table 5.10: Best ten cutting conditions evaluated by the geometric mean of DFs

f	a_p	v_c	F_p	VB_m	t	$d_1(F_p)$	$d_2(VB_m)$	$d_3(t)$	D_g
0.09	0.24	200	97.7724	79.0608	275.1475	0.5456	0.2790	0.8463	0.5051
0.09	0.24	199	97.8333	79.0520	276.6264	0.5444	0.2792	0.8441	0.5044
0.09	0.24	198	97.8943	79.0432	278.1234	0.5432	0.2794	0.8419	0.5037
0.09	0.23	200	96.4878	79.4782	286.6209	0.5709	0.2699	0.8289	0.5036
0.09	0.24	197	97.9555	79.0344	279.6385	0.5420	0.2796	0.8397	0.5030
0.09	0.23	199	96.5456	79.4703	288.1739	0.5698	0.2701	0.8264	0.5029
0.09	0.24	196	98.0170	79.0256	281.1721	0.5407	0.2798	0.8374	0.5022
0.09	0.23	198	96.6035	79.4625	289.7457	0.5687	0.2703	0.8239	0.5022
0.09	0.24	195	98.0786	79.0168	282.7243	0.5395	0.2800	0.8350	0.5015
0.09	0.23	197	96.6617	79.4547	291.3364	0.5676	0.2704	0.8213	0.5014

As a benchmark for the solutions obtained from the proposed methods, the best ten cutting parameters which are evaluated by the geometric mean (D_g) and the arithmetic mean of the DFs (D_a), are shown accordingly in table 5.10 and 5.9.

The solutions from D_a where correlation information has not been utilized, can be used as benchmark, and when they are compared with the solutions obtained from D_{PCA} and $D_{\mathrm{a(adj)}}$, a smaller f resulting in a lower F_{p} is preferred by D_{PCA} and $D_{\mathrm{a(adj)}}$. From D_{PCA}, it is obvious that the importance of $d_1(F_{\mathrm{p}})$ would be increased, since $d_1(F_{\mathrm{p}})$ has only negative correlation as shown in figure 5.3 and the first eigenvector $\vec{a_1}$ has a negative 1st element a_{11} while 2nd a_{12} and 3rd a_{13} elements are positive; thus, $d_1(F_{\mathrm{p}})$ would possess approximately half of weight from the first eigenvalue. Because the benefit of having a smaller f is a reduction in F_{p}, the optimal solutions from D_{PCA} should have a smaller f than D_{a}. The results of $D_{\mathrm{a(adj)}}$ can be simply described by the value of $\vec{\alpha}$ estimated previously that α_1 has the highest value in $\vec{\alpha}$, and therefore $d_1(F_{\mathrm{p}})$ has the highest contribution in $D_{\mathrm{a(adj)}}$.

When the solutions obtained from D_{g} are compared with the solutions from $D_{\mathrm{g(adj)}}$, only small differences can be observed, e.g., $f = 0.23$ mm is preferred by $D_{\mathrm{g(adj)}}$ and $f = 0.24$ mm by D_{g}. According to the value of $\vec{\alpha}$, the effects of correlation on the optimal solutions are supposed to be remarkable because the importance of $d_1(F_{\mathrm{p}})$ raises by approximately 47 percents, unfortunately D_{g} and $D_{\mathrm{g(adj)}}$ are heavily dependent on the small values of $d_2(VB_{\mathrm{m}})$ which in this case can dominate the effects from the correlations.

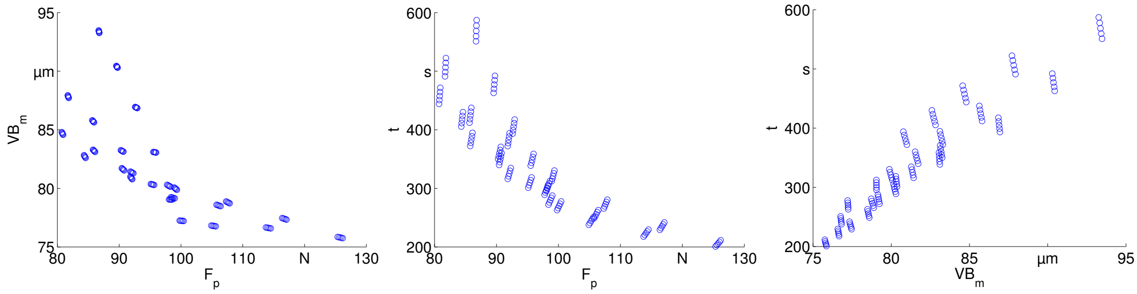
5.2.2 Optimization using Local Correlations

As there are interference patterns found in from correlations shown in figure 5.3, the range of cutting parameters used to estimate the correlations and covariances are to be restricted. The restricted range of cutting conditions is defined according to the favorable range which were found in tables 5.6, 5.7, 5.10 and 5.9. Additionally, the parameter range $f > 0.1$ mm will be eliminated from the parameter space due to dissatisfaction of $Rz_{95} \leq 3$ µm.

In order to avoid confusions, the correlations and covariances obtained from the restricted cutting parameters are referred as local correlations and local covariances respectively, and the correlations and covariances in figures 5.1, 5.3 and 5.4 will

Table 5.11: Restricted cutting parameters

Parameter	Notation	Unit	Values
Feed	f	mm/rev	0.05, . . . , 0.1
Depth of cut	a_{p}	mm	0.2, . . . , 0.3
Cutting speed	v_{c}	m/min	190 . . . ,200

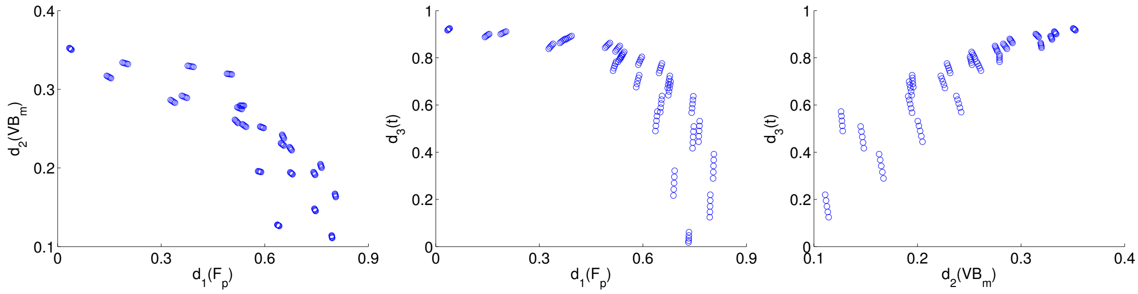


(a) $r_{(F_{\mathrm{p}},VB_{\mathrm{m}})}$ = -0.7500 (b) $r_{(F_{\mathrm{p}},t)}$ = -0.8461 (c) $r_{(VB_{\mathrm{m}},t)}$ = 0.9520

Figure 5.5: Scatter plots of the performance measures in restricted cutting parameters

be referred as global correlations and global covariances. The scatter plots of F_{p}, VB_{m} and t and their correlation coefficients are shown in figure 5.5. The coefficients $r_{(F_{\mathrm{p}},VB_{\mathrm{m}})}$ and $r_{(F_{\mathrm{p}},t)}$ shown in figure 5.5 are moderately stronger than which shown in figure 5.1, and the local correlations show a strong linear behavior.

After the transformation using Harrington's DFs is performed, the scatter plots of $d_1(F_{\mathrm{p}})$, $d_2(VB_{\mathrm{m}})$ and $d_3(t)$ can be illustrated as figure 5.6. It can be seen that most of zero values of $d_1(F_{\mathrm{p}})$, $d_2(VB_{\mathrm{m}})$ and $d_3(t)$ in figure 5.3a, 5.3b and 5.3c have been removed through the restriction of cutting parameters; therefore, the values of the local correlations of performance measures are not remarkably influenced by the desirability transformation as it was by global correlations. In addition, it can be also observed that the correlations of $d_1(F_{\mathrm{p}})$, $d_2(VB_{\mathrm{m}})$ and $d_3(t)$ show slightly more nonlinear behavior than of F_{p}, VB_{m} and t.



(a) $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ = -0.7968 (b) $r_{(d_1(F_\mathrm{p}),d_3(t))}$ = -0.7404 (c) $r_{(d_2(VB_\mathrm{m}),d_3(t))}$ = 0.9318

Figure 5.6: Scatter plots of the desirability scores in restricted cutting parameters

Table 5.12: Local covariance of the desirability scores

Variable	$d_1(F_\mathrm{p})$	$d_2(VB_\mathrm{m})$	$d_3(t)$
$d_1(F_\mathrm{p})$	0.0413	-0.0130	-0.0363
$d_2(VB_\mathrm{m})$	-0.0130	0.0065	0.0181
$d_3(t)$	-0.0363	0.0181	0.0584

Table 5.13: Eigenvectors, eigenvalues, and normalized weights of PCs computed with local correlation

	1st PC	2nd PC	3rd PC
Eigenvector	$\begin{bmatrix} -0.5986 \\ 0.2498 \\ 0.7611 \end{bmatrix}$	$\begin{bmatrix} -0.7962 \\ -0.0809 \\ -0.5996 \end{bmatrix}$	$\begin{bmatrix} 0.0882 \\ 0.9649 \\ -0.2473 \end{bmatrix}$
Eigenvalue	0.0929	0.0126	0.0006
W_j	0.8755	0.1185	0.0060

Following by the PCA-transformation and $d_1(F_\mathrm{p})$, $d_2(VB_\mathrm{m})$ and $d_3(t)$ are likewise transformed into uncorrelated PCs using their local covariances shown in table 5.12. Eigenvectors, eigenvalues, and normalized weights which are derived from the local covariances are listed in table 5.13. With the given local covariances, the first PC accounts almost 87 percents of the total weight and it can be also expected in advance that the degree of importance of $d_1(F_\mathrm{p})$ will be raised whereas the degree of importance of $d_2(VB_\mathrm{m})$ will be reduced by PCA-based DI. In order to avoid confusions, the PCA-based DI which is based on the given local covariances will be denoted as $D_{\mathrm{PCA(l)}}$, and the solutions ranking obtained from $D_{\mathrm{PCA(l)}}$ is shown in table 5.14. When compared the results shown in table 5.14 to the results shown in table 5.6, there are only small differences which means that in this case the difference of using the global covariances and the local covariances in PCA-based desirability approach is small.

Table 5.14: Best ten cutting conditions in the restricted region evaluated by PCA-based DI

f	a_p	v_c	F_p	VB_m	t	$d_1(F_\mathrm{p})$	$d_2(VB_\mathrm{m})$	$d_3(t)$	$D_{\mathrm{PCA(l)}}$
0.07	0.25	200	89.3172	82.2197	337.0605	0.6954	0.2124	0.7304	0.6520
0.07	0.26	200	90.9546	81.6625	324.7461	0.6696	0.2238	0.7581	0.6509
0.07	0.25	199	89.3592	82.2033	338.9506	0.6948	0.2128	0.7260	0.6500
0.07	0.26	199	90.9989	81.6456	326.5507	0.6689	0.2241	0.7542	0.6491
0.07	0.25	198	89.4015	82.1868	340.8635	0.6941	0.2131	0.7214	0.6480
0.07	0.26	198	91.0434	81.6287	328.3771	0.6681	0.2245	0.7502	0.6473
0.08	0.24	200	93.0247	81.0747	309.1512	0.6347	0.2359	0.7896	0.6469
0.07	0.25	197	89.4440	82.1703	342.7993	0.6935	0.2134	0.7167	0.6459
0.07	0.26	197	91.0882	81.6118	330.2256	0.6674	0.2248	0.7461	0.6454
0.08	0.24	199	93.0753	81.0624	310.8570	0.6338	0.2362	0.7863	0.6452

Next, for the weight adjusted DI, the weight adjustment factors $\vec{\alpha_l}$ are to be calculated from the values of correlations shown in figure 5.6 with $\eta = 1$. The values of α_1, α_2 and α_3 can be computed as following:

$$\alpha_1 = 1 - \frac{1}{3}(-0.7968 + (-0.7404)) = 1.5124$$

$$\alpha_2 = 1 - \frac{1}{3}(-0.7968 + 0.9318) = 0.9550$$

$$\alpha_3 = 1 - \frac{1}{3}(-0.7404 + 0.9318) = 0.9362,$$

and $\vec{\alpha_l} = [1.5124\ 0.9550\ 0.9362]^T$ can be obtained. In this case, $\vec{\alpha_l}$ is only slightly different from $\vec{\alpha}$ because the local correlations of DFs are only slightly different from the global correlations. The best 10 cutting parameters obtained using the weight adjusted DI using arithmetic mean $D_{a(adj,l)}$ and geometric mean of DFs $D_{g(adj,l)}$ are listed in table 5.15 and 5.16 correspondingly. The results show that the differences of using $D_{a(adj)}$ and $D_{a(adj,l)}$ are very small so that the same best 1-9 cutting parameters are obtained from both indices and only the 8th and the 9th are reversed. From $D_{g(adj)}$ and $D_{g(adj,l)}$, the same optimal result can be found and there are only small differences in results that from the 3rd to 9th there are some changes in order detected.

Table 5.15: Best ten cutting conditions in the restricted region evaluated by weight adjusted arithmetic mean of DFs

f	a_p	v_c	F_p	VB_m	t	$d_1(F_p)$	$d_2(VB_m)$	$d_3(t)$	$D_{a(adj,l)}$
0.07	0.25	200	89.3172	82.2197	337.0605	0.6954	0.2124	0.7304	0.5695
0.07	0.26	200	90.9546	81.6625	324.7461	0.6696	0.2238	0.7581	0.5688
0.07	0.25	199	89.3592	82.2033	338.9506	0.6948	0.2128	0.7260	0.5681
0.07	0.26	199	90.9989	81.6456	326.5507	0.6689	0.2241	0.7542	0.5675
0.07	0.25	198	89.4015	82.1868	340.8635	0.6941	0.2131	0.7214	0.5667
0.07	0.26	198	91.0434	81.6287	328.3771	0.6681	0.2245	0.7502	0.5662
0.08	0.24	200	93.0247	81.0747	309.1512	0.6347	0.2359	0.7896	0.5654
0.07	0.25	197	89.4440	82.1703	342.7993	0.6935	0.2134	0.7167	0.5652
0.07	0.26	197	91.0882	81.6118	330.2256	0.6674	0.2248	0.7461	0.5649
0.06	0.27	200	87.8573	82.2774	358.1020	0.7171	0.2113	0.6775	0.5643

Table 5.16: Best ten cutting conditions in the restricted region evaluated by weight adjusted geometric mean of DFs

f	a_p	v_c	F_p	VB_m	t	$d_1(F_p)$	$d_2(VB_m)$	$d_3(t)$	$D_{g(adj,l)}$
0.09	0.23	200	96.4878	79.4782	286.6209	0.5709	0.2699	0.8289	0.5127
0.09	0.23	199	96.5456	79.4703	288.1739	0.5698	0.2701	0.8264	0.5119
0.08	0.25	200	94.4243	80.5931	297.3696	0.6097	0.2461	0.8110	0.5113
0.09	0.23	198	96.6035	79.4625	289.7457	0.5687	0.2703	0.8239	0.5111
0.08	0.24	200	93.0247	81.0747	309.1512	0.6347	0.2359	0.7896	0.5106
0.08	0.25	199	94.4775	80.5800	298.9964	0.6088	0.2463	0.8082	0.5106
0.09	0.23	197	96.6617	79.4547	291.3364	0.5676	0.2704	0.8213	0.5103
0.09	0.24	200	97.7724	79.0608	275.1475	0.5456	0.2790	0.8463	0.5100
0.08	0.25	198	94.5309	80.5670	300.6430	0.6078	0.2466	0.8053	0.5099
0.08	0.24	199	93.0753	81.0624	310.8570	0.6338	0.2362	0.7863	0.5098

5.2.3 Summary and Analysis

To summarize the results obtained from this case study, the optimal solutions obtained from each index with given global and local correlations are listed in table 5.17. Since the traditional DIs D_a and D_g do not utilize the correlations of DFs, their results do not depend on correlations. For the reason that the values of each index are incomparable, i.e., the value of $D_{PCA} = 0.6170$ cannot be compared with $D_{a(adj)} = 0.5702$, their values are excluded from table 5.17. In table 5.17, it has been shown that when the global correlations are replaced by the local correlations, the results obtained from D_{PCA}, $D_{a(adj)}$ and $D_{g(adj)}$ do not change remarkably. When the correlations are taken into account, the importance of $d_1(F_p)$ which has only negative correlations is raised, and it can be observed by comparing the results obtained from D_a to D_{PCA}, $D_{a(adj)}$, $D_{PCA(l)}$ and $D_{a(adj,l)}$ that the differences of integrating correlation information into the weight geometric average index are much smaller than for the weight arithmetic average index, as the results obtained from D_g differ only slightly to the results from $D_{g(adj)}$ and $D_{g(adj,l)}$. In this case study, since $d_2(VB_m)$ has the lowest value and much less than the other DFs, D_{g}, $D_{\mathrm{g(adj)}}$ and $D_{\mathrm{g(adj,l)}}$ are heavily weighted by the values of $d_2(VB_{\mathrm{m}})$, and as a result, the effects of correlations are mostly dominated in $D_{\mathrm{g(adj)}}$ and $D_{\mathrm{g(adj,l)}}$.

Table 5.17: Optimal cutting conditions obtained from optimization

			Global correlation			Local correlation		
Index	D_{a}	D_{g}	D_{PCA}	$D_{\mathrm{a(adj)}}$	$D_{\mathrm{g(adj)}}$	$D_{\mathrm{PCA(l)}}$	$D_{\mathrm{a(adj,l)}}$	$D_{\mathrm{g(adj,l)}}$
f	0.09	0.09	0.07	0.07	0.09	0.07	0.07	0.09
a_{p}	0.24	0.24	0.25	0.25	0.23	0.25	0.25	0.23
v_{c}	200	200	200	200	200	200	200	200
F_{p}	97.7724	97.7724	89.3172	89.3172	96.4878	89.3172	89.3172	96.4878
VB_{m}	79.0608	79.0608	82.2197	82.2197	79.4782	82.2197	82.2197	79.4782
t	275.1475	275.1475	337.0605	337.0605	286.6209	337.0605	337.0605	286.6209
$d_1(F_{\mathrm{p}})$	0.5456	0.5456	0.6954	0.6954	0.5709	0.6954	0.6954	0.5709
$d_2(VB_{\mathrm{m}})$	0.2790	0.2790	0.2124	0.2124	0.2699	0.2124	0.2124	0.2699
$d_3(t)$	0.8463	0.8463	0.7304	0.7304	0.8289	0.7304	0.7304	0.8289
Rz_{95}	2.7739	2.7739	2.2937	2.2937	2.7767	2.2937	2.2937	2.7767

Table 5.18: Normalized weights of the optimization using deterministic models

	$W_{d_1(F_{\mathrm{p}})}$	$W_{d_2(VB_{\mathrm{m}})}$	$W_{d_3(t)}$
D_{a}	0.3333	0.3333	0.3333
D_{g}	0.3333	0.3333	0.3333
D_{PCA}	0.4933	0.1856	0.3210
$D_{\mathrm{a(adj)}}$	0.4388	0.2796	0.2815
$D_{\mathrm{g(adj)}}$	0.4388	0.2796	0.2815
$D_{\mathrm{PCA(l)}}$	0.5019	0.1174	0.3807
$D_{\mathrm{a(adj,l)}}$	0.4444	0.2806	0.2751
$D_{\mathrm{g(adj,l)}}$	0.4444	0.2806	0.2751

Note. All numbers are rounded to 4 digit accuracy after decimal point.

In order to confirm the conclusion obtained from table 5.17, the normalized weights used in each index are estimated as shown in table 5.18. The normalized weights for $D_{\mathrm{a(adj)}}$, $D_{\mathrm{g(adj)}}$, $D_{\mathrm{a(adj,l)}}$ and $D_{\mathrm{g(adj,l)}}$ can be easily analytically derived from $\vec{\alpha}$ and $\vec{\alpha}_{\mathrm{l}}$ which have been computed. For D_{PCA} and $D_{\mathrm{PCA(l)}}$, although the analytical solution for the normalized weights may be possible, it required less effort and is much easier to obtain the normalized weights using multivariate linear regression, and the obtained standard errors are approximately zero. Caution, however, for D_{PCA} and $D_{\mathrm{PCA(l)}}$ since the normalized weights shown in table 5.13 and 5.5 are for the PC scores which are not identical to the normalized weights for $d_1(F_{\mathrm{p}})$, $d_2(VB_{\mathrm{m}})$ and $d_3(t)$. When comparing the proposed indices (D_{PCA}, $D_{\mathrm{a(adj)}}$ and $D_{\mathrm{g(adj)}}$) to traditional DIs (D_{a} and D_{g}), the proposed indices which account the correlation information, trend to give a higher importance for $d_1(F_{\mathrm{p}})$ than the traditional indices. As a consequence, the importance of $d_2(VB_{\mathrm{m}})$ and $d_3(t)$ also decrease for the proposed indices. Especially, in D_{PCA}, the importance $d_2(VB_{\mathrm{m}})$ drops significantly due to the effects from the covariance matrices in which the variance of $d_2(VB_{\mathrm{m}})$ is relatively small when compared to $d_1(F_{\mathrm{p}})$ and $d_3(t)$. Since the covariance matrices shown in tables 5.4 and 5.12 are determined from the experimental design, the small variance of $d_2(VB_{\mathrm{m}})$ can be also viewed that the improvement of $d_2(VB_{\mathrm{m}})$ which can be achieved by changing cutting conditions is very small. Therefore, D_{PCA} not only considers the correlation information but also give priority to the performance measures which have potentials to be improved in the decided parameter space.

5.2.4 PCA-based Desirability Approach using Correlation Matrix

According to the results of this section that PCA-based DI is affected by variances of desirability scores, in this subsection, an alternative way to apply PCA-based DI that will not be affected by variances of desirability scores are to be demonstrated and discussed. The first possibility would be to standardize the values of desirability scores using the following formula:

$$\hat{d}_j = \frac{d_j - \text{mean}(d_j)}{\sigma_{d_j}} \tag{5.6}$$

where $\hat{d}_j$ denotes the standardized value of the jth desirability score, d_j denotes the value of the jth desirability score and σ_{d_j} denotes the standard deviation of d_j. As consequences, the covariances of $\hat{d}_j$ would be identical to the correlation coefficients shown in figure 5.6, the monotonicity of PC scores is no longer valid when using 3.18 due to the existence of negative $\hat{d}_j$ and a formulation of a monotone PCA-based DI would be very difficult.

5.3 Robust Optimization

Due to the reason that turning is a stochastic process in practice, and the mathematical models such as Kriging and regression model are usually constructed with stochastic errors, the stochastic error terms are to be included into the case study of hard turning of AISI 6150.

5.3.1 Optimization using Stochastic Models

Using the optimization model which is described in section 5.1 and the restricted range of cutting parameters as in table 5.11 with the stochastic mathematical models for F_p, VB_m, t and Rz defined as

$$F_\mathrm{p} = \hat{f}_1(f, a_\mathrm{p}, v_\mathrm{c}) + \epsilon_{F_\mathrm{p}} \tag{5.7}$$

$$VB_\mathrm{m} = \mathrm{e}^{(\hat{f}_2(f, a_\mathrm{p}, v_\mathrm{c}) + \epsilon_{VB_\mathrm{m}})} \tag{5.8}$$

$$t = \mathrm{e}^{(\hat{f}_3(f, a_\mathrm{p}, v_\mathrm{c}) + \epsilon_t)} \tag{5.9}$$

where $\hat{f}_1$, $\hat{f}_2$ and $\hat{f}_3$ are functions used to predict the values of F_p, VB_m and t respectively and ϵ_{F_p}, ϵ_{VB_m} and ϵ_t are their stochastic error terms which are assumed to be distributed normally with mean zero and independent and identically distributed (i.i.d.). The model of Rz remains as defined in equation 5.5. Since the real value of ϵ_t is in general very small and depends primarily on the machine precision, its value is assumed to be zero, whereas the variances of ϵ_{F_p}, ϵ_{VB_m} are estimated by cross-validation.

The uncertainty analysis is performed using the Monte-Carlo method with 1 million iterations and its procedure can be described as follows. For each iteration, the following steps are to be performed:

Step 1 : The values of $\hat{f}_1$, $\hat{f}_2$ and $\hat{f}_3$ are to be generated from Kriging models, according to the experimental design.

Step 2 : The values of ϵ_{F_p} and ϵ_{VB_m} are to be generated using random number generator.

Step 3 : The values of F_p, VB_m and t can be obtained using equation 5.7, 5.8 and 5.9, and their correlation coefficients are to be computed.

Step 4 : The values of $d_1(F_\mathrm{p})$, $d_2(VB_\mathrm{m})$ and $d_3(t)$ are computed from F_p, VB_m and t.

Step 5 : The correlation coefficients and covariances of $d_1(F_\mathrm{p})$, $d_2(VB_\mathrm{m})$ and $d_3(t)$ are to be computed, and repeat from step 2 for the next iteration.

Then, the expected value of correlation coefficients and covariances are calculated from their average values. The expected values of the correlation coefficients of F_p, VB_m, t, $d_1(F_\mathrm{p})$, $d_2(VB_\mathrm{m})$ and $d_3(t)$ are listed in table 5.19.

When comparing eigenvectors in table 5.21 with 5.13, small differences in values can be found due to the existence of error terms. For this extended case, the first PC accounts only about 77.72 percent of D_PCA which dropped due to the weaker correlations than the previous case study.

When there are no stochastic errors in the optimization model, only the operating parameter set that maximizes the value of DI is to be searched. In this extended

Table 5.19: Correlation coefficients of performance measures and desirability scores

Correlation coefficients	Expected value
$r_{(F_{\mathrm{p}},VB_{\mathrm{m}})}$	-0.4576
$r_{(F_{\mathrm{p}},t)}$	-0.6952
$r_{(VB_{\mathrm{m}},t)}$	0.7068
$r_{(d_1(F_{\mathrm{p}}),d_2(VB_{\mathrm{m}}))}$	-0.4788
$r_{(d_1(F_{\mathrm{p}}),d_3(t))}$	-0.6218
$r_{(d_2(VB_{\mathrm{m}}),d_3(t))}$	0.6706

Table 5.20: Covariance of the desirability scores

Variable	$W_{d_1(F_{\mathrm{p}})}$	$W_{d_2(VB_{\mathrm{m}})}$	$W_{d_3(t)}$
$d_1(F_{\mathrm{p}})$	0.0531	-0.0119	-0.0346
$d_2(VB_{\mathrm{m}})$	-0.0119	0.0116	0.0174
$d_3(t)$	-0.0346	0.0174	0.0584

Table 5.21: Eigenvectors, eigenvalues, and normalized weights of PCs for the extended case study

	1st PC	2nd PC	3rd PC
Eigenvector	$\begin{bmatrix} -0.6520 \\ 0.2411 \\ 0.7189 \end{bmatrix}$	$\begin{bmatrix} -0.7581 \\ -0.1878 \\ -0.6245 \end{bmatrix}$	$\begin{bmatrix} 0.0156 \\ 0.9522 \\ -0.3052 \end{bmatrix}$
Eigenvalue	0.0956	0.0216	0.0058
W_j	0.7772	0.1756	0.0472

study, since the stochastic error terms are included, the values of DIs for a given operating parameters are not constant. Therefore, in the optimization, not only the expected value of DIs, but also the worst case representative, the 5th percentile which is estimated by Monte-Carlo method, are selected as the second objective in the optimization. As a consequence, the optimization problem is no longer a single objective optimization problem. The optimization is performed by computing the expected value of DIs and their 5th percentile for all possible combinations of parameters, then using an algorithm to sort out the Pareto solutions which is developed by [4].

For the weight adjustment method, the values of α_1, α_2 and α_3 can be computed as:

$$\alpha_1 = 1 - \frac{1}{3}(-0.4788 + (-0.6218)) = 1.3669$$
$$\alpha_2 = 1 - \frac{1}{3}(-0.4788 + 0.6706) = 0.9361$$
$$\alpha_3 = 1 - \frac{1}{3}(-0.6218 + 0.6706) = 0.9837,$$

which leads to $\vec{\alpha} = [1.3669\ 0.9361\ 0.9837]^{\mathrm{T}}$. The optimization results obtained from the optimization of desirability indices are listed in table 5.22. The results show that for the traditional DIs and $D_{\mathrm{g(adj)}}$, the parameter $f = 0.09$ mm with $a_{\mathrm{p}} = 0.23$-0.24 mm are preferred, but for D_{PCA} and $D_{\mathrm{a(adj)}}$ the parameter $f = 0.07$ mm with $a_{\mathrm{p}} =$ 0.25-0.26 mm which result in a lower F_{p} are preferred. The results shown in table 5.22 agree with the normalized weights in table 5.23 that with the correlation information, the importance of $d_2(F_{\mathrm{p}})$ would be increased, and the optimal solutions obtained from D_{PCA} and $D_{\mathrm{a(adj)}}$ should result in lower F_{p} than the optimal solutions from D_{a}. For the geometric indices (D_{g} and $D_{\mathrm{g(adj)}}$), effects from the low values of $d_2(VB_{\mathrm{m}})$ are still found to be strong, but the effects of correlations on $D_{\mathrm{g(adj)}}$ are noticeable so that the parameters $f = 0.07$ mm and $a_{\mathrm{p}} = 0.26$ mm are also optimal for $D_{\mathrm{g(adj)}}$.

Table 5.22: Optimal cutting conditions obtained from robust optimization

Index	Cutting parameters			Performance measures			Overall performance	
	f	a_{p}	v_{c}	$\mathrm{E}(F_{\mathrm{p}})$	$\mathrm{E}(VB_{\mathrm{m}})$	$\mathrm{E}(t)$	E(DI)	DI_{05}
D_{a}	0.09	0.24	200	97.7777	79.1505	275.1475	0.5534	0.4569
	0.09	0.23	200	96.4827	79.5658	286.6209	0.5527	0.4577
	0.08	0.25	200	94.4341	80.6933	297.3696	0.5514	0.4592
	0.08	0.24	200	93.0124	81.1645	309.1512	0.5492	0.4593
	0.07	0.26	200	90.9498	81.7581	324.7461	0.5462	0.4600
D_{g}	0.09	0.24	200	97.7777	79.1505	275.1475	0.4921	0.3686
	0.09	0.23	200	96.4827	79.5658	286.6209	0.4911	0.3703
D_{PCA}	0.07	0.25	200	89.3063	82.3114	337.0605	0.6334	0.5280
$D_{\mathrm{a(adj)}}$	0.07	0.26	200	90.9498	81.7581	324.7461	0.5633	0.4619
	0.07	0.25	200	89.3063	82.3114	337.0605	0.5627	0.4656
$D_{\mathrm{g(adj)}}$	0.09	0.23	200	96.4827	79.5658	286.6209	0.5019	0.3718
	0.08	0.25	200	94.4341	80.6933	297.3696	0.4994	0.3751
	0.08	0.24	200	93.0124	81.1645	309.1512	0.4982	0.3771
	0.07	0.26	200	90.9498	81.7581	324.7461	0.4963	0.3790

Table 5.23: Normalized weights of the robust optimization

	$W_{d_1(F_{\mathrm{p}})}$	$W_{d_2(VB_{\mathrm{m}})}$	$W_{d_3(t)}$
D_{a}	0.3333	0.3333	0.3333
D_{g}	0.3333	0.3333	0.3333
D_{PCA}	0.4738	0.1417	0.3846
$D_{\mathrm{a(adj)}}$	0.4159	0.2848	0.2993
$D_{\mathrm{g(adj)}}$	0.4159	0.2848	0.2993

Note. All numbers are rounded to 4 digit accuracy after decimal point.

5.3.2 Optimization using Stochastic Model with Correlated Errors

Considering the fact that F_{p}, VB_{m} and t are correlated, it would be reasonable to formulate their error terms (ϵ_j) as correlated variables. These error terms should be also dependent on the given parameter set $\vec{x}_k$ =$[f_k\ a_{\text{p}_k}\ v_{\text{c}_k}]^{\text{T}}$, since the correlations of performance measures as well as desirability scores may change due to different operating conditions. However, to estimate the correlations and covariances of F_{p}, VB_{m} and t for each $\vec{x}_k$ would be really expensive, and may not possible in practice.

For this reason, an assumption that the correlations of ϵ_j do not change over the time space must be assumed, and this assumption would be reasonable when the cutting conditions do not shift during the operation. For this case study, since ϵ_t is assumed as zero, $r_{(\epsilon_{F_{\text{p}}},\epsilon_t)}$ and $r_{(\epsilon_{VB_{\text{m}}},\epsilon_t)}$ are zero as well. The correlation of $\epsilon_{F_{\text{p}}}$ and $\epsilon_{VB_{\text{m}}}$ for each $\vec{x}_k$ is to be estimated by generating F_{p} and VB_{m} data from various cutting path lengths (L_{c}). Due to the reason that the models in [41] are formulated from L_{c} between 2322 and 5000 m, the correlation of ϵ_j is supposed to be determined from L_{c} between 2500 m and 5000 m. However, due to some measurement errors for L_{c} between 4000 m and 5000 m, the range of L_{c} used to estimated $r_{(\epsilon_{F_{\text{p}}},\epsilon_{VB_{\text{m}}})}$ is between 2500 m and 4000 m. For example, for the parameters f = 0.07 mm, a_{p} = 0.25 mm and v_{c} = 200 m/min the data of F_{p} and VB_{m} are computed as shown in table 5.24, in which the values of F_{p} and VB_{m} are generated from the Kriging models without stochastic errors. Additionally, the volume of material removal varies depending on parameters f, a_{p} and L_{c}. It can be clearly observed that the values of VB_{m} raise as the value of F_{p} becomes higher so that $r_{(F_{\text{p}},VB_{\text{m}})} = 0.9751$. According to equation 5.8, VB_{m} is modeled on the logarithmic scale, in order to estimate $r_{(\epsilon_{F_{\text{p}}},\epsilon_{VB_{\text{m}}})}$, the values of $\ln(VB_{\text{m}})$ must be calculated, and therefore they are listed in table 5.24. As a result, for $\vec{x} = [0.07\ 0.25\ 200]^{\text{T}}$, $r_{(\epsilon_{F_{\text{p}}},\epsilon_{VB_{\text{m}}})} = 0.9673$ can be obtained. Note that the volume of material removal is not fixed during the estimation of $r_{(\epsilon_{F_{\text{p}}},\epsilon_{VB_{\text{m}}})}$, and the variances of the generated F_{p} and VB_{m} are generated according to the differences

Table 5.24: Data generated for determining the correlation of the error terms of F_p and VB_m

Cutting parameters				Generated data		
f	a_p	v_c	L_c	F_p	VB_m	$\ln(VB_\mathrm{m})$
0.07	0.25	200	2500	150.3712	94.1020	4.5444
0.07	0.25	200	2600	150.8701	96.1546	4.5660
0.07	0.25	200	2700	151.1386	98.1440	4.5864
0.07	0.25	200	2800	151.4010	100.1064	4.6062
0.07	0.25	200	2900	151.7094	102.0669	4.6256
0.07	0.25	200	3000	152.1875	104.0485	4.6449
0.07	0.25	200	3100	154.4310	106.0897	4.6643
0.07	0.25	200	3200	156.8442	108.1490	4.6835
0.07	0.25	200	3300	159.3049	110.2027	4.7023
0.07	0.25	200	3400	161.7725	112.2364	4.7206
0.07	0.25	200	3500	164.1984	114.2390	4.7383
0.07	0.25	200	3600	166.1689	116.2020	4.7553
0.07	0.25	200	3700	168.0673	118.1083	4.7716
0.07	0.25	200	3800	169.9040	119.9405	4.7870
0.07	0.25	200	3900	171.6549	121.6780	4.8014
0.07	0.25	200	4000	173.2114	123.2842	4.8145

in the material removal volume; therefore, only the correlation coefficient of ϵ_{F_p} and ϵ_{VB_m} will be determined from the method explained above and their covariance will be computed combining this correlation with the same variance values of ϵ_{F_p} and ϵ_{VB_m} as in section 5.3.1.

The optimization problem for this section follows from section 5.3.1 with F_p, VB_m and t defined in equation 5.7, 5.8 and 5.9 respectively. The uncertainty analysis can be performed with the procedure described in section 5.3.1, using the multivariate random number generator in MATLAB [30] for which the covariance of ϵ_{F_p} and ϵ_{VB_m} is computed from the values of $r_{(\epsilon_{F_\mathrm{p}},\epsilon_{VB_\mathrm{m}})}$ estimated from the method described in the beginning of this section with the same variance values of ϵ_{F_p} and ϵ_{VB_m} as in section

5.3.1.

The computation time required to perform the Monte-Carlo simulation is approximately 335 hours and the expected values of correlations and covariance are shown in table 5.25 and 5.26. From the results of the simulation, the values of $r_{(F_\mathrm{p},VB_\mathrm{m})}$ and $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ are found to be so small, because the correlation of F_p and VB_m on the parameter space is negative and their error terms, ϵ_{F_p} and ϵ_{VB_m}, are positively correlated. The other correlations $r_{(F_\mathrm{p},t)}$ and $r_{(VB_\mathrm{m},t)}$ remain almost unchanged from table 5.19, since the value of ϵ_t is assumed to be zero.

Table 5.25: Correlation coefficients of performance measures and desirability scores

Correlation coefficients	Expected value
$r_{(F_\mathrm{p},VB_\mathrm{m})}$	-0.0904
$r_{(F_\mathrm{p},t)}$	-0.6952
$r_{(VB_\mathrm{m},t)}$	0.7068
$r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$	-0.1204
$r_{(d_1(F_\mathrm{p}),d_3(t))}$	-0.6218
$r_{(d_2(VB_\mathrm{m}),d_3(t))}$	0.6706

Table 5.26: Covariance of the desirability scores

Variable	$d_1(F_\mathrm{p})$	$d_2(VB_\mathrm{m})$	$d_3(t)$
$d_1(F_\mathrm{p})$	0.0531	-0.0029	-0.0346
$d_2(VB_\mathrm{m})$	-0.0029	0.0116	0.0174
$d_3(t)$	-0.0346	0.0174	0.0584

From the covariance matrix shown in table 5.26, eigenvalues and eigenvectors are derived as shown in table 5.27. Due to the reason that $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ becomes smaller, the value of a_{21} derived is also small (0.1809), and the contribution of $d_2(VB_\mathrm{m})$ on D_PCA would be less than for all the previous case studies.

Table 5.27: Eigenvectors, eigenvalues, and normalized weights of PCs for the extended case study

	1st PC	2nd PC	3rd PC
Eigenvector	$\begin{bmatrix} -0.6502 \\ 0.1809 \\ 0.7379 \end{bmatrix}$	$\begin{bmatrix} 0.7161 \\ 0.4705 \\ 0.5156 \end{bmatrix}$	$\begin{bmatrix} 0.2539 \\ -0.8637 \\ 0.4354 \end{bmatrix}$
Eigenvalue	0.0932	0.0262	0.0037
W_j	0.7571	0.2128	0.0301

For the weight adjustment method, the values of α_1, α_2 and α_3 can be computed as:

$$\alpha_1 = 1 - \frac{1}{3}(-0.1204 + (-0.6218)) = 1.2474$$

$$\alpha_2 = 1 - \frac{1}{3}(-0.1204 + 0.6706) = 0.8166$$

$$\alpha_3 = 1 - \frac{1}{3}(-0.6218 + 0.6706) = 0.9837,$$

which lead to $\vec{\alpha} = [1.2474\ 0.8166\ 0.9837]^{\mathrm{T}}$. From the value of $\vec{\alpha}$, it can be expected that when the weight adjusted desirability approach is used, $d_1(F_{\mathrm{p}})$ would have the highest contribution on $D_{\mathrm{a(adj)}}$ but its contribution is reduced when compared to the previous case studies.

The optimization results are shown in table 5.28. The optimal parameter combinations obtained are the same set as in the previous extended case study in which the error terms are assumed to be i.i.d., and the expected value of indices E(DI) are almost identical to the values those shown in table 5.22. However, the predicted worst case scenarios DI_{05} seem worse than in the previous case. This can be explained by a strong positive correlation of $d_1(F_{\mathrm{p}})$ and $d_2(VB_{\mathrm{m}})$, i.e., higher than 0.9 over the selected parameter space, when the value of $d_2(VB_{\mathrm{m}})$ becomes low, then it is quite certain that the value $d_1(F_{\mathrm{p}})$ might become low as well, and vice versa. As a consequence, the variance of all DIs become larger as the correlations of desirability scores become stronger positive. Conversely, if the correlations are negative, the variance of DIs may become smaller.

Table 5.28: Optimal cutting conditions obtained from robust optimization

Index	Cutting parameters			Performance measures			Overall performance	
	f	a_p	v_c	$E(F_p)$	$E(VB_m)$	$E(t)$	E(DI)	DI_{05}
D_a	0.09	0.24	200	97.7777	79.1505	275.1475	0.5533	0.4239
	0.09	0.23	200	96.4827	79.5658	286.6209	0.5526	0.4247
	0.08	0.25	200	94.4341	80.6933	297.3696	0.5515	0.4273
	0.08	0.24	200	93.0124	81.1645	309.1512	0.5492	0.4280
	0.07	0.26	200	90.9498	81.7581	324.7461	0.5462	0.4298
D_g	0.09	0.24	200	97.7777	79.1505	275.1475	0.4970	0.3268
	0.09	0.23	200	96.4827	79.5658	286.6209	0.4957	0.3292
D_{PCA}	0.07	0.25	200	89.3063	82.3114	337.0605	0.6300	0.5084
$D_{a(adj)}$	0.07	0.26	200	90.9498	81.7581	324.7461	0.5730	0.4470
	0.07	0.25	200	89.3063	82.3114	337.0605	0.5717	0.4503
$D_{g(adj)}$	0.09	0.23	200	96.4827	79.5658	286.6209	0.5177	0.3420
	0.08	0.25	200	94.4341	80.6933	297.3696	0.5155	0.3456
	0.08	0.24	200	93.0124	81.1645	309.1512	0.5139	0.3487
	0.07	0.26	200	90.9498	81.7581	324.7461	0.5114	0.3525

Table 5.29: Normalized weights of the robust optimization with correlated errors

	$W_{d_1(F_p)}$	$W_{d_2(VB_m)}$	$W_{d_3(t)}$
D_a	0.3333	0.3333	0.3333
D_g	0.3333	0.3333	0.3333
D_{PCA}	0.4736	0.1483	0.3781
$D_{a(adj)}$	0.4093	0.2679	0.3228
$D_{g(adj)}$	0.4093	0.2679	0.3228

Note. All numbers are rounded to 4 digit accuracy after decimal point.

Regarding to the values of normalized weights shown in table 5.29, although the correlation $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ drops from -0.4788 (section 5.3.1) to -0.1204, changes in $W_{d_1(F_\mathrm{p})}$ values are so small, e.g., -0.0002 by D_PCA and -0.0066 by $D_\mathrm{a(adj)}$. This explains why the optimal cutting parameters shown in table 5.28 are identical to the optimal cutting parameters shown in table 5.22. For this extended case study, it has been shown that an increase of $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ by 0.3584 does not change the optimal solutions obtained from D_PCA, $D_\mathrm{a(adj)}$ and $D_\mathrm{g(adj)}$ which could imply that the optimal solutions of this case study does not seem to be so sensitive to changes in correlations.

5.4 An Optimization using Conditional Correlations

In the previous case studies, correlations and covariances of desirability scores are estimated using F_p, VB_m and t generated according to the experimental design shown in table 5.3. These correlations and covariances are used to represent the values of correlations and covariances on the selected parameter space. The values of $r_{(F_\mathrm{p},VB_\mathrm{m})}$ on the selected parameter space are all found to be negative due to the effects of changes in a_p value, and as already been mentioned in section 5.2.1 this negative correlation contradicts to the correlations found in [9, 41, 62]. This means that values of correlations and covariances could vary depending on sources of data or the design of experiment. Furthermore, since $r_{(F_\mathrm{p},VB_\mathrm{m})}$ are found to be positive in [9, 41, 62], it means that the correlations of performance measures mentioned in engineering studies are different from correlations which have been used in our optimization studies.

Instead of using correlations and covariances estimated from the experimental design, conditional correlations and covariances of $d_1(F_\mathrm{p})$, $d_2(VB_\mathrm{m})$ and $d_3(t)$ are used in the optimization. With an assumption that the correlation of F_p and VB_m does not change over the time space, the conditional correlation of F_p and VB_m can be estimated using the method explained in section 5.3.2 an example of which is illustrated in table 5.24.

The correlations $r_{(F_\mathrm{p},VB_\mathrm{m})}$ and $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ are plotted in figure 5.7 in which the grey transparent surface indicates the value of $r_{(F_\mathrm{p},VB_\mathrm{m})}$, and the another plane indicates the value of $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$. For the surface plot, the parameter v_c is fixed at 200 m/min, since v_c has small effects on F_p and VB_m and all optimal results obtained from the previous case studies contain v_c = 200 m/min. The surface plot shows that the values of $r_{(F_\mathrm{p},VB_\mathrm{m})}$ fluctuate only slightly in a range between 0.9615 and 0.9812 with the average value of 0.9740. By contrast, the values of $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ fluctuate moderately from 0.6754 to 0.9932 with the average value of 0.9080. The fluctuations in $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ are caused by the desirability transformation, e.g., for $f = 0.1$ mm, $a_\mathrm{p} = 0.3$ mm and $v_\mathrm{c} = 200$ m/min the value of F_p becomes large so that the values of $d_1(F_\mathrm{p})$ are approximately zero for all L_c while $VB_\mathrm{m} = 85.9369$ µm ($d_2(VB_\mathrm{m}) = 0.1429$) is generated at $L_\mathrm{c} = 2500$ m, and $VB_\mathrm{m} = 100.5124$ µm ($d_2(VB_\mathrm{m}) = 0.0086$) is reached at $L_\mathrm{c} = 3500$ m. Then, the values of $d_2(VB_\mathrm{m})$ afterwards (for $L_\mathrm{c} \geq 3500$ m) would be approximately zero; hence, for such cases, $r_{(F_\mathrm{p},VB_\mathrm{m})}$ is deteriorated by the desirability transformation and $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ is weaker than $r_{(F_\mathrm{p},VB_\mathrm{m})}$.

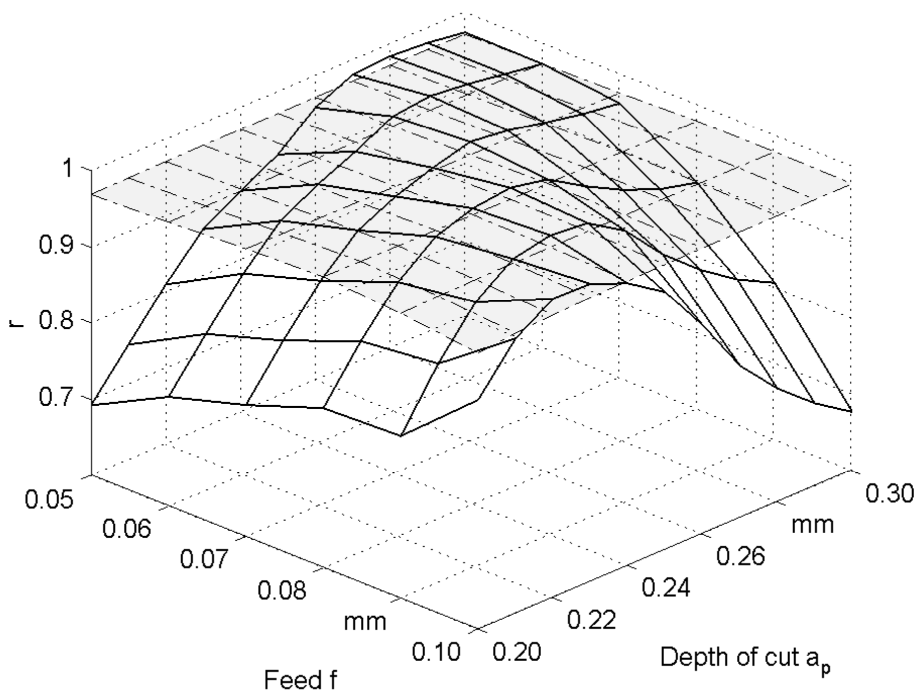


Figure 5.7: Surface plot of $r_{(F_{\mathrm{p}},VB_{\mathrm{m}})}$ and $r_{(d_1(F_{\mathrm{p}}),d_2(VB_{\mathrm{m}}))}$ at $v_{\mathrm{c}} = 200$ m/min

In such a case, it would be also reasonable to use correlations of performance measures in place of correlations of desirability scores in the optimization. Since the differences between the expected value of $r_{(F_{\mathrm{p}},VB_{\mathrm{m}})}$ and $r_{(d_1(F_{\mathrm{p}}),d_2(VB_{\mathrm{m}}))}$ are not so large ($\mathrm{E}(r_{(F_{\mathrm{p}},VB_{\mathrm{m}})}) = 0.9744$ and $\mathrm{E}(r_{(d_1(F_{\mathrm{p}}),d_2(VB_{\mathrm{m}}))}) = 0.9055$) and it has been demonstrated in previous case studies that small changes in correlations tend to have only small effects, the results obtained using $\mathrm{E}(r_{(F_{\mathrm{p}},VB_{\mathrm{m}})})$ and $\mathrm{E}(r_{(d_1(F_{\mathrm{p}}),d_2(VB_{\mathrm{m}}))})$ are expected to be similar.

The optimization problem used in this case is the optimization problem with correlated error terms as in section 5.3.2. The different between this section and section 5.3.2 is that conditional correlations and conditional covariances are used to adjusted the weights of desirability scores, while in section 5.3.2, conditional correlations are assumed for stochastic error terms and the correlations used to adjust the weights of

Table 5.30: Conditional covariance of the desirability scores

Variable	$d_1(F_\mathrm{p})$	$d_2(VB_\mathrm{m})$	$d_3(t)$
$d_1(F_\mathrm{p})$	0.0161	0.0088	0
$d_2(VB_\mathrm{m})$	0.0088	0.0055	0
$d_3(t)$	0	0	0

Table 5.31: Eigenvectors, eigenvalues, and normalized weights of PCs for the extended case study

	1st PC	2nd PC
Eigenvector	$\begin{bmatrix} -0.8706 \\ -0.4920 \end{bmatrix}$	$\begin{bmatrix} 0.4920 \\ -0.8706 \end{bmatrix}$
Eigenvalue	0.0211	0.0005
W_j	0.9756	0.0244

desirability scores are determined from the parameter space. The covariance matrix for PCA transformation is shown in table 5.30, of which the zero column and row of $d_3(t)$ are resulted from the assumption that the stochastic error of t is zero. Since ϵ_t is assumed to be zero, the expected conditional covariance matrix of desirability scores becomes a singular matrix, if PCA transformation is performed using this matrix, it is obvious that the results obtained from PCA-based DI are biased towards variances of $d_1(F_\mathrm{p})$ and $d_2(VB_\mathrm{m})$. Moreover, since $d_3(t)$ is known to be independent, there is no necessity for $d_3(t)$ to be decorrelated; hence, PCA transformation will be performed only with $d_1(F_\mathrm{p})$ and $d_2(VB_\mathrm{m})$, and the last row and column of the conditional covariance matrix are to be removed from the matrix.

Next, eigenvalues and eigenvectors are derived as shown in table 5.31. Then, the 1st PC and 2nd PC are transformed into PC scores and these PC scores are combined using the W_j shown in table 5.31 into a component score ($N_{1\&2}$). Again, in order to integrate $d_3(t)$ with $N_{1\&2}$, the formula based on the idea of weight adjusted desirability approach is used to compute D_PCA.

$$D_{\text{PCA}} = \frac{2 * \left[1 - \frac{1}{3}(r_{(d_1(F_\text{p}),d_2(VB_\text{m}))})\right] * N_{1\&2} + d_3(t)}{2 * \left[1 - \frac{1}{3}(r_{(d_1(F_\text{p}),d_2(VB_\text{m}))})\right] + 1} \tag{5.10}$$

For the weight adjustment method, using correlations of desirability scores, the values of α_1, α_2 and α_3 can be computed as:

$$\alpha_1 = 1 - \frac{1}{3}(0.9055 + 0) = 0.6982$$

$$\alpha_2 = 1 - \frac{1}{3}(0.9055 + 0) = 0.6982$$

$$\alpha_3 = 1 - \frac{1}{3}(0 + 0) = 1.0000,$$

which lead to $\vec{\alpha} = [0.6982\ 0.6982\ 1.0000]^\text{T}$. For the weight adjustment method, using correlations of performance measures, the values of $\hat{\alpha_1}$, $\hat{\alpha_2}$ and $\hat{\alpha_3}$ can be computed as:

$$\hat{\alpha_1} = 1 - \frac{1}{3}(0.9744 + 0) = 0.6752$$

$$\hat{\alpha_2} = 1 - \frac{1}{3}(0.9744 + 0) = 0.6752$$

$$\hat{\alpha_3} = 1 - \frac{1}{3}(0 + 0) = 1.0000,$$

which lead to $\vec{\hat{\alpha}} = [0.6752\ 0.6752\ 1.0000]^\text{T}$.

The results obtained from optimization are shown in table 5.32. The parameters $f = 0.09$ mm, $a_\text{p} = 0.24$ mm and $v_\text{c} = 200$ m/min are optimal for all indices except D_{PCA}. Since the optimal solutions obtained from D_{PCA} are likely to produce less F_p but slightly higher VB_m and t, it can be expected that influences of F_p on D_{PCA} are greater than on D_a, $D_{\text{a(adj)}}$ and $\hat{D}_{a(\text{adj})}$. For the geometric indices, the effects of small $d_2(VB_\text{m})$ seem to dominate the effects of correlation so that the same set of optimal solutions are obtained from D_g, $D_{\text{g(adj)}}$ and $\hat{D}_{g(\text{adj})}$. The differences between using correlations of desirability scores and using correlations of performance measures are also very small, as the same set of optimal solutions can be obtained from $D_{\text{a(adj)}}$ and $\hat{D}_{a(\text{adj})}$. Note that the results shown in table 5.28 are obtained from a different simulation run. The obtained values for $E(D_a)$, $E(D_g)$, D_{a05} and D_{g05} might be slightly different from table 5.32 due to the randomness of generator with errors approximately ± 0.0002.

Table 5.32: Optimal cutting conditions obtained using conditional correlations

Index	Cutting parameters			Performance measures			Overall performance	
	f	a_p	v_c	$E(F_p)$	$E(VB_m)$	$E(t)$	E(DI)	DI_{05}
D_a	0.09	0.24	200	97.7777	79.1505	275.1475	0.5534	0.4239
	0.09	0.23	200	96.4827	79.5658	286.6209	0.5527	0.4247
	0.08	0.25	200	94.4341	80.6933	297.3696	0.5516	0.4275
	0.08	0.24	200	93.0124	81.1645	309.1512	0.5492	0.4282
	0.07	0.26	200	90.9498	81.7581	324.7461	0.5462	0.4297
D_g	0.09	0.24	200	97.7777	79.1505	275.1475	0.4971	0.3268
	0.09	0.23	200	96.4827	79.5658	286.6209	0.4958	0.3293
D_{PCA}	0.08	0.25	200	94.4341	80.6933	297.3696	0.6117	0.4935
	0.08	0.24	200	93.0124	81.1645	309.1512	0.6096	0.4945
	0.07	0.26	200	90.9498	81.7581	324.7461	0.6066	0.4961
$D_{a(adj)}$	0.09	0.24	200	97.7777	79.1505	275.1475	0.5903	0.4771
$D_{g(adj)}$	0.09	0.24	200	97.7777	79.1505	275.1475	0.5304	0.3684
	0.09	0.23	200	96.4827	79.5658	286.6209	0.5278	0.3699
$\hat{D}_{a(adj)}$	0.09	0.24	200	97.7777	79.1505	275.1475	0.5939	0.4822
$\hat{D}_{g(adj)}$	0.09	0.24	200	97.7777	79.1505	275.1475	0.5338	0.3727
	0.09	0.23	200	96.4827	79.5658	286.6209	0.5311	0.3741

Table 5.33: Normalized weights of the optimization using conditional correlations

	$W_{d_1(F_\mathrm{p})}$	$W_{d_2(VB_\mathrm{m})}$	$W_{d_3(t)}$
D_a	0.3333	0.3333	0.3333
D_g	0.3333	0.3333	0.3333
D_PCA	0.3703	0.2124	0.4173
$D_\mathrm{a(adj)}$	0.2913	0.2913	0.4173
$D_\mathrm{g(adj)}$	0.2913	0.2913	0.4173
$\hat{D}_{a(\mathrm{adj})}$	0.2873	0.2873	0.4255
$\hat{D}_{g(\mathrm{adj})}$	0.2873	0.2873	0.4255

Note. All numbers are rounded to 4 digit accuracy after decimal point.

For the further investigation the normalized weights for index optimization are determined as shown in table 5.33. The values of $W_{d_3(t)}$ are equal for D_PCA, $D_\mathrm{a(adj)}$ and $D_\mathrm{g(adj)}$ because the D_PCA is adapted based on the same concept of weight adjustment; hence, the differences of D_PCA from $D_\mathrm{a(adj)}$ are the weight allocation of $W_{d_1(F_\mathrm{p})}$ and $W_{d_2(VB_\mathrm{m})}$. For D_PCA, it has been shown in table 5.30 that $d_1(F_\mathrm{p})$ has approximately thrice the variance of $d_2(VB_\mathrm{m})$ and there are only 2 variables involved in PCA transformation, so it is clear that $W_{d_1(F_\mathrm{p})}$ should be greater than $d_2(VB_\mathrm{m})$. For this case study, since the covariances shown in table 5.30 are conditional covariances, D_PCA is an index which allocates importance of desirability scores according to the conditional correlations and conditional variances which means that its variance bias would prioritize desirability scores with large stochastic errors. In addition, it has been demonstrated that the concept of PCA-based DI is not compatible with singular covariance matrices such in table 5.30.

5.5 Alternative Optimization Problem

According to the negative value of $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ determined from the parameter space, it is possible that the effects of a_p and f on F_p might be too large. For this reason, the specific passive force k_p which is passive force per unit area of cutting, might be a better performance measure for F_p. In general, k_p is defined as a function of the chip width b and the chip thickness h as

$$k_\mathrm{p} = \frac{F_\mathrm{p}}{b * h}. \tag{5.11}$$

Since b and h can be derived from the following equations:

$$b = \frac{a_\mathrm{p}}{\sin(\kappa)}, \tag{5.12}$$

$$h = f * \sin(\kappa), \tag{5.13}$$

where κ denotes the cutting edge angle, equation 5.11 can be extended as

$$k_\mathrm{p} = \frac{F_\mathrm{p}}{b * h} = \frac{F_\mathrm{p}}{\frac{a_\mathrm{p}}{\sin(\kappa)} * f * \sin(\kappa)} = \frac{F_\mathrm{p}}{f * a_\mathrm{p}}. \tag{5.14}$$

When the conditional correlation of k_p and VB_m is determined, f and a_p are set as constant, it is obvious that k_p in equation 5.14 is a linear transformation of F_p, and $r_{(F_\mathrm{p},VB_\mathrm{m})}$ is identical to $r_{(k_\mathrm{p},VB_\mathrm{m})}$. However, $r_{(d_1(F_\mathrm{p}),d_2(VB_\mathrm{m}))}$ may not be identical to $r_{(d_1(k_\mathrm{p}),d_2(VB_\mathrm{m}))}$ because the DFs are not linear transformations.

For the alternative model, since there is no information on the favorable range of parameters available, the range of parameters of table 5.2 will be used. The mathematical model of k_p can be reformulated from equation 5.2, as is formulated as:

$$k_\mathrm{p} = \frac{\hat{f}_1(f, a_\mathrm{p}, v_\mathrm{c}) + \epsilon_{F_\mathrm{p}}}{a_\mathrm{p} * f}. \tag{5.15}$$

There are problems with selecting specifications for k_p, since k_p is a performance measure which is not used often in optimizations. It is known that the yield strength of alloy steel AISI-6150 lies approximately from 412 MPa to 1690 MPa depending on the type heat treatment and the temperature of treatment. In general, yield strength is measured by using a tensile testing machine to pull the metal apart, so it may not be compared with F_p and k_p, and in the turning process, plastic deformation can be found from material, e.g., as found in [47]; hence, the yield strength of workpiece cannot be used as the upper specification limit. In contrast, PCBN cutting tools are known to have excellent strength and wear resistance, their strength is apparently too high for the upper specification limit of k_p. For these reasons, the upper specification limit of k_p is assumed to be 5,000 N/mm^2, and a value of k_p lower than 2,000 N/mm^2 is assumed to provide no further improvement. In fact, the values of $k_p \leq$ 2,000 N/mm^2 are almost impossible to be induced in this case study, especially for parameters which contain small f and a_p because the denominators for equation 5.14 are small. On the other hand, parameters which have large f and a_p produce also high F_p. For example, $F_p \leq 128$ N should be induced in order to achieve $k_p \leq$ 2,000 N/mm^2 with $f = 0.16$ mm and $a_p = 0.4$ mm, nevertheless it was found in the experiments of [41] that $F_p \approx 230$ N are induced from $f = 0.13$ mm and $a_p = 0.4$ mm. The configuration for Harrington's function are defined as $(k_p^{(1)}, d_1^{(1)}) = (2000,\ 0.99)$ and $(k_p^{(2)}, d_1^{(2)}) = (5000, 0.01)$. The desirability transformation of k_p is illustrated in 5.8.

Since the value of F_p cannot be controlled through k_p for this case, an additional constraint of F_p is added in order to assure the stability of the operation.

$$F_{p95} \leq 200 \quad \text{N}, \tag{5.16}$$

where F_{p95} denotes the 95th percentile of F_p, and the value of $F_p \approx 240$ N is approximately the maximum value of F_p found in [41], so by setting $F_{p95} \leq 200$ N, the stability of the operation could be ensured.

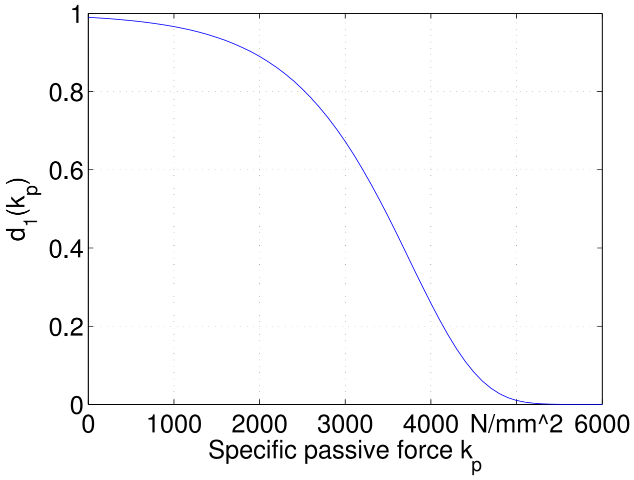
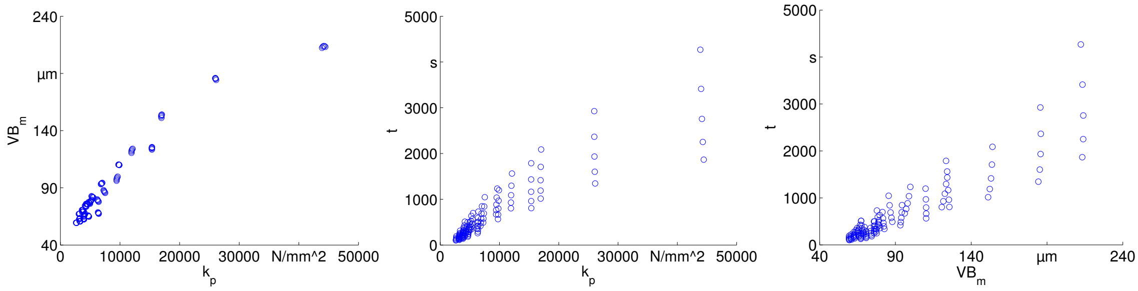


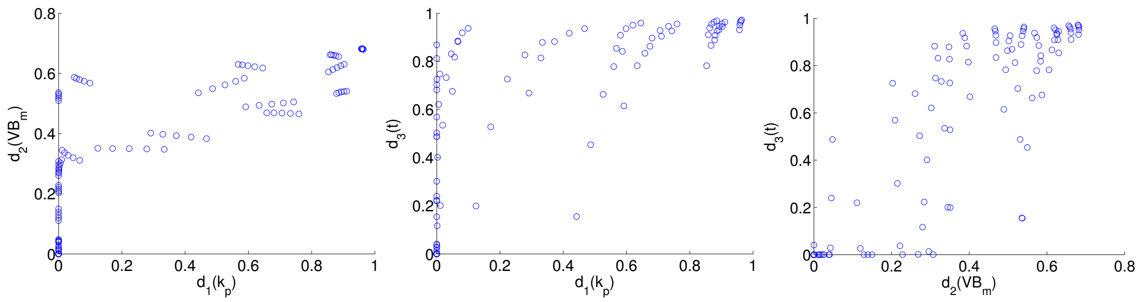
Figure 5.8: Configured Harrington's one-sided DF for k_{p}

From sections 5.3.1 and 5.3.2, it has been found that the correlation of DFs are found to be smaller, when uncertainty analysis is performed, and the computational time is also long. Therefore, there would be no uncertainty analysis performed on correlations and covariances. Correlations and covariances are then generated from the 5^3 factorial design as performed in section 5.2.1. The scatter plots of k_{p}, VB_{m} and t are illustrated in figure 5.9, and all correlations are found to be positive. According to the fact that k_{p}, VB_{m} and t are objectives to be minimized, their very strong positive correlations in the parameter space reflect that conflicts between performance measures might be absent or not significant. For this case, the optimal parameters are expected to be the highest combination of f, a_{p} and v_{c} from which the constraints of Rz in equation 5.1 and F_{p} in equation 5.16 are satisfied.



(a) $r_{(k_\mathrm{p},VB_\mathrm{m})} = 0.9587$ (b) $r_{(k_\mathrm{p},t)} = 0.9122$ (c) $r_{(VB_\mathrm{m},t)} = 0.9190$

Figure 5.9: Scatter plots of the performance measures



(a) $r_{(d_1(k_\mathrm{p}),d_2(VB_\mathrm{m}))} = 0.7860$ (b) $r_{(d_1(k_\mathrm{p}),d_3(t))} = 0.7678$ (c) $r_{(d_2(VB_\mathrm{m}),d_3(t))} = 0.8846$

Figure 5.10: Scatter plots of the desirability scores

After the desirability transformation is performed, the scatter plots of desirability scores are illustrated in figure 5.10. From figures 5.10a and 5.10b, there exist numerous of $d_1(k_\mathrm{p})$ which are approximately zero and the correlations $r_{(k_\mathrm{p},VB_\mathrm{m})}$ and $r_{(k_\mathrm{p},t)}$ are deteriorated by desirability transformation. For this case study, since F_p is replaced by k_p, the favorable range of parameters is still unknown. For PCA transformation, the covariance matrix of desirability scores is shown in table 5.34 and the derived eigenvectors and eigenvalues are shown in table 5.35. Since $r_{(d_1(k_\mathrm{p}),d_2(VB_\mathrm{m}))}$, $r_{(d_1(k_\mathrm{p}),d_3(t))}$ and $r_{(d_2(VB_\mathrm{m}),d_3(t))}$ are positive, their values are very close, and according to diagonal components of the covariance matrix that $c_{3,3} > c_{1,1} > c_{2,2}$, it could be

Table 5.34: Covariance of the desirability scores

Variable	$d_1(k_\mathrm{p})$	$d_2(VB_\mathrm{m})$	$d_3(t)$
$d_1(k_\mathrm{p})$	0.1288	0.0702	0.1133
$d_2(VB_\mathrm{m})$	0.0702	0.0618	0.0905
$d_3(t)$	0.1133	0.0905	0.1692

Table 5.35: Eigenvectors, eigenvalues, and normalized weights of PCs

	1st PC	2nd PC	3rd PC
Eigenvector	$\begin{bmatrix} 0.5806 \\ 0.4110 \\ 0.7028 \end{bmatrix}$	$\begin{bmatrix} -0.8026 \\ 0.1441 \\ 0.5788 \end{bmatrix}$	$\begin{bmatrix} -0.1366 \\ 0.9002 \\ -0.4135 \end{bmatrix}$
Eigenvalue	0.3157	0.0345	0.0096
W_j	0.8773	0.0959	0.0268

expected that PCA-based DI would assign $d_3(t)$ as the most important for the scores and $d_2(VB_\mathrm{m})$ as the least important. It also agrees with the data shown in table 5.35 that the first eigenvector $\vec{a_1}$ contains only positive elements with a_{12} as the smallest element and a_{13} as the largest element.

For the weight adjustment method, the values of α_1, α_2 and α_3 can be computed as:

$$\alpha_1 = 1 - \frac{1}{3}(0.7860 + 0.7678) = 0.4821$$

$$\alpha_2 = 1 - \frac{1}{3}(0.7860 + 0.8846) = 0.4431$$

$$\alpha_3 = 1 - \frac{1}{3}(0.7678 + 0.8846) = 0.4492,$$

which lead to $\vec{\alpha} = [0.4821\ \ 0.4431\ \ 0.4492]^\mathrm{T}$. Since all correlation coefficients are strongly positive, the values of the weight adjustment factors become small. Due to the small difference between values of α_1, α_2 and α_3, the effects of weight adjustment factors can be expected to be so small.

The optimal results obtained from DI optimization are shown in table 5.36. It has been shown that for this case study, $f = 0.1$ mm, $a_\mathrm{p} = 0.4$ mm and $v_\mathrm{c} = 200$ m/min is the only optimal solution. In previous case studies, F_p was an obstacle of raising parameters f and a_p which is replaced by k_p and appear in this case study as a constraint. For this case, there is no disadvantage against the objectives for raising f and a_p, and $f = 0.1$ mm and $a_\mathrm{p} = 0.4$ mm are the highest combination which can satisfy the constraints. The results show that the effects of correlations and covariances could not affect results obtained; therefore, this alternative model is not used as the main model to demonstrate the optimization methods in this research.

Table 5.36: Optimal cutting conditions obtained using conditional correlations

Index	Cutting parameters			Performance measures			Overall performance	
	f	a_p	v_c	$\mathrm{E}(k_\mathrm{p})$	$\mathrm{E}(VB_\mathrm{m})$	$\mathrm{E}(t)$	E(DI)	DI_{05}
D_a	0.1	0.4	200	3,973.3	63.5975	144.5324	0.7070	0.6025
D_g	0.1	0.4	200	3,973.3	63.5975	144.5324	0.6835	0.5499
D_PCA	0.1	0.4	200	3,973.3	63.5975	144.5324	0.7340	0.6349
$D_\mathrm{a(adj)}$	0.1	0.4	200	3,973.3	63.5975	144.5324	0.7039	0.5967
$D_\mathrm{g(adj)}$	0.1	0.4	200	3,973.3	63.5975	144.5324	0.6804	0.5439

Table 5.37: Normalized weights of the optimization using alternative model

	$W_{d_1(k_\mathrm{p})}$	$W_{d_2(VB_\mathrm{m})}$	$W_{d_3(t)}$
D_a	0.3333	0.3333	0.3333
D_g	0.3333	0.3333	0.3333
D_PCA	0.3519	0.2356	0.4125
$D_\mathrm{a(adj)}$	0.3508	0.3224	0.3268
$D_\mathrm{g(adj)}$	0.3508	0.3224	0.3268

Note. All numbers are rounded to 4 digit accuracy after decimal point.

The normalized weights are shown in table 5.37. As it has been expected, as correlations between desirability scores are approximately the same, PCA-based DI would allocate importance of desirability scores depending mainly on their variance. From the overall point of view, the weights of desirability scores are adjusted only slightly for this case.

When the conditional correlation is used it is obvious that $W_{d_1(k_\mathrm{p})}$ and $W_{d_2(VB_\mathrm{m})}$ would be moderately reduced, while $W_{d_3(t)}$ would be increased. As it has been described in equation 5.14 that the conditional $r_{(F_\mathrm{p},VB_\mathrm{m})}$ is identical with $r_{(k_\mathrm{p},VB_\mathrm{m})}$, if the conditional correlations of performance measures are used in the optimization, The adjusted normalized weights using $D_{\mathrm{a(adj)}}$ and $D_{\mathrm{g(adj)}}$ would be very close to the results in table 5.33. The correlations $r_{(k_\mathrm{p},VB_\mathrm{m})}$ and $r_{(d_1(k_\mathrm{p}),d_2(VB_\mathrm{m}))}$ at $v_\mathrm{c} = 200$ m/min are plotted in figure 5.11 in which the grey transparent surface indicates the value of $r_{(k_\mathrm{p},VB_\mathrm{m})}$, and the other plane indicates the value of $r_{(d_1(k_\mathrm{p}),d_2(VB_\mathrm{m}))}$. The cause of negative $r_{(k_\mathrm{p},VB_\mathrm{m})}$ are unknown but it can be suspected that there might be some measurement errors in small a_p, or condition of the operation might be different. If the conditional correlations are to be used in the optimization, it is recommended that parameters with such a_p smaller than 0.2 mm should be excluded.

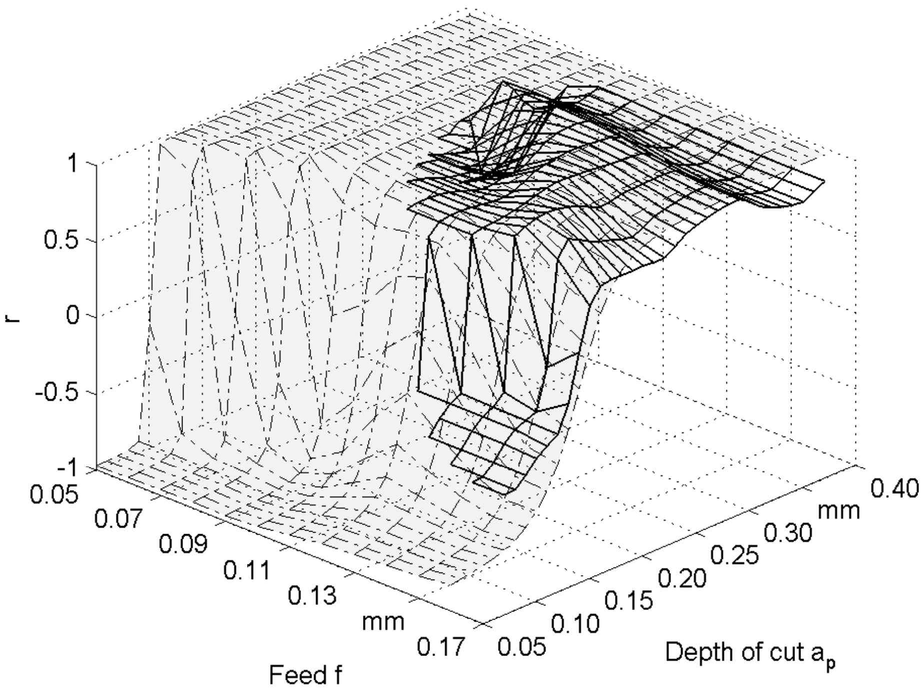


Figure 5.11: Surface plot of $r_{(k_{\rm p},VB_{\rm m})}$ and $r_{(d_1(k_{\rm p}),d_2(VB_{\rm m}))}$ at $v_{\rm c}$ = 200 m/min

An experimental optimization has been performed with this model, assuming that $r_{(d_1(k_{\rm p}),d_2(VB_{\rm m}))} = 1$, so that $W_{d_1(k_{\rm p})}$, $W_{d_2(VB_{\rm m})}$ and $W_{d_3(t)}$ are adjusted with the maximum effects which can be adjusted by $\vec{\alpha}$ with $\eta = 1$. The optimal results obtained using $D_{\rm a(adj)}$ and $D_{\rm g(adj)}$ are still $f = 0.1$ mm, $a_{\rm p} = 0.4$ mm and $v_{\rm c} = 200$ m/min with the values $\mathrm{E}(D_{\rm a(adj)}) = 0.7428$, $D_{\rm a(adj)05} = 0.6530$, $\mathrm{E}(D_{\rm g(adj)}) = 0.7167$ and $D_{\rm g(adj)05} = 0.5951$. Thus, the same solution would be also obtained when the conditional correlations are used.

The facts that have been learned from this case study are; first, the use of correlations in the parameter space can indicate conflicts between performance measures that might occur in the optimization. Second, $k_{\rm p}$ has a potential in practice to be considered as a performance measure in optimization, since it could be used to indicate the condition of cutting tool and the effectiveness of turning. Its correlations with

VB_{m} are found to be positive for both correlation in parameter space and conditional correlation. Third, the value of correlation coefficients are also found to be lower after the DF transformation, the correlation coefficients of performance measures could be used instead, as it has been demonstrated in section 5.4. Finally, the conditional correlations of k_{p} with other performance measures are identical to the conditional correlations of F_{p} with the others, since in that case k_{p} is a linear transformation of F_{p}.

5.6 Summary and Conclusion

The PCA-based desirability approach and weight adjusted desirability approach have been demonstrated in this chapter, using case studies in which different correlations and mathematical models are used in optimizations. The purpose of this section is to review the results which have been shown in the previous sections, and give a summary of the advantages and disadvantages of using the proposed desirability indices (DIs).

In order to compare the optimization results which are obtained from different correlation information, the results of section 5.2.1 is compared with section 5.2.2 with correlations calculated from a smaller parameter space which are stronger than those of section 5.2.1. It is clear that correlations have effects on optimization results but such small changes as in section 5.2.1 and section 5.2.2 may not affect the results. The results obtained from geometric indices such D_{g} and $D_{\mathrm{g(adj)}}$ are found to have no significant differences, since they are heavily weighted by the small values of $d_2(VB_{\mathrm{m}})$. When the results of weight adjusted indices are compared with the PCA-based index, variance biases can be found with the results of PCA-based desirability approach. In order to solve the variance biases issue, a modification of the PCA-based index will be necessary of as it has been discussed in section 5.2.4.

Robust optimizations have been demonstrated in section 5.3 in which uncertainty analysis is performed. In section 5.3.1 the stochastic errors of performance measures are assumed to be independent and identically distributed (i.i.d.), whereas they are correlated in section 5.3.2. The values of correlation and covariances are estimated from a Monte-Carlo method with 1 million iterations, and it has been found that the computational effort required is high. In practice, if the decision is needed to be made promptly, uncertainty analysis should be performed only for performance measures, as small changes in correlations may not affect the solutions. Moreover, large uncertainty of correlations indicates lack of information which means that further investigations might be necessary. The results have shown that with correlated stochastic errors, the expected value of DIs may change only very slightly but their variance could can change remarkably. Therefore, it is highly recommended to use correlated stochastic errors for best/worst case analysis.

Due to the existence of conditional correlations, a robust optimization using conditional correlations is performed in section 5.4 and the optimal results obtained are noticeably different from those of sections 5.3.1 and 5.3.2. This means that selecting correlations in optimization is also an important process. If correlations are used which do not reflect preferences, the optimization can mislead. When conditional correlations are used instead of correlations in parameter space, the PCA-based desirability approach shows some compatibility issues with conditional correlations, not only when the covariance matrix of desirability scores is singular but also when the PCA-based desirability approach is performed, the covariance matrix of desirability scores must be assumed to be equal all over the parameter space.

In section 5.5, an alternative optimization problem is introduced. With this alternate usage of correlations in parameter space the insignificance of conflicts between performance measures is detected. It has been shown that the specific passive force (k_{p}) which are found to have positive correlations, can be used to replace passive force (F_{p}).

Overall, the weight adjusted desirability approach is shown to have a better flexibility than PCA-based desirability approach. The definition of weight adjustment factors are defined as coefficients so that the original weights of performance measures can be excluded from the formula and the original formulas of DIs are modified only slightly; hence, we also have less variables and complexity than with the PCA-based desirability approach. On the other hand, a possible bias can be caused by weight adjusted desirability approach, when the number of performance measures becomes large as it has been explained in section 4.1.2.1 and 4.1.2.2.

For the current version of the PCA-based desirability approach, the known incompatibilities appear when the importance of performance measures are unequal and when the covariance matrix is a singular matrix. The variance biased characteristic of the PCA-based desirability approach allow the PCA-based DI to have some unique characteristics. When the covariances in the parameter space are used in PCA transformation D_{PCA} tends to give priority to performance measures which have strong negative correlations and high potential for being improved by changing operating parameters (variance). In contrast, when conditional covariances are used, D_{PCA} would allocate priority to performance measures which have strong negative correlations and high stochastic errors. Due to compatibility issues of the PCA-based desirability approach, it is recommended only when performance measures are equally important and correlations in parameter space are used.

The geometric indices such as D_{g} and $D_{\mathrm{g(adj)}}$ are absolutely preferred, if the optimization goals include to improve especially the weakest performance aspects and balance all performance aspects. The drawbacks of these indices are the by-products of their advantages, if particular values of the desirability score are relatively low, e.g., $d_2(VB_{\mathrm{m}})$ in the case studies in this chapter, D_{g} and $D_{\mathrm{g(adj)}}$ would give priority highly to such a performance measure. As consequences, the effects of correlation might be dominated and potentials for improving other performance measures could be diminished.

As a conclusion for this chapter, in an optimization of correlated performance measures using desirability approach, correlations and covariances should be estimated by the method from which the obtained correlations and covariances best match preferences of the decision maker. In general, it cannot be concluded whether correlations in parameter space or conditional correlations should be preferred; therefore, the choice would depend on the situation of the optimization problem and preference of the decision maker. Meanwhile, the desirability index which best match the preferences is to be selected for the optimization. For example, $D_{\mathrm{g(adj)}}$ when the balance among desirability scores is to be maintained while correlation information is to be taken into account.

Chapter 6

Summary and Conclusion

As a result of this research, 2 primary methodologies of desirability approach which are the principal component analysis (PCA) based desirability approach and the weight adjusted desirability approach have been developed and proposed.

The first optimization methodology, PCA-based desirability approach, has been inspired by the utilization of PCA in Taguchi's method that have been developed since 1997. The advantage of using the PCA-based desirability approach over PCA-based Taguchi is that the overall performance index, PCA-based desirability index (DI), is formulated based on the principle of strict monotonicity so that the optimality of results can be assured by the theorem of Legrand and Touati [26].

The alternative framework for PCA-based desirability approach which is called weight adjusted desirability approach, is developed in parallel aiming at a better simplicity and flexibility. The main idea of this method is to define and introduce weight adjustment coefficients for the traditional formulas of the DI. As a result from its flexibility, weight adjusted desirability approach has more potential to be adapted to match the expert's preferences, as an example demonstrates which is given at the end of section 4.1.1.

The effectiveness of the proposed methods has been verified with case studies of hard turning of AISI 6150 steel, in which inspections have been performed using not only deterministic and stochastic models but also comparisons between uses of different correlations. The results can be summarized as following:

- The range of parameters and experimental design have influence on the estimation of correlations estimated. If the optimal solutions are sensitive to changes in preferences, e.g., optimal solutions change with a small change in correlations, special caution must be taken. In case studies of hard turning of AISI 6150 steel, it has been found that optimal solutions are not sensitive to small changes in correlations of desirability scores, as the optimal parameter combinations obtained in sections 5.3.1 and 5.3.2 are identical although the difference in $r_{(d_1(F_{\mathrm{p}}),d_2(VB_{\mathrm{m}}))}$ is more than 0.3.

- Correlations of performance measures are not equal to correlations of desirability scores because desirability functions (DFs) are in general not linear transformations. There are possibilities for desirability scores to have much stronger than their performance measures as in section 5.2.1, or weaker correlations than their performance measures as in section 5.5. In case the correlations of performance measures are deteriorated by DFs, using the correlation coefficients of performance measures instead can be an alternative, as it has been demonstrated in section 5.4, when the weight adjusted desirability approach is applied.

- It has been analyzed at the end of section 5.2.3 that the PCA-based desirability approach is shown to be an optimization method which has unique characteristics which have not been offered by the traditional DIs. The PCA-based DI tends to prioritize performance measures which have more negative correlations and higher variances than others. When correlations in parameter space are utilized, e.g., in sections 5.2.1 and 5.2.2, the variance bias of the PCA-based desirability approach would give priority to performance measures which have potential for being improved by changing operating parameters. In case that conditional correlations are used, e.g., in section 5.4, priority would be given to performance measures which have high stochastic errors.

- The known limitations of the PCA-based desirability approach are that all performance measures should be equally important, its formulas are not customizable and difficult to modify, and especially, it have compatibility issues with some singular covariance matrices as it shows in examples 3.2.4 and 3.2.5. Therefore, in section 5.4, the cutting time t, an independent measure was handled separately and specially in the PCA-based desirability approach.

- The weight adjusted desirability approach is shown to be a simple, flexible and customizable method. It has been shown in case studies that the adjusted weights can be simply applied, have no particular issues with independent variable and singular correlation matrix which are found in section 5.4 and can be adapted to meet requirements.

- Geometric DIs can be heavily weighted by desirability scores which have a relatively low value, and there is a potential that this way effects of integrating correlations are dominated. The results obtained in all case studies for the geometric index D_{g} are found to be very similar with the results from the weight adjusted geometric index $D_{\mathrm{g(adj)}}$.

- Correlations in parameter space and conditional correlations have in general different meaning and applications. In multi-objective optimization of correlated performance characteristics, it is very essential that the correlations used match the preferences of the expert. If wrong correlations which do not match the expert's preferences are used, the outcomes of optimization might not match the expert's preferences, unless the values of correlations in parameter space and conditional correlations are very similar. For example, if the expert intends to use conditional correlations in an optimization (as performed in section 5.4), but correlations in parameter space is used instead (as performed in section

5.3.2) due to the availability of correlations in optimization problems. Then, the results obtained from the optimization are likely erroneous.

From previous literature, there was no guideline provided whether correlations in parameter space or conditional correlations should be used in optimization. As an outcome of this research, it is recommended that conditional correlations should be used if the optimization problem concerns with long-term production or mass production, since conditional correlations could indicate the degree of dependence between measures without influences from changes in parameters and in mass production, changes in parameters would not be so large so that the operating conditions could significantly change. When the optimization is dealing with short-term decision making, correlations in parameter space would be recommended.

The field of applications of the PCA-based desirability approach and the weight adjusted desirability approach is not limited to only the turning process. They are expected to be beneficial for any optimization problems which have correlated performance characteristics. For a correlated multi-objective optimization problem, as a lack of knowledge regarding performance characteristics could lead to unintended results, it is strongly recommended that investigations on performance characteristics and their correlations should be prior to the optimization.

As recommendations for further research topics, it is recommended that Harrington's DFs should be modified before performing the derivation of asymptotic distribution of DIs, since it was already proven that the distribution of Harrington's DFs have non-trivial distributions, e.g., double log-normal. Due to the reason that Harrington's one-sided DF was developed to convert measures from real number to $[0, 1]$, it is constructed with 2 exponentials. Actually, most of performance characteristics are non-negative and have one-sided specifications, for example, processing time, tool wears, surface roughness, costs, power required and magnitude of cutting forces. Moreover, all of the aforementioned characteristics are smaller-the-better (STB) variables. According to the aforementioned reasons, there are possibilities to develop alternative DFs, e.g., with only 1 exponential and has a log-normal distribution. Subsequently, the derivation of asymptotic distribution of weight adjusted DIs should be much less complicate.

On the other hand, the asymptotic distribution of PCA-based DI seems to be very complicated, if uncertainty analysis is performed on covariances and eigenvectors, as it has been demonstrated in example 3.2.6 where elements of eigenvectors even were not continuously changing.

Bibliography

[1] E. Y. T. Adesta et al. Tool wear and surface finish investigation in high speed turning using cermet insert by applying negative rake angles. *European Journal of Scientific Research*, 38(2):180–188, 2009.

[2] J. Antony. Multi-response optimization in industrial experiments using Tagchis quality loss function and principal component analysis. *Quality and Reliability Engineering International*, 16(1):3–8, February 2000.

[3] M. Bashiri and A. Salmasnia. Decision making for interactive optimization of correlated desirability functions. In *Industrial Engineering and Engineering Management, 2009. IEEM 2009. IEEE International Conference on*, pages 2075 – 2079, dec. 2009.

[4] Y. Cao. Pareto front. MATLAB Central File Exchange, `http://www.mathworks.com/matlabcentral/fileexchange/17251`. Retrieved July 29, 2008.

[5] Y. K. Chou and C. J. Evans. Tool wear mechanism in continuous cutting of hardened tool steels. *Wear*, 212(1):59–65, 1997.

[6] B. S. Choudhury, S. Datta, R. S. Sen, B. Oraon, and G. Majumdar. Parametric optimization of electroless Ni-P coating using weighted principal component analysis (WPCA) and Taguchi method. *International Journal of Applied Engineering Research*, 5(4):601–618, 2010.

[7] S. Datta, S. S. Mahapatra, and A. Bandyopadhyay. Elimination of multi-response correlation while applying Taguchi philosophy in optimization of submerged arc weld. *National Seminar on Joining Processes: Challenges for Quality, Design and Development, organized by Mechanical and Production Engineering Department*, March 2010.

[8] E. P. DeGarmo, J. T. Black, and R. A. Kohser. *DeGarmo's Materials and Processes in Manufacturing*. Wiley, 10th edition, August 2007.

[9] B. Denkena, D. Boehnke, and R. Meyer. Reduction of wear induced surface zone effects during hard turning by means of new tool geometries. *Production Engineering*, 2:123–132, 2008.

[10] G. Derringer. A balancing act: Optimizing a product's properties. *Quality Progress*, 27(6):51–58, June 1994.

[11] G. Derringer and R. Suich. Simultaneous optimization of several response variables. *Journal of Quality Technology*, 12(4):214–219, 1980.

[12] DIN EN ISO 4288: Geometrical Product Specifications (GPS) - Surface texture: Profile method - rules and procedures for the assessment of surface texture. ISO, Geneva, Switzerland, 1998.

[13] C.-X. Feng. An experimental study of the impact of turning parameters on surface roughness. Number 2036, Texas, USA, May 2001. Industrial Engineering Research Conference.

[14] D. Fuller and W. Scherer. The desirability function: underlying assumptions and application implications. In *1998 IEEE International Conference on Systems, Man, and Cybernetics*, volume 4, pages 4016 –4021, oct 1998.

[15] M. P. Groover. *Fundamentals of Modern Manufacturing: Materials, Processes, and Systems*. Wiley, 3rd edition, March 2006.

[16] W. Härdle and L. Simar. *Applied Multivariate Statistical Analysis*. Springer, 2003.

[17] J. Harrington. The desirability function. *Industrial Quality Control*, 21(10):494–498, 1965.

[18] N. Henkenjohann. *Eine adaptive sequentielle Prozedur zur effizienten Optimierung des CNC-gesteuerten Drückprozesses*. Phd-thesis, Technische Universität Dortmund, December 2006.

[19] H. Hotelling. Analysis of a complex of statistical variables into principal components. *Journal of Educational Psychology*, 24:417–441 and 498–520, 1933.

[20] R. A. Johnson and D. W. Wichern. *Applied Multivariate Statistical Analysis*. Prentice Hall, 6th edition, April 2007.

[21] H. F. Kaiser. The application of electronic computers to factor analysis. *Educational and Psychological Measurement*, 20(1):141–151, April 1960.

[22] K. Kandananond. Characterization of FDB sleeve surface roughness using the Taguchi approach. *European Journal of Scientific Research*, 33(2):330–337, 2009.

[23] E. KIlIçkap, O. ÇakIr, M. Aksoy, and A. Inan. Study of tool wear and surface roughness in machining of homogenised SiC-p reinforced aluminium metal matrix composite. *Journal of Materials Processing Technology*, 164-165:862 – 867, 2005. AMPT/AMME05 Part 2.

[24] K.-J. Kim and D. K. J. Lin. Simultaneous optimization of mechanical properties of steel by maximizing exponential desirability functions. *Journal of the Royal Statistical Society Series C*, 49(3):311–325, 2000.

[25] E. D. Kirby. Optimizing the turning process toward an ideal surface roughness target. *Journal of Industrial Technology*, 26(1), January 2010.

[26] A. Legrand and C. Touati. How to measure efficiency? In *Proceedings of the 2nd International Conference on Performance Evaluation Methodologies and Tools*, ValueTools '07, pages 8:1–8:8, Institute for Computer Sciences, Social-Informatics and Telecommunications Engineering (ICST), Brussels, Belgium, 2007.

[27] H.-C. Liao. Multi-response optimization using weighted principal component. *The International Journal of Advanced Manufacturing Technology*, 27:720–725, 2006.

[28] S. N. Lophaven, H. B. Nielsen, and J. Søndergaard. DACE A matlab Kriging Toolbox, August 2002.

[29] S. S. Mahapatra, A. Patnaik, and P. K. Patnaik. Parametric analysis and optimization of cutting parameters for turning operations based on Taguchi method. Coimbatore, India, July 2006. International Conference on Global Manufacturing and Innovation.

[30] MATLAB. *version 7.9.0.529 (R2009b)*. The MathWorks Inc., Natick, Massachusetts, 2009.

[31] S. Moshat, S. Datta, A. Bandyopadhyay, and P. K. Pal. Optimization of CNC end milling process parameters using PCA-based Taguchi method. *International Journal of Engineering, Science and Technology*, 2(1):92–102, 2010.

[32] S. Mostaghim, H. Trautmann, and O. Mersmann. Preference-based multi-objective particle swarm optimization using desirabilities. In *Proceedings of the 11th International Conference on Parallel Problem Solving from Nature: Part II*, PPSN'10, pages 101–110, Berlin, Heidelberg, 2010. Springer-Verlag.

[33] P. O'Neil. *Advanced Engineering Mathematics*. CL Engineering, 2011.

[34] K. Pearson. On lines and planes of closest fit to systems of points in space. *Philosophical Magazine*, 2(6):559–572, 1901.

[35] S. B. Rao. Tool wear monitoring through the dynamics of stable turning. *ASME Journal of Engineering for Industry*, 108:183–190, 1986.

[36] B. Routara, S. Mohanty, S. Datta, A. Bandyopadhyay, and S. Mahapatra. Combined quality loss (CQL) concept in WPCA-based Taguchi philosophy for optimization of multiple surface quality characteristics of uns C34000 brass in cylindrical grinding. *The International Journal of Advanced Manufacturing Technology*, 51:135–143, 2010.

[37] B. C. Routara, A. Bandyopadhyay, and P. Sahoo. Use of desirability function approach for optimization of multiple performance characteristics of the surface roughness parameters in CNC turning. pages 1–6, Dhaka, Bangladesh, December 2007. International Conference on Mechanical Engineering.

[38] C. Scheffer. Monitoring of tool wear in turning operations using vibration measurements. Master's thesis, University of Pretoria, December 1999.

[39] T. Sibalija and V. Majstorovic. Multi-response optimisation of thermosonic copper wire-bonding process with correlated responses. *The International Journal of Advanced Manufacturing Technology*, 42:363–371, 2009.

[40] A. Siddiquee, Z. Khan, and Z. Mallick. Grey relational analysis coupled with principal component analysis for optimisation design of the process parameters in in-feed centreless cylindrical grinding. *The International Journal of Advanced Manufacturing Technology*, 46:983–992, 2010.

[41] B. Sieben, T. Wagner, and D. Biermann. Empirical modeling of hard turning of AISI 6150 steel using design and analysis of computer experiments. *Production Engineering*, 4:115–125, 2010.

[42] T. Srikanth and V. Kamala. A real coded genetic algorithm for optimization of cutting parameters in turning. *International Journal of Computer Science and Network Security*, 8(6):189–193, June 2008.

[43] D. Steuer. *Statistische Eigenschaften der Multikriteriellen Optimierung mittels Wünschbarkeiten*. Phd-thesis, Technische Universität Dortmund, January 2005.

[44] C.-T. Su and L.-I. Tong. Multi-response robust design by principal component analysis. *Total Quality Management*, 8(6):409–416, 1997.

[45] A. H. Suhail, N. Ismail, S. V. Wong, and N. A. A. Jalil. Optimization of cutting parameters based on surface roughness and assistance of workpiece surface temperature in turning process. *American Journal of Engineering and Applied Sciences*, 3(1):102–108, 2010.

[46] S. V. Tatjana and M. D. Vidosav. Novel approach to multi-response optimisation for correlated responses. *FME Transactions*, 38:39–48, 2010.

[47] D. G. Thakur, B. Ramamoorthy, and L. Vijayaraghavan. Effect of high speed cutting parameters on the surface characteristics of superalloy Inconel 718. In *Proceedings of the World Congress on Engineering (WCE 2010)*, volume 3, June-July 2010.

[48] S. Thamizhmanii and S. Hasan. Analyses of roughness, forces and wear in turning gray cast iron. *Journal of Achievements in Materials and Manufacturing Engineering,*, 17(1-2):401–404, July-August 2006.

[49] M. Thomas, Y. Beauchamp, A. Y. Youssef, and J. Masounave. Effect of tool vibrations on surface roughness during lathe dry turning process. *Computers & Industrial Engineering*, 31(3-4):637 – 644, 1996. 18th International Conference on Computers and Industrial Engineering.

[50] F. H. Tientcheu. Wünschbarkeitsindizes für korrelierte Qualitätsmerkmale. Master's thesis, Technische Universität Dortmund, Dortmund, Germany, 2011.

[51] S. T. N. Ting. Effect of cutting speed and depth of cut on surface roughness of mild steel in turning operation. Bachelor's thesis, Universiti Malaysia Pahang, November 2009.

[52] L. Tong and C. Wang. Multi-response optimization using principal component analysis and grey relational analysis. *International Journal of Industrial Engineering*, 9:343–350, 2002.

[53] L.-I. Tong, C.-H. Wang, and H.-C. Chen. Optimization of multiple responses using principal component analysis and technique for order preference by similarity to ideal solution. *The International Journal of Advanced Manufacturing Technology*, 27:407–414, 2004.

[54] H. Trautmann and C. Weihs. On the distribution of the desirability index using harringtons desirability function. *Metrika*, 63:207–213, 2006.

[55] S. Vajpayee. Analytical study of surface roughness in turning. *Wear*, 70(2):165–175, 1981.

[56] T. Wagner and H. Trautmann. Integration of preferences in hypervolume-based multiobjective evolutionary algorithms by means of desirability functions. *Evolutionary Computation, IEEE Transactions on*, 14(5):688 –701, oct. 2010.

[57] C.-H. Wang. Dynamic multi-response optimization using principal component analysis and multiple criteria evaluation of the grey relation model. *The International Journal of Advanced Manufacturing Technology*, 32:617–624, 2007.

[58] K. Wonggasem and C. Weihs. PCA-based desirability index for multi-objective optimization. In *Proceedings of the 5th PSU-UNS International Conference on Engineering and Technology (ICET-2011)*, May 2011.

[59] C. F. J. Wu and M. Hamada. *Experiments: Planning, Analysis and Parameter Design Optimization*. John Wiley & Sons, Inc., New York, 2000.

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

[61] G. Yule and M. Kendall. *An Introduction to the Theory of Statistics*. Griffin books on statistics and mathematics. C. Griffin, 1950.

[62] J. Zhou, M. Andersson, and J. Stahl. The monitoring of flank wear on the CBN tool in the hard turning process. *The International Journal of Advanced Manufacturing Technology*, 22:697–702, 2003.