Robust optimization and tailoring of scatter in metal forming processes

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Robust Optimization and Tailoring of Scatter in Metal Forming Processes

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ROBUST OPTIMIZATION AND TAILORING OF SCATTER IN METAL FORMING PROCESSES

DISSERTATION

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Summary

Metal forming is the process of deforming metals into desired shapes. To obtain a specific shape, process settings must be adjusted. Decades ago, analytical approximations and trial-and-error methods were used to find appropriate process settings, which was time-consuming and costly. Availability of computers for numerical calculations opened a new horizon for searching for an optimal process setting. Computer simulations replaced the costly experiments, and optimization algorithms were programmed to find the optimal process design efficiently.

In a forming process, there are many sources of disturbance such as variation in material properties, forming temperature, and thickness. Those noise variables are either out of control or costly to control and they lead to variations in the shape of the product. The challenge is to obtain an accurate shape and reduce its variation. It is performed by adjusting the parameters that can be controlled (design variables). A class of optimization techniques that is used to reduce the sensitivity of output to the input is known as robust optimization. As the simulations of metal forming processes are costly and the computational sources are usually limited, an approximate model of the process, a metamodel, is used to describe the relation between the input and responses. The simulations are then performed only on specific combinations of parameters (design of experiments). Then the optimization algorithm searches for an optimum design at which the process has the least sensitivity to disturbances. This approach is referred to as metamodel-based robust optimization. Metamodel-based robust optimization comprises many building blocks and the accuracy and efficiency of the method depends on the choices in each step. In this thesis, an analytical approach is presented to speeding up the calculation of the statistics of a response distribution determined by a Kriging metamodel or Gaussian radial basis function networks. It also includes the calculation of the gradient of the mean and the standard deviation of the response, and the uncertainty of
the objective function value. This method is validated by comparing the results with that of the Monte Carlo method. Moreover, the significance of the analytical evaluation of uncertainty of the objective function value is shown during the sequential improvement of the metamodel. The results confirm that the robust optimum can be achieved accurately with less computational effort than when using Monte Carlo.

A general assumption in robust optimization is that all inputs and outputs follow a normal probability distribution. An investigation is made of how non-normality of input and the propagation of a normal input via non-linear models lead to non-normal response. In this case, the objective function and constraints for robust optimization are re-defined based on a reliability level. For this purpose, two metal forming processes are investigated. Stretch-bending a dual-phase steel sheet and forming an automotive component (B-pillar) were optimized considering non-normality of input and response. It is demonstrated that by accounting for non-normal input and response a higher reliability is achieved than when considering a normal distribution.

Performing robust optimization allows the minimum variation of response around the target mean to be achieved. This is referred to as a forward problem and can be inverted. In a first scenario, if the minimum variation of response does not have a satisfactory level and further reduction of variation is required, the tolerance for the noise variables must be tightened. Since it is expensive to suppress all noise variables, the cheapest combination of tolerances for noise is preferred while the response is within a specified tolerance. In a second scenario, if the variation already meets the tolerances, a cheaper process is obtained by allowing greater noise. Based on these two scenarios, a new method is developed to determine the acceptable material and process scatter from the specified product tolerance by inverse robust optimization. This problem is referred to as tailoring of scatter. A gradient-based approach is used based on the analytical evaluation of the characteristics of output distribution to solve the inverse problem. As the evaluation of the robust optimum is computationally affordable using the analytical approach, the inverse analysis is also efficient. Tailoring of scatter in forming the B-pillar is performed based on the proposed approach. This leads to Pareto fronts which show the optimal adjustment of the tolerance for each noise variable such that the specified output tolerance is met. This method is used successfully to obtain the cheapest combinations of tolerances for noise variables to meet the required quality of the process.
Samenvatting

In metaalomvormprocessen worden metalen omgevormd tot de gewenste vorm. Om een specifieke vorm te verkrijgen moeten procesinstellingen worden aangepast. Decennia geleden werden analytische benaderingen en trial-and-error methoden gebruikt om de geschikte procesinstellingen te vinden, een tijdrovende en kostbare werkwijze. De beschikbaarheid van computers voor numerieke berekeningen bood nieuwe perspectieven in de zoektocht naar de optimale procesinstellingen. Computersimulaties vervingen de dure trial-and-error techniek en nieuwe optimalisatiealgoritmen werden geprogrammeerd om de optimale procesinstellingen efficiënt te kunnen vinden.

In een metaalomvormproces kunnen zich verschillende bronnen van ruis voordoen, bijvoorbeeld door variatie in materiaaleigenschappen, omvormtemperatuur en plaatdikte. Deze bronnen van ruis zijn niet beheersbaar of kostbaar om te onderdrukken. De variaties in materiaaleigenschappen en processtoestand leiden tot variatie in de vorm van het eindproduct. Een nauwkeurige vorm verkrijgen en de variatie reduceren ondanks de bronnen van ruis is een uitdaging die kan worden volbracht door het instellen van de beheersbare procesparameters. Robuuste optimalisatie methoden kunnen worden gebruikt om de gevoeligheid van het proces voor de bronnen van ruis te minimaliseren. De simulaties van metaalomvormprocessen zijn hedendaags nog steeds kostbaar. Aangezien rekenkracht gewoonlijk schaars is, wordt een benadering van de simulatie gebruikt, een zogenaamd metamodel, om de relatie tussen de procesinvoer en respons te beschrijven. De simulaties worden dan alleen uitgevoerd op een aantal specifieke combinaties van parameters verkregen door een Design of Experiments. Het optimalisatiealgoritme zoekt op basis van het metamodel naar de optimale procesinstellingen bij welke het proces het minst gevoelig is voor verstoringen. Deze aanpak wordt ook wel metamodel-gebaseerde robuuste optimalisatie genoemd. Metamodel-gebaseerde robuuste optimalisatie
bestaat uit vele verschillende bouwstenen. De nauwkeurigheid en efficiëntie van de optimale procesinstellingen hangt af van de keuzes in elke stap. In dit proefschrift zal een analytische beschrijving gepresenteerd worden om de karakteristieken van de responseverdeling snel te kunnen verkrijgen. Deze analytische beschrijving zal worden gepresenteerd voor Kriging metamodellen en Gaussische radiale basis functie interpolatie. De karakteristieken van de responsverdeling omvatten de eerste vier genormaliseerde momenten, de gradint van het gemiddelde en de standaarddeviatie en de onzekerheid van de waarde van de doelfunctie. Een Branin-testfunctie zal worden gebruikt om de voordelen van de analytische beschrijving ten opzichte van de Monte Carlo methode aan te tonen. Bovendien zal de significantie van de analytische beschrijving van de onzekerheid van de waarde van de doelfunctie worden aangetoond bij sequentiele verbetering van het metamodel. De resultaten bevestigen dat het robuuste optimale ontwerp accuraat en met minder rekenkracht kan worden gevonden in vergelijking met de Monte Carlo methode.

Een algemene aanname in robuuste optimalisatie is dat de bronnen van ruis en proces respons een normale verdeling volgen. Niet-normaal verdeelde input en de propagatie van normaal verdeelde input door niet-lineaire modellen lijdt tot een niet-normaal verdeelde respons. In dit geval zullen de doelfunctie en de randvoorwaarden worden geherdefinieerd op basis van betrouwbaarheid. Twee metaalomvormprocessen zullen worden onderzocht om dit te demonstreren, het trekbuigen van een twee-fasen staal en het dieptrekken van een B-stijl. Het meenemen van een niet-normaal verdeelde invoer in de berekening verbeterde de zoektocht naar de optimale procesinstellingen.

Het uitvoeren van een robuuste optimalisatie zorgt voor minimale variatie rondom het gemiddelde. Deze procedure kan omgedraaid worden tot een inverse probleem. In een eerste scenario is verdere reductie van deze uitgangsvariatie nodig, en zal de spreiding in de ruis verkleind moeten worden. Aangezien het kostbaar is om de toleranties op alle bronnen van ruis te verminderen, zal de voorkeur uitgaan naar de meest economische combinatie van ruis toleranties, zolang de respons binnen de toegestane toleranties valt. In een tweede scenario zal worden gekeken of eenzelfde variatie rondom het gemiddelde kan worden bereikt met wijdere spreiding in de bronnen van ruis, wat zal leiden tot een goedkoper proces. Op basis van beide scenarios is een nieuwe methode ontwikkeld voor het vaststellen van de spreiding op de bronnen van ruis door het inverteren van de robuuste optimalisatie. Deze inverse robuuste opti-
malisatie methode word het op maat maken van spreiding genoemd. Een gradint-gebaseerde aanpak word gebruikt voor de analytische evaluatie van karakteristieken van de responsverdeling om het inverse probleem op te lossen. Omdat de evaluatie van een robuust optimum weinig rekenkracht vraagt dankzij de analytische beschrijving, is de inverse analyse ook efficiënt uit te voeren. Het op maat maken van spreiding bij het vormen van de B-stijl is met succes uitgevoerd op basis van de voorgestelde aanpak. Deze benadering resulteert in Pareto-grenzen die de optimale aanpassing van de tolerantie voor elke bron van ruis tonen, zodat aan de vereiste uitgangstolerantie wordt voldaan. Deze methodie is succesvol toegepast voor het bepalen van de meest economische samenstelling van toleranties op alle bronnen van ruis, waarbij aan de vereiste nauwkeurigheid van het proces voldaan wordt.
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Chapter 1

Introduction

The discovery of metals has heavily influenced the development of civilization. From the earliest times, metals such as copper, gold, silver, and lead were formed to make a variety of primitive tools, decorative items and ornaments. Subsequent developments by early societies contributed to expanding the existing knowledge of metallurgy. Nowadays, metal forming industry plays a key role in our society and it is one of the major contributors to the world’s economy.

The components produced via metal forming processes affect all aspects of human life. Metal forming processes are rapidly improving owing to the development of new theoretical and numerical methods. This chapter provides a brief overview on metal forming processes.

1.1 Metal forming processes

Metal forming is the process of the deformation of metals into the desired shape. As the metallic products are supplied in a variety of forms, the processes are generally categorized into two broad classes, bulk metal forming processes (namely forging and extrusion) and sheet metal forming processes (namely deep-drawing and stamping).

Several factors play a part in the metal forming processes. Complexity of the geometry of a component, tooling, and material properties are factors which introduce a lot of complicated issues during the forming process. Combined effects of these factors make it difficult to improve the quality of components and reduce the rejection rate of the parts only with experimental tests.
1.2 Application of the finite element method in metal forming

The finite element method was derived from the work of several researchers during the 1940s and 1950s and it was generalized for everyday use by the pioneering work of Turner et al. (1956). Later, many researchers contributed to the development of FEM, which is currently being used for many applications in civil, mechanical and aeronautical engineering.

To gain an insight and to investigate the influence of different factors in metal forming processes, employing computation methods has a big advantage over trial and error using experiments. It reduces the costs, efforts, and the time required to develop, to test and to modify a component.

FEM can be used to optimize a forming process. Finding the best solution out of all possible solutions in a certain domain is the main goal of mathematical optimization. An objective should be defined to be minimized (or maximized) by adapting certain input factors. Optimization helps to improve a component in advance before the manufacturing starts.

1.3 Including uncertainty in FEM

Finite element (FE) simulation is performed in a deterministic manner. A single value is usually assigned to each input parameter of FE simulations and the results obtained from those inputs are also deterministic. Consequently, repeating the same simulation with the same input parameters will lead to the same result.

When doing experiments, repeating the same process in the same condition results in slightly different results due to uncertainties. These uncertainties originate from unavoidable variation in process conditions (Figure 1.1). To be able to capture the variation in the results using FEM, the variation of process conditions must be taken into account.

Classic FEM cannot directly handle a stochastic input. One of the methods of handling a stochastic input is to perform many deterministic simulations using the parameters drawn from the stochastic input. This helps to obtain a description of the variation of the output. A large number of simulations are required to obtain a reliable description of output. However, this will increase the computation time significantly.
1.4. Optimization under uncertainty

(a) Repeating a finite element simulation

(b) Repeating an experiment

\[ \theta_1 = \theta_2 \]

\[ \theta_1 \neq \theta_2 \]

Figure 1.1: (a) Same results obtained from repeating a finite element model with the same input parameters, (b) different results obtained from repeating an experiment due to variation in material input or process condition

This is specifically important for nonlinear processes.

1.4 Optimization under uncertainty

One can modify the deterministic optimization to incorporate uncertain inputs in the optimization. Robust optimization is one of the methods that are used to optimize process settings based on minimization of the process variations considering stochastic input. This is very important
in metal forming processes as a proper use of material often pushes the forming process towards the limits. Then a small perturbation can lead to quality issues. In mass production, the lack of quality in the produced components causes delays in production, problems in assembly, or issues when the product is in use. Therefore, optimization in the presence of uncertainty of input parameters has become a common exercise in various fields of study (Marton et al., 2015; Picheny et al., 2017; Yazdi, 2017; Zhou et al., 2018).

1.5 Research objective and outline

The main goals of this research are to investigate the robust optimization technique, to make robust optimization more accurate and efficient, and to study the possibilities of inverting it to tailor the scatter of input based on requirements on the output. This thesis is organized as follows. The building blocks of robust optimization and possible steps that can be taken to improve both accuracy and efficiency of finding a robust optimum are presented in Chapter 2. In Chapters 3 and 4, an analytical approach is presented and validated to speed up the process of obtaining the characteristics of output distribution. In Chapter 5, the consequences of using higher order statistical moments of the output in robust optimization are presented. The FE simulation of a stretch-bending process is used to show the relevance of considering higher order statistical moments during robust optimization. In Chapter 6, the influence of the correlations between the noise parameters is shown. Moreover, a method to account for bimodal input is presented based on experiments on a large number of samples prepared from various coils of DP800 steel sheet. The results of optimizing an automotive component (B-pillar) with correlated input and bimodal distribution are shown in this chapter. The inverse of robust optimization is presented in Chapter 7, along with the procedure for obtaining the acceptable variation of input based on requirements for the output.

This study is performed with a focus on metal forming processes and most of the examples presented in this thesis are forming-related processes. However, the outcomes of this research and the methods developed throughout this thesis are applicable in other fields of study.
Chapter 2

Robust optimization and tailoring of scatter

In this thesis, the focus is on the influence of uncertainty in metal forming processes. In deterministic optimization of a process, the input variables are assumed to have no variation and an optimum design setting is found based on this assumption. In many problems, some of the input variables are not known exactly, but they can be described using a probabilistic distribution. Such disturbances are a challenge in optimizing the processes. The main concern is to predict their effects on the uncertainty of the response of the process and to minimize the sensitivity of the process to these noise variables. This problem is very common in various disciplines including engineering, physics, biology and economy. For instance, the uncertainty of the response has been assessed in large-scale energy-economic policy models (Kann and Weyant, 2000), zero-defect manufacturing (Myklebust, 2013), maintenance modelling (Gao and Zhang, 2008), study of groundwater flow (Dettinger and Wilson, 1981), engineering design (Kang et al., 2012), weather forecast (Palmer, 2000) and health related issues (Barchiesi et al., 2011). The processes optimized in this thesis relate mainly to metal forming. However, the methods developed in this thesis are applicable in various disciplines.

For optimization under the influence of uncertainty, the input vari-
ables are considered in two categories. The variables that can be adjusted to get an optimum process are called design variables and those which are difficult to control are referred to as noise variables. The goal of robust optimization is to find a set of design variables at which the process is least sensitive to the disturbances.

Computer models are often used for optimizing processes. Optimizing a process under the influence of uncertainty using computer models requires many evaluations of the model and is therefore computationally expensive. Often an approximate model of the process, a so-called metamodel, is built from results of computer simulations. The metamodels are then used to efficiently perform the optimization in the presence of uncertainty.

In this chapter, this robust optimization approach is reviewed and its building blocks are presented. The current approaches and recent advances are discussed and the potential steps that can be taken to improve the accuracy and speed of this method are presented. In addition, the potential of inverting the robust optimization technique to work back from the allowable response variation to acceptable noise variation is explained and discussed. This is referred to in this thesis as tailoring of scatter.

### 2.1 Metamodel-based robust optimization

Consider a process model with one design variable, $x$, as the input that leads to the output, $y$. This is referred to as a black-box function evaluation and it implies that only the inputs and the output are of interest. When noise is not present, the process model will calculate a deterministic value of $y$, $y = f_1(x)$, as shown in Figure 2.1(a).

In the presence of a noise variable, $z$, the output is a function of both $x$ and $z$, $y = f_2(x, z)$. Since $z$ is a stochastic input variable, the uncertainties will be present in the response as shown in Figure 2.1(b). The challenge is to calculate the probability distribution of response based on the probability distribution of $z$. Process models generally handle all inputs deterministically. This means that $y$ can be evaluated for one specific value of $x$ and $z$. Therefore, to obtain the probability distribution of the output, $p(y)$, for a specific $x$, many model evaluations are required for different $z$ values. In this case, the response must be evaluated using various values of $z$ drawn from the probability distribution, $p(z)$.
When the process model is computationally expensive, a metamodel can replace the black-box function. Then the response of the metamodel is an approximation of the output of the process model. Therefore, the result of metamodel evaluation is referred to as $r$ to distinguish it from the result of the black-box evaluation $y$. The idea behind using a metamodel of the process is that the evaluation of the response on a metamodel is much faster than on the model itself (Dellino et al., 2015; Koziel et al., 2011; Zhuang et al., 2015).

The procedure of obtaining a design setting, $x_{opt}$, at which the response of the process has the least sensitivity to the noise variables is referred to as robust optimization. In addition, robust optimization can handle the constraints on the uncertain responses based on the probabilities of meeting the specification limits. The building blocks of such a procedure are explained in the next section.

### 2.2 Building blocks of robust optimization

Before starting the optimization procedure, design variables, noise variables and responses must be identified. Since models can have many inputs, it is recommended to perform a sensitivity analysis to determine...
the importance of the model inputs and to decide which variables to account for in the optimization. This step is performed based on factorial designs and by evaluating the main effects of input variables (Bonte, 2007).

A typical metamodel-based robust optimization procedure is shown in Figure 2.2 and consists of several building blocks. First a design of experiments (DOE) is generated in the combined design and noise variables space. Then the responses of the black-box function are evaluated for the discrete DOE points. It is assumed that a constraint is present in the optimization. In Figure 2.2, \( r_c \) denotes a response on which a constraint is defined. In the third step, metamodels which are the mathematical fits of the responses are constructed. The search for the robust optimum design consists of uncertainty propagation (step 4) and the repetitive evaluation of objective function value and constraints (step 5), which subsequently leads to the optimal setting, \( x_{opt} \).

The robust optimum is evaluated on a metamodel of the process. As the metamodel is an approximate representation of the process, the reliance on a metamodel might lead to loss of accuracy in the evaluation of the robust optimum. To reduce the prediction error, iterative improvement of the metamodel can be applied. For this purpose, new points are added to the initial DOE to get an improved metamodel of the process. A new infill point is selected in combined design and noise variable space (step 7) and is added to the initial DOE. This procedure can be repeated until the updated metamodel does not lead to further improvement of the predicted robust optimum design.

For each building block of robust optimization shown in Figure 2.2, various methods exist and a variety of choices can be combined to perform the optimization (Huang et al., 2006; Kitayama and Yamazaki, 2014; Marzat et al., 2013; ur Rehman et al., 2014). Some of the methods that are used to perform each step of the robust optimization procedure are shown in Figure 2.3. This figure illustrates the modular nature of the metamodel-based robust optimization. It means that, the choice of a method within each block is independent from other choices in other blocks. The methods that are commonly used in the literature are introduced and reviewed in the next seven sections.

### 2.2.1 Design of experiments

The steps of robust optimization in Figure 2.2 were illustrated using one design and one noise variable. Usually there are more than one
2.2. Building blocks of robust optimization

1. Making a DOE

2. Black-box function evaluation

3. Metamodelling

4. Uncertainty propagation

5. Objective function and constraints

6. Search for the robust optimum design

7. Iterative improvement of the metamodel

Figure 2.2: Schematic illustration of the steps of robust optimization with iterative improvement

design and one noise variables. The vector of design variables is referred to as \( \mathbf{x} \) and the vector of noise variables is referred to as \( \mathbf{z} \). The vector \( \mathbf{v} = (\mathbf{x}, \mathbf{z}) \) is input for the process model. The process model is evaluated for a selected number of different values of \( \mathbf{v} \), the Design of Experiments (DOE).
Figure 2.3: Various choices of building blocks of metamodel-based robust optimization

The DOE can be made using various schemes such as factorial design, central composite, random sampling, Latin hypercube sampling (LHS), and orthogonal sampling (Cavazzuti, 2013; Ferreira et al., 2007; Tang, 1993). It is desirable to have a small number of DOE points since the process model is often expensive to evaluate. In addition, the goal is to sample uniformly to get an accurate approximation of the underlying
relationship between input and output in the whole design-noise domain.

Figure 2.4 shows schematically different sampling techniques for two input variables. In a full factorial or fractional factorial sampling (Figure 2.4-(a,b)), extreme values of each variable are used. For the design variables, the lower and the upper bound are selected as extreme values. The extreme values for a noise variable are generally $\mu_z \pm 3\sigma_z$ in which $\mu_z$ is the mean and $\sigma_z$ is the standard deviation of that noise variable.

In random sampling the DOE points are generated without considering the previously generated points (Figure 2.4(c)). Therefore, it is very probable that the points are not evenly distributed. A central composite design (Figure 2.4(d)) consists of three types of points. Full factorial design, the centre point, and axial (star) points. In LHS the range of each variable is divided into $n_{DOE}$ equiprobable bins and each bin is sampled once (McKay et al., 1979) (Figure 2.4(e)). Orthogonal sampling is an extension to LHS in which the sampling domain is divided into sub-domains and, similarly to LHS, the domain is sampled such that each subdomain has the same density of points (Figure 2.4(f)). The LHS method can be implemented in such a way that the minimum distance between the points is maximized (Maximin). In that case, a uniform and disperse sample can be obtained (Figure 2.4(g)). The Maximin approach can also be used for combination of LHS and full factorial design(Figure 2.4(h)).

The choice of the size of the sample to build the DOE directly influences the accuracy of the metamodel and the computational effort required to build the metamodel. As a rule of thumb, it is proposed to select the number of sampling points equal to 10 times the number of input variables for moderately complex functions (Schonlau, 1997). This number can be altered if a highly nonlinear process response is expected. Nevertheless, it is feasible to start using a small number of sample points and add infill points to the initial DOE at later stages of the robust optimization to improve the accuracy of the metamodel where necessary.

2.2.2 Black-box function evaluation

The black-box function is evaluated in each DOE point to obtain the output. The output can be the result of a computer simulation or evaluation of the analytical models. These models and simulations are an approximation of a real process and therefore are not exact. They must be accurate enough to capture the influence of variation in the input
variables. If the difference between the predicted response and the real response is large, the process model must be improved. Furthermore, it is recommended to perform a study on the numerical noise of the model before running the optimization procedure, to make sure that the order of variation due to numerical noise is lower than the order of variation caused by noise variables (Wiebenga and van den Boogaard, 2014).
2.2.3 Generating a metamodel

The metamodel describes the relationship between \( r \) (or \( r_c \)) and the input vector \( \mathbf{v} = (\mathbf{x}, \mathbf{z}) \). The metamodel is an approximate representation of the output obtained from black-box function evaluation. An estimation of the prediction error at each point can be evaluated. This error evaluation can be used to improve the prediction of metamodel iteratively.

A metamodel built on the discrete responses obtained from evaluations of a black-box function is required to search for the robust optimum design. One can choose from several methods of metamodelling, such as Kriging models, radial basis functions, neural networks or regression models (Luo and Lu, 2014). The choice of the metamodel depends on the complexity of the response with respect to input variables. Kriging, a widely used method which is based on the work of Krige (1951), is described by:

\[
    r(\mathbf{v}) = \mathbf{\phi}^T \mathbf{R}^{-1} \mathbf{y}
\]

In this equation, the vector \( \mathbf{\phi} \) contains the correlations between the point \( \mathbf{x} \) and the DOE points, \( \mathbf{R} \) is an \( n_{\text{DOE}} \times n_{\text{DOE}} \) matrix that contains the spatial correlations between all DOE points, and \( \mathbf{y} \) is the vector containing the responses of the black-box function on the DOE points. The error estimate, \( \hat{s}_r \) at every point can be calculated by:

\[
    \hat{s}_r(\mathbf{v}) = \hat{\sigma}^2 [1 - \mathbf{\phi}^T \mathbf{R}^{-1} \mathbf{\phi}]
\]

\[
    \hat{\sigma}^2 = \frac{\mathbf{y}^T \mathbf{R}^{-1} \mathbf{y}}{n_{\text{DOE}}}
\]

The main assumption in Kriging is that the data is a realization of a Gaussian random field which means that the responses are spatially correlated. The distance between the DOE points is used to determine the correlation between them. Kriging is considered a semiparametric model, which allows moderate level of flexibility in modelling. A parametric model is a model that has a fixed set of parameters, for example polynomial regression. In this case, the number of fitting parameters is independent of the size of the input data \( n_{\text{DOE}} \). In a nonparametric model there are no bounds on the number of the parameters. This means that the number of fitting parameters can grow as the size of input data grows. The Kriging metamodel is categorized as a semi-parametric model (Rasmussen, 2003). In Equation (2.1) the fact that the size of the correlation matrix is dependent on the number of DOE points, reveals
Chapter 2. Robust optimization and tailoring of scatter

Table 2.1: Commonly used radial basis functions

<table>
<thead>
<tr>
<th>Type of basis function</th>
<th>$\psi(\hat{r})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian</td>
<td>$e^{(-c\hat{r})^2}$</td>
</tr>
<tr>
<td>Multiquadric</td>
<td>$\sqrt{1 + (c\hat{r})^2}$</td>
</tr>
<tr>
<td>Inverse Multiquadric</td>
<td>$\frac{1}{\sqrt{1+(c\hat{r})^2}}$</td>
</tr>
<tr>
<td>Inverse Multiquadradic</td>
<td>$\frac{1}{1+(c\hat{r})^2}$</td>
</tr>
<tr>
<td>Polyharmonic spline</td>
<td>$\hat{r}^k$    $k$ odd</td>
</tr>
<tr>
<td>Thin plate spline</td>
<td>$\hat{r}^k\ln(\hat{r})$    $k$ even</td>
</tr>
</tbody>
</table>

the parametric nature of Kriging models. However, the fact that the data is assumed to be a realization of a Gaussian random field highlights the nonparametric component of the Kriging model, hence limiting its flexibility.

An example of a more flexible family of models, so-called non-parametric models, is radial basis function (RBF) networks that can be used for function approximation:

$$r(v) = \psi^T\Psi^{-1}y$$ (2.3)

in which $\psi$ is a vector that contains the correlations between the point $x$ and the DOE points. The correlation between two points is a function of the Euclidean distance, $\hat{r}$, between them. Commonly used radial basis functions are summarized in Table 2.1. In fact, choosing Gaussian basis functions with the same model parameters as in Kriging leads to the same prediction of response. The flexibility of choosing the correlation function is a big advantage of using RBF networks. However, RBF networks do not include an explicit uncertainty measure as Kriging does. This can be regarded as a disadvantage of RBF networks.

In some studies, the metamodel is built of the mean and standard deviation of the response instead of building a metamodel on the response itself. This approach is generally referred to as the dual response surface method (Myers and Carter, 1973; Vining and Myers, 1990). In this approach, fitting a metamodel is performed after noise propagation on individual design points. The dual response surface method is not used in this thesis.
2.2.4 Evaluating the robust optimum design

Generally, an optimization problem in the presence of constraints can be expressed as:

\[
\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad h(x) = 0 \\
& \quad g(x) \leq 0 \\
& \quad lb < x < ub
\end{align*}
\]  

(2.4)

where \( f(x) \) is the objective function, \( h(x) \) are the equality constraints, \( g(x) \) are the inequality constraints, \( lb \) are the lower bounds of \( x \) and \( ub \) are the upper bounds of \( x \). This formulation can be used for both deterministic and probabilistic optimization. The difference is in the definition of the objective function and constraints. The definition of the objective function and constraints for a robust optimization approach will be presented in the next section. The focus in this section is to introduce the methods that are used to solve such an optimization problem specifically when the objective function, the constraints, or both are nonlinear. In that case, Equation (2.4) is referred to as a constrained nonlinear problem. To solve such a problem, constrained nonlinear optimization algorithms can be employed (Baginski et al., 2005). There are two main classes of algorithms namely derivative-free or stochastic techniques such as genetic algorithm (GA), and iterative methods which require the derivatives such as iterative quadratic programming (SQP) and trust region algorithms. A genetic algorithm maintains a large population of candidate solutions (Homaifar et al., 1994) in contrast to iterative search methods in which a single potential solution is generated at each iteration. GA is on the basis of bio-inspired operators (e.g. mutation, crossover and selection) and a population of candidate solutions evolves toward better solutions.

Iterative methods are categorized in two main classes: line search methods and trust region methods (Nocedal and Yuan, 1998). The classic methods of optimization are combined with line search algorithms. This is based on an initial guess and the construction of an approximate model from first order and second order derivatives near the current point and iteratively improving the solution. This approach is also used in trust region algorithm, but in that case the approximate model is trusted only in a region near the current solution (Omojokun, 1990).
2.2.5 Objective function and constraints

One of the earliest methods for robust process design originates from the work of Taguchi (1987). The Taguchi method is generally used to classify robust design problems. The objective in robust design is one of the following:

- The smaller the better
- The larger the better
- On target is best

When the focus is mainly on the performance of the process (mean of the response), the first two approaches are employed. For the third approach, the Taguchi approach is often a two-step procedure. In the first step, some design variables are identified to reduce variability of the response. In the second step, other design variables are used to shift the mean to the target value.

A common approach is to simultaneously minimize the variability of the response and set the mean on the target value which is used in this thesis. At the same time the constraints must be satisfied. To use a measure for variability of the response and handling the constraints under the influence of uncertainties many methods can be used. The satisfaction of the constraints in robust optimization is directly related to the probability of failure. The main challenge for analyzing the constraints is the evaluation of the probability of the failure since the response probability density function is not known. A moment matching technique is often used to approximate the reliability based on the statistical moments of the response. More specifically, mean and standard deviation are used to estimate the reliability of the satisfaction of a constraint using:

\[ \mu_{r_c}(x) + n\sigma_{r_c}(x) \leq 0 \]  \hspace{1cm} (2.5)

where \( \mu_{r_c}(x) \) and \( \sigma_{r_c}(x) \) are the mean and standard deviation of the response of a constraint. The mean and standard deviation are simple to compute using limited stochastic data and therefore this method is widely used in the literature (Du and Chen, 2000, 2002). The choice of \( n \) is related to the probability of constraint satisfaction assuming a normal distribution for the response of the constraint. Figure 2.5 shows schematically the reliability of constraint satisfaction for different values of \( n \) in the presence of an upper bound.
2.2. Building blocks of robust optimization

For a lower bound constraint:

\[ \mu_{rc}(x) - n\sigma_{rc}(x) \geq 0 \]  \hspace{1cm} (2.6)

To define the objective function, many approaches can be used as a measure for the variability of the response. The standard deviation of the response is one of the measures that shows the spread of a set of data around the mean value. For a robustness measure that minimizes the variation of response in addition to the difference between mean and target value, \( C_r \), several expressions are proposed in the literature such as (Koch et al., 2004):

\[
\text{minimize } \left( (\mu_r(x) - C_r)^2 + w\sigma_r^2(x) \right) \hspace{1cm} (2.7)
\]

or (Havinga et al., 2017; Wiebenga et al., 2012):

\[
\text{minimize } (|\mu_r(x) - C_r| + w\sigma_r(x)) \hspace{1cm} (2.8)
\]

In Equations (2.7) and (2.8), \( w \) is a weighting factor to adjust the optimization objective between mean on target and response variation. By varying \( w \), this weighted sum formulation can lead to a set of optimal solutions. Then a set of Pareto optimal solutions is obtained which indicates the trade-off between the deviation of the mean from the target and the variation of the response.

Using these objective functions does not imply that the response actually follows a normal probability distribution, even if the input is normally distributed. In some studies, specification limits exist on the response, and the reliability of the response is of interest. In this case, the

\[ \text{Upper specification limit} \]

84.13% 97.73% 99.87%

\[ \text{Upper specification limit} \]

Figure 2.5: Reliability of satisfaction of an upper bound constraint
response probability distribution must be defined. For instance, \( n \) sigma
design quality (Koch et al., 2004) in which the probability of response
falling in a particular range defined by a lower and an upper bound
is obtained from a normal probability distribution (Figure 2.6). The
percentage variation within the specification limits can be calculated
and is referred to as short-term sigma quality. In contrast, long-term
sigma quality corresponds to the variation within the specification limits
if the mean shifts for about 1.5\( \sigma \). Table 2.2 shows the short-term sigma
quality and long-term sigma quality for various values of \( n \).

In the definition of objective function and constraints, the super-
scripts \( r \) and \( r_c \) denote respectively the main response and the response
of a constraint. As an example, in metal forming processes, a specific
dimension in the product can be considered as the main response for
which the variation must be minimized. The thinning due to forming
which is related to the reliability of the process can be considered as
a constraint. It is of interest only if it exceeds the upper specification
limit, in which case the product will be damaged. Consequently, the
robust optimization leads to reduction of the variation of that specific
dimension by setting its mean on target, while considering the limits
on thinning. In some research both constraint and objective function
are defined on the same response. Therefore, as a result of robust opti-
mization the response shrinks to minimize the variation and it shifts to
satisfy the specification limits (Koch et al., 2004).

Figure 2.6: Sigma design quality level by choosing \( n =1, 2 \) and \( 3 \)
2.2. Building blocks of robust optimization

Table 2.2: Short-term and long-term quality level for n sigma design

<table>
<thead>
<tr>
<th>$n$ sigma quality level</th>
<th>Percent variation</th>
<th>Defect per million (Short-term)</th>
<th>Defect per million (Long-term)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>68.26</td>
<td>317400</td>
<td>697700</td>
</tr>
<tr>
<td>2</td>
<td>95.46</td>
<td>45400</td>
<td>308733</td>
</tr>
<tr>
<td>3</td>
<td>99.73</td>
<td>2700</td>
<td>66803</td>
</tr>
<tr>
<td>4</td>
<td>99.9937</td>
<td>63</td>
<td>6200</td>
</tr>
<tr>
<td>5</td>
<td>99.999943</td>
<td>0.57</td>
<td>233</td>
</tr>
<tr>
<td>6</td>
<td>99.9999998</td>
<td>0.002</td>
<td>3.4</td>
</tr>
</tbody>
</table>

2.2.6 Noise propagation

The criteria used for evaluation of objective function and constraints are usually based on the statistical moments of the response (mean and standard deviation). Finding the statistical moments of the response from the noise variables is referred to as noise propagation. Several methods for noise propagation have been developed over past decades. Monte Carlo (MC) and its variations, perturbation methods, Gaussian Quadrature (GQ), polynomial chaos, Bayesian statistical modelling, method of moments (Taylor-series expansion) and stochastic collocation have been widely used (Heijungs and Lenzen, 2014; Lee and Chen, 2009; Leil, 2014). Dimensionality of the problem (Fuchs and Neumaier, 2008) and fidelity of the model (Ng and Willcox, 2014) determine the efficiency and effectiveness of these methods.

Monte Carlo (MC) analysis is one of the most widely used methods in the literature for propagation of noise (Helton and Davis, 2003; Keating et al., 2010; Martinelli and Duvigneau, 2010; Pacheco et al., 2016; Putko et al., 2002; Zhou et al., 2018). It requires sampling from the noise variable which is generally assumed to have a normal probability distribution. There are several methods of sampling from a normal probability distribution and the concept is basically similar to the sampling techniques described in Section 2.2.1. The main difference is that in that section the aim is to sample uniformly, while here the samples are taken from a probability distribution. The concept of random sampling and LHS from a normal probability distribution is shown in Figure 2.7. The sampling is performed by choosing random numbers between 0 and 1 from the cumulative probability distribution (CDF) of a normal
distribution and translating them to the noise domain. Using random sampling, there is no consideration with respect to the previously sampled points and the points can belong to any particular subset of the sampling domain. In LHS, the CDF is divided into sub-domains of equal size, and sampling is done by adding new points avoiding selection of more than one point in each domain.

After choosing the samples, the approximate mean and standard deviation are evaluated by:

\[
\mu_r(x) \simeq \frac{1}{N_{mc}} \sum_{s=1}^{N_{mc}} r(x, z_s)
\]
\[
\sigma_r^2(x) \simeq \frac{1}{N_{mc}} \sum_{s=1}^{N_{mc}} \left( r(x, z_s) - \mu_r(x) \right)^2
\]

where \( N_{mc} \) is the number of sample points drawn from the noise probability distribution, \( p(z) \).

### 2.2.7 Improving metamodel accuracy

An optimum design found by using the metamodel is not always equal to the optimum of the underlying black-box function. This occurs when the prediction behaviour of the metamodel around the predicted optimum is
poor when there are no sampling points around the optimum. Therefore, it is necessary to use an update procedure to improve the metamodel and subsequently obtain an accurate robust optimum. For this purpose, new points are added to the initial DOE. Two types of iterative sampling techniques are used in the literature: space-filling and adaptive sampling techniques. In the space-filling approach, the points are added to the initial DOE in the sparsely-sampled regions. The adaptive techniques require a criterion to add an infill point where it is needed most. In some cases, the infill point is added at the predicted optimum. However, in most cases the infill criterion is based on the metamodel estimation error, \( \hat{s} \). Using this potential error, various methods can be developed to add infill points. A simple approach is to add an infill point where \( \hat{s} \) has the biggest value.

One of those adaptive methods is based on expected improvement (Jones et al., 1998) that has been proposed to take into account both local and global search for new infill points in deterministic optimization. The expected improvement is defined by:

\[
EI(x) = (r_{min}^* - \hat{r})\Phi\left(\frac{r_{min}^* - \hat{r}}{\hat{s}_r}\right) + \hat{s}_r\phi\left(\frac{r_{min}^* - \hat{r}}{\hat{s}_r}\right)
\] (2.10)

In this equation, \( \phi \) is the standardized normal distribution, \( \Phi \) is the cumulative distribution of a standardized normal distribution and \( r_{min}^* \) is the minimum value of the response at the DOE points examined so far. \( \hat{r} \) and \( \hat{s}_r \) are the predicted value and uncertainty of the predicted response. The procedure is to search for a point that has the highest \( EI \) value to add it to the initial DOE.

Equation (2.10) is used to optimize the response of a process (deterministic optimization). It can be altered to be used in a robust optimization procedure (ur Rehman and Langelaar, 2016; Wiebenga et al., 2012). A new infill point \( (x', z') \) must be selected in the combined design and noise space. The objective function value, \( f(x) \), replaces the response, \( r(x) \). Moreover, to evaluate \( f(x) \) and get the minimum value of the objective function at the DOE points, \( f_{min}^* \), one needs to calculate \( \mu_r(x) \) and \( \sigma_r(x) \). Therefore, the objective function values are not a result of evaluations of the black-box function, but of a prediction using a metamodel. Thus, there is a prediction uncertainty at the current best point. The minimum objective function value at the DOE points has an uncertainty of \( \hat{s}^* \). A suitable estimation for the prediction error at any design, \( \hat{s}(x) \), is also required. The uncertainty measure on metamodel
(\hat{s}_r) is dependent on both design variables and noise variables. To obtain the uncertainty of the objective function value (\hat{s}_f) an integral over noise space is usually evaluated (calculating mean value of mean square error (MSE))(Havinga et al., 2017; Wiebenga et al., 2012):

\[
\hat{s}_f^2(x) = \int_z \hat{s}^2(x, z)p(z) dz
\]  

(2.11)

The influence of uncertainty of the best point, \( \hat{s}^* \), is ignored and expected improvement is evaluated using (Sóbester et al., 2004):

\[
EI(x) = \bar{\omega}(f_{\text{min}}^* - f) \Phi \left( \frac{f_{\text{min}}^* - f}{\hat{s}_f} \right) + (1 - \bar{\omega})\hat{s}_f \phi \left( \frac{f_{\text{min}}^* - f}{\hat{s}_f} \right)
\]

(2.12)

More details about including the influence of \( \hat{s}^* \) can be found elsewhere (Jurecka, 2007; Jurecka et al., 2007). The first term in Equation (2.12) is related to local search (near the predicted optimum) and the second term is related to global search. One can adjust the search in the global and local domain by choosing a proper weight factor such that 0 < \( \bar{\omega} \) < 1.

Maximizing expected improvement using (2.12) leads to an infill point in the design space, \( x' \). At that design, a point in noise space must be selected to be able to evaluate the black-box function. For this purpose \( z' = \arg\max_z (\hat{s}^2(x', z)p(z)) \) is employed. The point \( (x', z') \) is then added to the initial DOE, a new metamodel is fitted and the robust optimum is evaluated again using the updated metamodel.

### 2.2.7.1 Termination criterion

The termination criterion for adding infill points can be defined in various ways. One can limit the maximum number of iterations. Another approach is to terminate when root-mean-square error (RMSE) at robust optimum (\( \hat{s}_f(x_{\text{opt}}) \)) is below a specific threshold.

Wiebenga and van den Boogaard (2014) introduced an efficient termination approach based on a measure for the magnitude of the numerical noise. They proposed that if infill points fall within the noise bandwidths the iterative improvement is to be terminated. They also suggested that if no numerical noise is present, a threshold for \( EI \) has to be chosen to terminate the iterative improvement.
2.3 Overview of commonly used strategies for robust optimization

In recent years, metamodel-based robust optimization has been implemented in a variety of fields to optimize the processes in the presence of unavoidable noise variables. Sun et al. (2014) applied it to improve the crashworthiness and robustness of a foam-filled thin-walled structure. In that work the initial DOE comprised 32 sample points generated using the Latin hypercube sampling (LHS) approach and 12 sampling points were added by iterative sampling strategy in a two-dimensional variable space. They showed the influence of improvement steps on the accuracy of the metamodel and predicted the robust optimum. Choi et al. (2018) implemented a robust optimization method for designing a tandem grating solar absorber. A Kriging method was used to build a metamodel in a five-dimensional input space and the search for robust design was conducted using GA. It was shown that in the robust optimum design a solar absorptance of greater than 0.92 was achieved with a probability of 90%. That was a significant improvement on the reference design in a previous work in which only 22% of samples could satisfy that condition. The capability of metamodel-based robust optimization to solve an industrial V-bending process was investigated by Wiebenga et al. (2012). Various initial DOEs were generated using LHS on a six-dimensional design-noise variable space. A Kriging metamodel was used and uncertainty propagation was evaluated using the MC method.

Metal forming processes are influenced by the scatter of both material and process conditions. Robust optimization is therefore an essential approach to enhancing the production quality in forming processes. Recently, robust optimization has been implemented for cold roll forming (Wiebenga et al., 2013), stretch-drawing of a hemispherical cup (Wiebenga et al., 2015), extrusion-forging (Hu et al., 2007), and V-bending (Havinga et al., 2017).

Table 2.3 summarizes some of the most recent articles related to the metamodel-based robust optimization of forming-related processes. The process that has been optimized (second row), the choices that have been made for each building block of robust optimization explained in the previous sections (3rd to 9th row), and the input probability distribution (10th row) are reflected in this table.
Table 2.3: The choices for building blocks of robust optimization in the literature

<table>
<thead>
<tr>
<th>Reference</th>
<th>Process</th>
<th>DOE</th>
<th>Black-box</th>
<th>Metamodel</th>
<th>Uncertainty</th>
<th>Objective function</th>
<th>Search algorithm</th>
<th>Iterative improvement</th>
<th>Input distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wei et al. (2018)</td>
<td>Multi-rib</td>
<td>BoxBehnken and Uniform design</td>
<td>Finite element</td>
<td>Dual-RSM</td>
<td>(second order polynomial)</td>
<td>$f(\mu, \sigma)$</td>
<td>Genetic algorithm</td>
<td>-</td>
<td>Normal and uncorrelated</td>
</tr>
<tr>
<td>Heng et al. (2017)</td>
<td>Tube bending</td>
<td>Taguchi orthogonal array</td>
<td>Finite element</td>
<td>Dual-RSM</td>
<td>(second order polynomial)</td>
<td>$f(\mu, \sigma)$</td>
<td>-</td>
<td>Space-filling</td>
<td>Normal</td>
</tr>
<tr>
<td>Tang and Chen (2009)</td>
<td>Cup deep</td>
<td>Latin hypercube sampling</td>
<td>Finite element</td>
<td>RSM</td>
<td>Adaptive importance sampling</td>
<td>$\tilde{f}(\mu, \sigma)$</td>
<td>Monte Carlo</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sun et al. (2010)</td>
<td>Drawbead design</td>
<td>Taguchi orthogonal array</td>
<td>Finite element</td>
<td>Dual-RSM</td>
<td>(second order polynomial)</td>
<td>$\tilde{f}(\mu, \sigma)$</td>
<td>Particle swarm</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
## 2.3. Overview of commonly used strategies for robust optimization

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>Process</td>
<td>Deep-drawing of a square cup</td>
<td>V-bending</td>
<td>foam-filled thin-walled structure</td>
<td>Deck lid inner panel stamping</td>
</tr>
<tr>
<td>DOE</td>
<td>Integration of Taguchi orthogonal design and CCD</td>
<td>LHS</td>
<td>LHS</td>
<td>Uniform design</td>
</tr>
<tr>
<td>Black-box</td>
<td>Finite element</td>
<td>Finite element</td>
<td>Finite element</td>
<td>Finite element</td>
</tr>
<tr>
<td>Metamodel</td>
<td>Dual-RSM (Third-order polynomial)</td>
<td>Kriging (second-order)</td>
<td>Dual-RSM (Kriging) (second order polynomial)</td>
<td>Dual-RSM (Kriging) (second order polynomial)</td>
</tr>
<tr>
<td>Uncertainty propagation</td>
<td>Monte Carlo</td>
<td>Monte Carlo</td>
<td></td>
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</tr>
<tr>
<td>Objective function</td>
<td>( \tilde{f}(\mu, \sigma) )</td>
<td>( \hat{f}(\mu, \sigma) )</td>
<td>( \hat{f}(\mu, \sigma) )</td>
<td>( \tilde{f}(\mu, \sigma) )</td>
</tr>
<tr>
<td>Search algorithm</td>
<td>-</td>
<td>Genetic Algorithm</td>
<td>SQP</td>
<td>Monte Carlo</td>
</tr>
<tr>
<td>Iterative improvement</td>
<td>-</td>
<td>Adaptive (Jurecka (2007))</td>
<td>Adaptive (optimal solution)</td>
<td>-</td>
</tr>
<tr>
<td>Input distribution</td>
<td>-</td>
<td>Normal</td>
<td>Normal and uncorrelated</td>
<td>Normal and uncorrelated</td>
</tr>
</tbody>
</table>
### The choices for building blocks of robust optimization in the literature (continued)

<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>Process</td>
<td>V-bending</td>
<td>U-shaped forming</td>
<td>Stamping process</td>
</tr>
<tr>
<td>DOE</td>
<td>LHS and Full-factorial</td>
<td>LHS</td>
<td>Box-Behnken design</td>
</tr>
<tr>
<td>Black-box</td>
<td>Finite element</td>
<td>Finite element</td>
<td>Finite element</td>
</tr>
<tr>
<td>Metamodel</td>
<td>Kriging, RBF</td>
<td>RBF</td>
<td>RSM (second order)</td>
</tr>
<tr>
<td>Uncertainty propagation</td>
<td>Monte Carlo</td>
<td>finite difference on Metamodel</td>
<td>Monte Carlo</td>
</tr>
<tr>
<td>Objective function</td>
<td>$\tilde{f}(\mu, \sigma)$</td>
<td>$\tilde{f}(\mu, \sigma)$</td>
<td>Percentage of rejected products</td>
</tr>
<tr>
<td>Search algorithm</td>
<td>SQP</td>
<td>-</td>
<td>Monte Carlo</td>
</tr>
<tr>
<td>Iterative improvement</td>
<td>Adaptive (Jurecka (2007))</td>
<td>Adaptive (optimal solution)</td>
<td>-</td>
</tr>
<tr>
<td>Input distribution</td>
<td>Normal</td>
<td>-</td>
<td>Normal</td>
</tr>
</tbody>
</table>
Inspection of Table 2.3 reveals that some assumptions are very common during robust optimization. For instance, the input probability distribution is generally assumed to follow a normal distribution. Moreover, the objective function is usually a function of the mean and standard deviation of the response. It is also notable that various choices for each building block can be mixed with any other choice in another building block. Based on this information, the challenges and approaches in this thesis are introduced briefly in the next section.
2.4 Approaches and challenges addressed in this thesis

The computational effort during metamodel-based robust optimization and the accuracy of the results depend directly on the methods selected for each building block of robust optimization. There are some steps, e.g. calculation of uncertainty propagation and objective function uncertainty, that require the biggest portion of the computational effort and have a large influence on the accurate prediction on the robust optimum. Therefore, using more accurate and efficient approaches in those steps are the subject of this thesis. MC method which is generally used in the literature for noise propagation is a brute force method that is based on direct function evaluations. In Chapter 3 an analytical approach is presented that replaces MC in the evaluation of the noise propagation. In addition, the analytical method improves the search for the robust optimum by directly providing the gradients of the objective function and constraints. Moreover, it can be employed in the analysis of metamodel uncertainty and therefore a remarkable improvement in the robust optimization is expected. This method is implemented and the results are compared with that of MC in terms of accuracy and efficiency in Chapter 4.

In Chapter 5 the consequences of the non-normality of the response is discussed. The formulation of constraints and the reliance on sigma design quality level are based on the normal probability distribution of the response. However, in practice the response might not follow a normal distribution and therefore corrections to the formulation of constraint and robustness measure are required. It is shown how to implement skewness and kurtosis of the response to consider the reliability and robustness more accurately. Skewness, the normalized third central moment, is a measure of symmetry and is denoted by $\gamma_1(x)$. Kurtosis, the normalized fourth central moment, is a measure of tailedness and is denoted by $\gamma_2(x)$. Figure 2.8 shows how the response distribution changes by varying the skewness and kurtosis values. These changes in the distribution of response can significantly affect the reliability of constraints satisfaction and the sigma-level quality.
2.4. Approaches and challenges addressed in this thesis

\[ \gamma_1 > 0 \quad \gamma_1 = 0 \quad \gamma_1 < 0 \]

\[ \gamma_2 > 3 \quad \gamma_2 = 3 \quad \gamma_2 < 3 \]

Figure 2.8: The schematics of the effects of (a) skewness, \( \gamma_1 \) and (b) kurtosis, \( \gamma_2 \) on the appearance of a probability distribution (all curves have the same mean and standard deviation)

Figure 2.9: Schematic illustration of the propagation of a non-normal noise

In Chapter 6, the influence of non-normal noise distribution and the correlation between different noise variables are investigated. The propagation of a non-normal input through the model of a process is shown in Figure 2.9. The estimation of the resulting response with a normal distribution leads to errors in the prediction of reliability and sigma level process quality. Therefore, the criteria used for objective function and constraints must be adapted.
Robust optimum design is obtained by searching for the minimum variation of response around the target mean. A tighter product tolerance is achievable only by requiring less scatter of noise variables. This means for example that materials with a tighter specification must be ordered. The concept of tailoring noise variable is shown schematically in Figure 2.10-b.

Finding a solution to reduce the scatter of input noise and implementing that solution usually incur additional costs (Stockert et al., 2018). Therefore, the combination of noise variables having large variations while satisfying the required tolerances is of economic interest. A method will be presented in Chapter 7 to address this challenge. Tailoring material and process scatter are performed on an automotive part. The knowledge developed in the analysis of robust optimization (forward problem) in this thesis, is used as a basis for tailoring the scatter of noise variables (inverse problem) in an efficient manner.

Figure 2.10: (a) Noise propagation and (b) the concept of tailoring scatter
Chapter 3

Uncertainty evaluation based on analytical method

In the previous chapter, the building blocks of a robust optimization problem were introduced. In this chapter, an efficient method for uncertainty evaluation during the search for a robust optimum is developed. This method assesses the uncertainty propagation through integration of the mathematical description of the metamodel multiplied by noise probability distribution. This method can replace existing methods used for uncertainty evaluation such as Monte Carlo (MC) and Taylor series approximation.

The analytical method helps to perform several building blocks of robust optimization accurately and efficiently. It will be shown how to evaluate the propagation of uncertainty and calculate objective function value and constraints. In addition, the derivatives of responses with respect to each design variable will be evaluated which can improve the search for a robust optimum. Moreover, the uncertainty of the objective function value will be evaluated that can be used to perform iterative improvement of the metamodel.

In this chapter only the analytical method used in robust optimization is developed. In the following chapter, the results of analytical

This chapter contains content from:


method will be compared to the MC method which is widely used in the literature. This chapter is structured as follows: In Section 3.1 a general approach is presented to calculate the uncertainty propagation analytically. In Section 3.2 the method of calculation of derivatives is presented. The potential of the analytical approach to evaluating higher order statistical moments of the response is presented in Section 3.4. This method is used for uncertainty propagation through Kriging and RBF metamodels in Sections 3.5 and 3.6, respectively.

3.1 Calculation of the response mean and standard deviation

Assume a process that has $n_v$ inputs and one response. The vector of input variables is considered as $\mathbf{v} \in \mathbb{R}^{n_v}$ which includes design parameters, $\mathbf{x} \in \mathbb{R}^{n_x}$, and noise variables, $\mathbf{z} \in \mathbb{R}^{n_z}$. Assume that the response of the process is defined as $r = r(\mathbf{v}) = r(\mathbf{x}, \mathbf{z})$. The mean and variance of response are expressed by:

$$
\mu_r(\mathbf{x}) = \int_{\mathbf{z}} r(\mathbf{x}, \mathbf{z}) p(\mathbf{z}) d\mathbf{z} \quad (3.1)
$$

$$
\sigma_r^2(\mathbf{x}) = \int_{\mathbf{z}} [r(\mathbf{x}, \mathbf{z}) - \mu_r(\mathbf{x})]^2 p(\mathbf{z}) d\mathbf{z} \quad (3.2)
$$

In this equation, $p(\mathbf{z})$ is the probability distribution function of the noise variables. A simple approach to solving the above-mentioned integrals is to use MC approximations:

$$
\hat{f}(\mathbf{x}) = \int_{\mathbf{z}} f(\mathbf{x}, \mathbf{z}) p(\mathbf{z}) d\mathbf{z} \simeq \frac{1}{N_{mc}} \sum_{s=1}^{N_{mc}} f(\mathbf{x}, \mathbf{z}_s) \quad (3.3)
$$

where $\mathbf{z}_s$ is the vector consisting of random sample points drawn from the noise probability distribution and $N_{mc}$ is the number of sample points. Using the MC method the first two statistical moments of the response can be calculated using:

$$
\mu(\mathbf{x}) \simeq \frac{1}{N_{mc}} \sum_{s=1}^{N_{mc}} r(\mathbf{x}, \mathbf{z}_s) \quad (3.4)
$$

$$
\sigma^2(\mathbf{x}) \simeq \frac{1}{N_{mc}} \sum_{s=1}^{N_{mc}} (r(\mathbf{x}, \mathbf{z}_s) - \mu(\mathbf{x}))^2 \quad (3.5)
$$
3.1. Calculation of the response mean and standard deviation

These equations are the approximations of the integrals in Equations (3.1) and (3.2). A large sample size is required to obtain an accurate result. Even when a metamodel is evaluated using these samples, considerable computational effort is still required. If the integrals of Equations (3.1) and (3.2) are evaluated analytically and a closed-form expression for those integrals is obtained, a significant improvement in accuracy and calculation time is expected.

It has been shown that if the response of a metamodel, \( r(v) \), can be expressed as a sum of tensor-product basis functions, the results of univariate integrals can be combined to evaluate multivariate integrals. (Chen et al., 2005). Multivariate tensor-product basis functions, \( B_i(v) \), can be written as a product of \( n_v \) univariate basis functions, \( b_i(v) \):

\[
B_i(v) = \prod_{t=1}^{n_v} b_{it}(v_t), \quad i = 1, 2, ..., N
\]  \hspace{1cm} (3.6)

where \( b_{it}(v_t) \) is a univariate basis function and \( N \) is the number of multivariate basis functions.

If a response function, \( r(v) \) can be defined using linear expansion of these multivariate basis functions, it can also be re-written in terms of univariate basis functions as follows:

\[
r(v) = a_0 + \sum_{i=1}^{N} a_i B_i(v) = a_0 + \sum_{i=1}^{N} \left\{ a_i \prod_{t=1}^{n_v} b_{it}(v_t) \right\}
\]  \hspace{1cm} (3.7)

Most of the metamodels which are commonly used, e.g. polynomial regression, Kriging, and Gaussian radial basis functions (RBF), can be expressed using tensor-product basis functions. Thus, the multivariate integrals of Equations (3.1) and (3.2) can be evaluated for those metamodels (Chen et al., 2005).

By substituting Equation (A.1) into (3.1), the mean of the response is obtained through:

\[
\mu_r(x) = a_0 + \sum_{i=1}^{N} \left\{ a_i \prod_{p=1}^{n_x} b_{ip}(x_p) \prod_{q=1}^{n_z} C_{1iq} \right\}
\]  \hspace{1cm} (3.8)

where \( C_{1iq} \) depends on the choice of the metamodel and the noise probability distribution:

\[
C_{1iq} = \int_{z_q} b_{iq}(z_q)p(z_q)dz_q
\]  \hspace{1cm} (3.9)
Similarly, by inserting Equations (A.1) and (3.8) into Equation (3.2) the standard deviation of the response is calculated using:

\[
\sigma^2_r(x) = \sum_{i=1}^{N} \sum_{j=1}^{N} \left\{ a_i a_j \prod_{p=1}^{n_x} b_{ip}(x_p)b_{jp}(x_p)(\prod_{q=1}^{n_z} C^2_{ijq} - \prod_{q=1}^{n_z} C^1_{iq} C^1_{jq}) \right\}
\]

(3.10)

where \(C^2_{ijq}\) depends on the choice of the metamodel and the noise probability distribution:

\[
C^2_{ijq} = \int_{z_q} b_{iq}(z_q)b_{jq}(z_q)p(z_q)dz_q
\]

(3.11)

The details of the derivation of \(\mu_r(x)\) and \(\sigma^2_r(x)\) are given in Appendix A. The evaluations of \(\mu_r(x)\) and \(\sigma^2_r(x)\) are generic and there is no specific assumption for basis functions and noise probability distribution. Once the basis functions for specific metamodel and the noise probability distribution are substituted in Equations (3.8) to (3.11), the specific results for the combination of metamodel and noise probability distribution can be obtained. Since Kriging and Gaussian RBF metamodels are usually used for metamodelling, the results of evaluations for both Kriging and Gaussian RBF metamodels are given in Sections 3.5 and 3.6 respectively.

It is assumed that the noise variables are statistically independent. If the noise variables are not statistically independent, this method is still applicable when principal component analysis (PCA) of the input noise is done. The PCA analysis should be performed to transform a set of correlated parameters into a set of linearly uncorrelated parameters. More details about employing PCA in robust optimization to decouple the input noise variables will be presented in Chapter 6.

### 3.2 Analytical gradients of mean and standard deviation

If the search for robust optimum design is performed using gradient-based methods, it is beneficial to provide the gradients of objective function and constraints analytically. As the objective function and the constraints are usually a function of mean and standard deviation of response, in this section the derivatives of mean and standard deviation are given so as to be able to calculate the derivatives of objective function and the constraints.
3.3 Iterative improvement of the metamodel

In gradient-based optimization algorithms, providing Analytical gradients of objective function and constraints increases the accuracy and the computational efficiency, specifically when a large number of input parameters are present. If the optimization algorithms are not provided with analytical gradients, the finite difference method is usually used to calculate those gradients. Nevertheless, finite difference is computationally more expensive than analytical calculation of gradients as it requires more function evaluations.

Analytical gradients of the mean and the standard deviation of the response with respect to each design variable can be calculated by:

\[
\frac{d\mu_r(x)}{dx_u} = \sum_{i=1}^{N} \left\{ a_i \times \frac{\frac{db_{iu}(x_u)}{dx_u}}{b_{iu}(x_u)} \prod_{p=1}^{n_x} b_{ip}(x_p) \prod_{q=1}^{n_z} C^{1iq} \right\} \tag{3.12}
\]

\[
\frac{d\sigma_r(x)}{dx_u} = \frac{1}{2\sigma_r(x)} \sum_{i=1}^{N} \sum_{j=1}^{N} \left\{ a_i a_j \times \frac{\frac{db_{iu}(x_u)}{dx_u} b_{ju}(x_u) + b_{iu}(x_u) \frac{db_{ju}(x_u)}{dx_u}}{b_{iu}(x_u) b_{ju}(x_u)} \prod_{p=1}^{n_x} b_{ip}(x_p) \prod_{p=1}^{n_z} b_{jp}(x_p) \times \left( \prod_{q=1}^{n_x} C^{2ijq} - \prod_{q=1}^{n_z} C^{1iq} C^{1jq} \right) \right\} \tag{3.13}
\]

where \(C^{1iq}\) and \(C^{2ijq}\) are as defined in Equations (3.9) and (3.11). Once these gradients are evaluated, the gradients of objective function and constraints can be calculated directly.

3.3 Iterative improvement of the metamodel

Iterative improvement of the metamodel during robust optimization requires prediction of the mean squared error (MSE) estimate \(\hat{s}^2(v) = \hat{s}^2(x, z)\). Therefore, the uncertainty of the objective function must be provided. The uncertainty measure on metamodel is dependent on both design variables and noise variables. In contrast, the uncertainty of the objective function value, \(\hat{s}_f(x)\) is dependent only on design variables. There are two main approaches to obtaining the uncertainty of the objective function value. As mentioned in Chapter 2, one method is to evaluate an integral over the noise space (evaluating mean value
of MSE) (Havinga et al., 2017; Wiebenga et al., 2012) and the other approach is a minimax robustness criterion (Jurecka, 2007; Jurecka et al., 2007). In this thesis, the first approach is used which is defined by:

\[
\hat{s}_f^2(x) = \int_z \hat{s}_f^2(x, z)p(z)dz
\]

(3.14)

This equation is similar to Equation (3.3) and the integral can be evaluated analytically in a similar way to that of Equation (3.10). The expression of \( \hat{s}_f^2 \) depends on the choice of metamodel and therefore it will be discussed in Sections 3.5 and 3.6.

### 3.4 Evaluation of higher order statistical moments of the response

It is feasible to extend the method presented in Section 3.1 for higher order statistical moments. Skewness, the normalized third central moment, is a measure of symmetry and is denoted by \( \gamma_1(x) \). Kurtosis, the normalized fourth central moment, is a measure of tailedness and is denoted by \( \gamma_2(x) \). Since the contribution of the tails of the response distribution to determining the robust optimum and evaluating the constraint is significant, the analytical approach is extended to find those statistical moments. They will be used in the following chapters to enhance the prediction of the robust optimum design. Skewness is calculated using:

\[
\gamma_1(x) = \frac{1}{\sigma_f^3(x)} \int_z [r(x, z) - \mu_r(x)]^3 p(z)dz
\]

(3.15)
By substituting Equation (A.1) in Equation (3.15):

\[
\gamma_1(x) = \frac{1}{\sigma_r^3(x)} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} a_i a_j a_k \times \left\{ \prod_{p=1}^{n_x} b_{ip}(x_p) b_{jp}(x_p) b_{kp}(x_p) \right. \\
\left. \prod_{q=1}^{n_x} \left(C_{3ijkq} - 3C_{2ijq}C_{1kq} + 2C_{1iq}C_{1jq}C_{1kq}\right) \right\}
\]

(3.16)

In this equation, \(C_{3ijkq}\) depends on the choice of metamodel (basis functions), and noise probability distribution:

\[
C_{3ijkq} = \int_{z_q} b_{iq}(z_q) b_{jq}(z_q) b_{kq}(z_q) p(z_q) \, dz_q
\]

(3.17)

Kurtosis is calculated using:

\[
\gamma_2(x) = \frac{1}{\sigma_r^4(x)} \int \left[ f(x,z) - \mu_r(x,z) \right]^4 p(z) \, dz
\]

(3.18)
By substituting Equation (A.1) in Equation (3.18):

\[
\gamma_{2r}(x) = \frac{1}{\sigma_{r}^{4}(x)} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} a_{i} a_{j} a_{k} a_{l} \times \\
\left\{ \prod_{p=1}^{n_{x}} b_{ip}(x_{p}) b_{jp}(x_{p}) b_{kp}(x_{p}) b_{lp}(x_{p}) \right. \\
\left. \times \prod_{q=1}^{n_{x}} \left( C_{4ijklq} - 4C_{3ijklq}C_{1lq} + 6C_{2ijklq}C_{1kq}C_{1lq} \\
- 3C_{1iq}C_{1jq}C_{1kq}C_{1lq} \right) \right\}
\]

(3.19)

In this equation:

\[
C_{4ijklq} = \int b_{iq}(z_{q}) b_{jq}(z_{q}) b_{kq}(z_{q}) b_{lq}(z_{q}) p(z_{q}) dz_{q} \quad (3.20)
\]

Once \(C_{3ijklq}\) and \(C_{4ijklq}\) are known for the specific metamodel and probability distribution, the skewness and kurtosis of the response can be evaluated on each design point. Details of the derivation of \(\gamma_{1r}(x)\) and \(\gamma_{2r}(x)\) are given in Appendix A.

### 3.5 Results for Kriging

Up to this section there was no assumption on basis functions (choice of metamodel) nor on probability distribution. One can employ the analytical approach as long as the integral of the basis function multiplied by probability distribution can be calculated directly. In this section and next section, the derivations will be provided for Kriging and Gaussian radial basis function (RBF) models, using normal probability distribution as noise distribution.

Calculation of the mean, the standard deviation, the derivatives, and the uncertainty of the objective function value requires the evaluation of \(C_{1iq}\) and \(C_{2iq}\). It should be noted that \(C_{1iq}\) and \(C_{2iq}\) are associated only with noise variables; they depend on the choice of metamodel for
3.5. Results for Kriging

noise variables and the noise probability distribution. A normal probability distribution is described using:

\[ N(z_q) = \frac{1}{\sigma_q \sqrt{2\pi}} \exp\left\{ -\frac{(z_q - \mu_q)^2}{2\sigma_q^2} \right\} \]  
\[ (3.21) \]

where \( \mu_q \) and \( \sigma_q \) are the mean and standard deviation of the input noise data.

An ordinary Kriging metamodel is described by:

\[ r(v) = a_0 + \sum_{i=1}^{N} \kappa_i \prod_{t=1}^{n_v} b_{it}(v_t) \]  
\[ (3.22) \]

In this equation, the basis functions for Kriging are:

\[ b_{it}(v_t) = \exp\left\{ -\theta_t^2(v_t - v_{it})^2 \right\} \]  
\[ (3.23) \]

where the values for \( \theta_t \) are obtained from fitting the Kriging metamodel.

Considering the basis functions in Equation (3.23) and a normal probability distribution, as described in Equation (3.21), the expressions for \( C_{1iq}^{N} \), \( C_{ijq}^{N} \), \( C_{ijkq}^{N} \) and \( C_{ijklq}^{N} \) are evaluated by:

\[ C_{1iq}^{Krig,N} = \frac{1}{\sqrt{2\sigma_q^2 + 1}} \exp\left\{ -\frac{\theta_q^2}{2\sigma_q^2 + 1}(\mu_q - z_{iq})^2 \right\} \]  
\[ (3.24) \]

\[ C_{ijq}^{Krig,N} = \frac{1}{\sqrt{4\sigma_q^2 + 1}} \exp\left\{ -\frac{\theta_q^2}{4\sigma_q^2 + 1} \times \right\} \]

\[ \left( (\mu_q - z_{iq})^2 + (\mu_q - z_{jq})^2 + 2\sigma_q^2 \theta_q^2(z_{iq} - z_{jq})^2 \right) \]  
\[ (3.25) \]
\[
C_{ij \kappa q}^{3\text{Krig.N}} = \frac{1}{\sqrt{6\sigma^2_q \theta^2_q + 1}} \exp\left\{ \frac{-\theta^2_q}{6\sigma^2_q \theta^2_q + 1} \times \left[ (\mu_q - z_{iq})^2 + (\mu_q - z_{jq})^2 + (\mu_q - z_{kq})^2 \right. \right. \\
\left. \left. + 2\sigma^2_q \theta^2_q (z_{iq} - z_{jq})^2 + (\mu_q - z_{kq})^2 \right. \right. \\
\left. \left. + (z_{iq} - z_{kq})^2 \right) \right\} 
\]
(3.26)

\[
C_{ijkl \lambda q}^{4\text{Krig.N}} = \frac{1}{\sqrt{8\sigma^2_q \theta^2_q + 1}} \exp\left\{ \frac{-\theta^2_q}{8\sigma^2_q \theta^2_q + 1} \times \left[ (\mu_q - z_{iq})^2 + (\mu_q - z_{jq})^2 \right. \right. \\
\left. \left. + (\mu_q - z_{kq})^2 + (\mu_q - z_{lq})^2 \right. \right. \\
\left. \left. + 2\sigma^2_q \theta^2_q (z_{iq} - z_{jq})^2 + (z_{iq} - z_{kq})^2 + (z_{iq} - z_{lq})^2 \right. \right. \\
\left. \left. + (z_{jq} - z_{kq})^2 + (z_{jq} - z_{lq})^2 + (z_{kq} - z_{lq})^2 \right) \right\} 
\]
(3.27)

Details of the derivation of \(C_{ij \kappa q}^{1\text{Krig.N}}\), \(C_{ij \kappa q}^{2\text{Krig.N}}\), \(C_{ij \kappa q}^{3\text{Krig.N}}\), and \(C_{ijkl \lambda q}^{4\text{Krig.N}}\) are given in Appendix B. For universal Kriging with a linear detrending, the linear part can be evaluated separately. Then the result of the linear part of the response and the Kriging fitted on the residuals can be combined to obtain the statistical moments of the response. For more details
about the uncertainty propagation using a Kriging metamodel with a linear or second order detrending, the reader is referred to Appendix B.

As mentioned earlier, the uncertainty measure for objective function value is another important parameter to obtain during sequential optimization. From Equation (3.14), for a Kriging metamodel combined with a normal distribution as noise input:

$$\hat{s}^2_f = \sigma^2 - \hat{\sigma}^2 \sum_{i=1}^{N} \sum_{j=1}^{N} R_{ij}^{-1} \left( \prod_{p=1}^{n_x} b_{ip} b_{jp} \prod_{q=1}^{n_x} C_{Krig,N}^{ijq} \right)$$  \hspace{1cm} (3.28)

More details about the calculation of $\hat{s}_f$ can be found in Appendix B.

### 3.6 Results for Gaussian RBFs

The basis functions for Gaussian RBF are:

$$b_{it}(v_t) = \exp \left\{ -\frac{\rho_t^2}{2\tau_i^2} (v_t - v_{it})^2 \right\}$$  \hspace{1cm} (3.29)

In these equations, $\rho_t$, and $\tau_i$ are the parameters obtained from fitting a Gaussian RBF model. More details about fitting and RBF model can be found elsewhere (Havinga et al., 2017).

The main difference of RBF with Kriging is that the weights in RBF are assigned to each basis function and each variable, whereas those weights in a Kriging model are assigned to each variable only. With this definition, Kriging is a special case of RBF when the basis functions are Gaussian and the weights assigned to each basis function are equal. For Gaussian RBF and normal distribution, $C_{1iq}^{GRBF,N}$ and $C_{2iq}^{GRBF,N}$ are obtained in a similar way to Kriging by:

$$C_{1iq}^{GRBF,N} = \frac{1}{\sqrt{\frac{\sigma_q^2 \rho_q^2}{\tau_i^2} + 1}} \exp \left\{ -\frac{\rho_q^2}{2\sigma_q^2 \rho_q^2 + 2\tau_i^2} (\mu_q - z_{iq})^2 \right\}$$  \hspace{1cm} (3.30)
\[ C_{ijq}^{2,GRBF,N} = \frac{\tau_i \tau_j}{\sqrt{\rho_q^2 \sigma_q^2 \tau_i^2 + \rho_q^2 \sigma_q^2 \tau_j^2 + \tau_i^2 \tau_j^2}} \times \exp \left\{ -\frac{\rho_q^2}{2(\rho_q^2 \sigma_q^2 \tau_i^2 + \rho_q^2 \sigma_q^2 \tau_j^2 + \tau_i^2 \tau_j^2)} \times \left( \tau_i^2 (\mu_q - z_{jq})^2 + \tau_j^2 (\mu_q - z_{iq})^2 + \rho_q^2 \sigma_q^2 (z_{iq} - z_{jq})^2 \right) \right\} \]

(3.31)

The expressions of \( C_{ijkq}^{3,GRBF,N} \) and \( C_{ijklq}^{4,GRBF,N} \) for Gaussian RBF and normal probability distribution can be evaluated in a similar way as described in Section 3.5. Those expressions are very similar but lengthy and therefore are not included in this section.

In contrast to the Kriging metamodel, RBF does not provide an explicit uncertainty measure. Nevertheless, there are several methods of estimating \( \hat{s}^2 \) for RBF in the literature (Havinga et al., 2017; Li et al., 2010; Sóbester et al., 2004) and one common approach is to use the same form as employed for Kriging (Gibbs, 1998). If the same form as for a Kriging model is employed, Equation (3.28) can be used to calculate \( \hat{s}_f \) by substituting the basis functions for RBF and \( C_{ijq}^{2,GRBF,N} \) in that equation.

### 3.7 Conclusions and remarks

In this chapter, an analytical approach for obtaining the normalized statistical moments of the response is presented. In addition, the derivatives of the response statistical moments with respect to each design variable and the uncertainty of the objective function value are expressed. The analytical evaluation can replace other methods for noise propagation such as MC and Taylor series approximation. Moreover, the analytical gradients can replace the numerical methods of approximation of gradients such as finite difference.

To use the analytical method, the noise variables must be independent of each other. In addition, it must be possible to express the metamodel as a sum of tensor-product basis functions. Those expres-
Conclusions and remarks

Evaluations can be obtained only for specific combinations of basis functions of metamodels and the noise probability distribution. The results for Kriging and Gaussian RBF metamodels combined with a normal probability distribution of the noise are presented. The validation of those expressions is performed in the next chapter and they are compared with the MC method.
Chapter 4

Validation of the analytical approach

In this chapter, the Branin function is used to validate the expressions in the previous chapter and to show the relevance and advantages of using the analytical approach in metamodel-based robust optimization. The exact robust optimum design of the Branin function can be evaluated directly, without employing a metamodel. Thus, it can be used as a reference value to compare with the results obtained through metamodels.

The analytical approach is used on the metamodels of the Branin function to evaluate the statistical moments of the response, gradients of the response with respect to each design parameter, and the uncertainty of the objective function. Those results are compared with the MC method. Moreover, those results are used to evaluate the robust optimum design of the Branin function and compare the accuracy of different methods.

This chapter contains content from:


4.1 The Branin function

The Branin function has two variables: one variable is designated as design parameter and the other one is noise variable:

\[ r(x, z) = (z - \frac{5.1x^2}{4\pi^2} + \frac{5x}{\pi} - 6)^2 + 10(1 - \frac{1}{8\pi})\cos(x) + 10 \quad (4.1) \]

where \( x \) is the design parameter and \( z \) is the noise variable that follows a normal distribution described by a given mean and standard deviation. It is assumed that no constraints are present. The optimization problem is expressed by:

\[
\begin{align*}
\text{minimize} & \quad f(x) = \mu_r(x) + 3\sigma_r(x) \\
\text{subject to} & \quad -5 \leq x \leq 10 \\
& \quad z \sim \mathcal{N}(7.5, 2.5)
\end{align*}
\]

(4.2)

4.2 Generating a DOE

Latin hypercube sampling (LHS) combined with full factorial design (FFD) is used to generate 14 DOE points. This is done by generating 10,000 DOE sets using LHS, merging each one with FFD, and evaluating the minimum distance between all DOE points in each set. Among these sets the one that has the biggest minimum distance between any two points is selected as the best DOE. Branin function values are evaluated at those points and are used to make a metamodel.

4.3 Metamodels of Branin function

The analytical approach presented in the previous chapter was developed based on Kriging and Gaussian RBF. Both Kriging and Gaussian RBF are used in this section to make the metamodel of the Branin function for robust optimization. To propagate the noise variable through the metamodel, to evaluate the derivatives, and to calculate the uncertainty of the objective function value, the analytical method and also MC are employed on the metamodels of the Branin function.

In addition, the exact robust optimum design of the Branin function which is obtained by substituting (4.1) in Equations (3.1) and (3.2) is used to compare the accuracy of the robust optimum design obtained using analytical and MC methods on metamodels of the Branin function.
4.4. Comparison of analytical method and MC using Kriging

The statistical moments of the response, the gradients of mean and standard deviation with respect to design parameters, and the uncertainty of the objective function value are evaluated for the Kriging metamodel of the Branin function using the analytical approach. The results are compared with the values obtained using MC. It has been suggested that the number of sample points for MC analysis should be between 100 and 1000 for each dimension (Bucher, 2009; Kleijnen, 2007). This range balances the accuracy versus computational effort. Therefore, these sample sizes are used in this chapter. It must be noted that exact values of response characteristics for the Branin function can also be calculated. However, they are not presented, as the purpose in this section is to compare the accuracy of uncertainty propagation through

The Branin function and its representative metamodels are illustrated in Figure 4.1.

![Figure 4.1: Branin function and its representative metamodels](image)
the metamodels.

4.4.1 Mean and standard deviation

To minimize the objective function in Equation (4.2), \( \mu_r(x) \) and \( \sigma_r(x) \) must be calculated. Figure 4.2 shows the values obtained for \( \mu_r(x) \) and \( \sigma_r(x) \) using the analytical approach, and the results of using MC method are also presented. In this figure, each point on each curve is a result of the MC evaluation at that \( x \). For different \( x \) values on each curve, MC evaluation is performed using a fixed sample drawn from a normal probability distribution. If a new random sample is taken for different \( x \) values of each curve, the curves generated by MC will not be smooth. For this reason, a fixed sample is used to plot these curves.

In Figure 4.2, each curve generated by MC represents a different sample. Due to the randomness of the MC sampling, various samples of the same size drawn from a given normal distribution, propagated using the same metamodel, lead to different results. It is shown in Figure 4.2 that a small sample size leads to large sample-to-sample variations in the prediction of the mean and the standard deviation. Sample-dependency of the results is a major disadvantage of the MC method. Even though increasing the sample size on the noise domain reduces the variation, it never vanishes. Additionally, the computational effort increases by increasing the sample size.

The sample-to-sample variation due to randomness leads to variations in the prediction of the objective function value in equation (4.2) and consequently results in unreliable prediction of the robust optimum design. The consistent result and relatively low computation cost of the analytical approach (compared to a large sample size in MC) makes it more advantageous than MC.

4.4.2 Derivatives with respect to each design parameter

Most nonlinear optimization algorithms require derivatives of the objective function and constraints. Approximation methods such as finite difference are widely used to obtain those gradients. However, providing analytical gradients improves the computational efficiency by reducing the number of function evaluations which are required to obtain gradients numerically (Nocedal and Wright, 1999). If required by the analytical method, second order derivatives (Hessian) of a function can additionally be obtained by using a similar approach.
4.4. Comparison of analytical method and MC using Kriging

Figure 4.2: Comparison of mean and standard deviation on design space obtained using analytical and MC method for Kriging metamodel
Chapter 4. Validation of the analytical approach

Figure 4.3: Comparison of gradients of mean and standard deviation on design space obtained using analytical and MC&FD method for a Kriging metamodel of the Branin function.
4.4. Comparison of analytical method and MC using Kriging

Figure 4.3 shows the comparison between gradients obtained using finite difference applied to MC results (MC&FD) and analytical approaches. Similarly to the mean and the standard deviation, their gradients obtained using various random samples of the same size drawn from a normal distribution show variations around the analytical gradients. The variations of gradients originate from the random sampling and not from the finite difference method. Analytical calculation of the gradients is even more efficient than finite difference as the number of function evaluations is less than in the finite difference method.

As discussed in the previous section, a fixed random sample is used for each curve generated by MC. This is critical in calculation of gradients and if a new random sample is taken for different $x$ values, MC&FD will lead to inaccurate and fluctuating gradients. This justifies the use of a fixed sample to obtain the curves by MC. Additionally, a bigger sample size on the noise domain increases the computational cost. The ratios of calculation time between analytical and MC methods to obtain the mean, the standard deviation and their derivatives are shown in Figure 4.4. This figure represents a single evaluation of each response which is done on the metamodel of the Branin function. Although the computational effort of the analytical method is similar to MC for small sample sizes, increased computational time specifically in high-dimensional problems is inevitable when using a larger sample size.

Taking into account the variations of the predictions as shown in Figures 4.2 and 4.3 and comparing them with the computational effort shown in Figure 4.4, the trade-off between the accuracy and computational time in the MC method is revealed. However, the analytical method is both fast and accurate and therefore highly recommended for robust optimization.

4.4.3 Skewness and kurtosis

In Section 3.4, it is argued that the analytical approach can be used to predict the higher order statistical moments of the response. Skewness and Kurtosis for a combination of the Kriging metamodel and normally distributed noise variable are shown in Figure 4.5. Moreover, MC results using different sample sizes are plotted in this figure. As shown in this figure, the higher order statistical moments of response calculated using the MC method show a larger sample-to-sample variation than those of the mean and the standard deviation of response. In most cases, their values deviate significantly from those calculated by the analytical
method. Drawing a random sample from a normally distributed noise generates some errors, e.g. the mean and standard deviation of the samples are not exactly equal to the desired mean and standard deviation of the noise. Large errors in MC predictions arise for two main reasons. First, the sampling error is propagated and is raised to the third or fourth power, and therefore the errors are larger than those of the mean and the standard deviation of the response. Second, calculation of skewness and kurtosis requires a division by $\sigma^3_r$ and $\sigma^4_r$, respectively. Therefore, the errors in calculation of $\sigma_r$ magnifies the errors in calculation of skewness and kurtosis.
4.4. Comparison of analytical method and MC using Kriging

Figure 4.5: Comparison of skewness and Kurtosis obtained using analytical approach and MC method for a Kriging metamodel of the Branin function

4.4.4 Iterative improvement for Kriging metamodels

The prediction of the uncertainty of the objective function, \( \hat{s}(x) \), is essential for improving the metamodel. Figure 4.6 shows \( \hat{s} \) for the Kriging model as a function of \( x \) obtained analytically and using the MC method with a sample size of 100. This figure shows that the MC evaluation of
\( \hat{s}(x) \) deviates significantly from that of the analytical approach. An accurate prediction of \( \hat{s}(x) \) is important as this value is calculated during each step of the iterative improvement of the metamodel to maximize the expected improvement (\( EI \)). A good prediction of \( EI \) increases the efficiency of the metamodel update by selecting a proper infill point. This is the topic of the next section in which the influence of the selection of a proper infill point during robust optimization is shown.

![Graph](image.png)

*Figure 4.6: Comparison of objective function uncertainty obtained using analytical and MC method for a Kriging metamodel of the Branin function*

### 4.5 Robust optimization based on analytical approach

In this section, robust optimization is performed based on the results obtained so far. The sequential quadratic programming (SQP) method is used to find the robust optimum design (Cheng and Li, 2015). Higher order statistical moments of the response are ignored in this section and the objective function of Equation (4.2) is used. To include the higher order statistical moments of the response in robust optimization, a different objective function must be defined which is the topic of Chapters 5 and 6. The initial Kriging metamodel is used for calculation of the uncertainty of the objective function. It is then used to obtain the new
4.5. Robust optimization based on analytical approach

infill points and to update the Kriging metamodel.

Table 4.1 shows the robust optimum design and the objective function values obtained from various approaches using the initial metamodel of the Branin function. The reference robust design optimum is at \( x_{\text{ref}} = -1.12 \) and has an objective function value of \( f_{\text{ref}} = 47.97 \). Using the MC method with different samples on the same metamodel leads to a different robust optimum value and robust design point due to sample-to-sample variation. Even using a random sample of size 1000 leads to around 8.0% difference in the prediction of robust optimum design and around 12.6% difference in the objective function value compared with the reference values. However, using the analytical method on the same metamodel leads to around 8.9% difference in the prediction of robust optimum design and around 7.2% difference in the objective function value compared with the reference values. The difference between \((x_{\text{opt}}, f_{\text{opt}})\) obtained using the analytical method and the reference solution of \((x_{\text{ref}}, f_{\text{ref}})\) originates from the metamodel error near the optimum, while the difference between the \((x_{\text{opt}}, f_{\text{opt}})\) obtained using the MC method and the reference solution of \((x_{\text{ref}}, f_{\text{ref}})\) originates from both metamodel error near the optimum and sampling. Therefore, using the analytical approach for propagating the noise variables eliminates the sampling error.

<table>
<thead>
<tr>
<th></th>
<th>Kriging</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( x_{\text{opt}} )</td>
</tr>
<tr>
<td>Reference</td>
<td>-1.12</td>
</tr>
<tr>
<td>Analytical</td>
<td>-1.02</td>
</tr>
<tr>
<td>MC-Rand100 #1</td>
<td>-1.42</td>
</tr>
<tr>
<td>MC-Rand100 #2</td>
<td>-0.95</td>
</tr>
<tr>
<td>MC-Rand100 #3</td>
<td>-0.67</td>
</tr>
<tr>
<td>MC-Rand1000 #1</td>
<td>-0.94</td>
</tr>
<tr>
<td>MC-Rand1000 #2</td>
<td>-1.06</td>
</tr>
<tr>
<td>MC-Rand1000 #3</td>
<td>-1.09</td>
</tr>
</tbody>
</table>

Iterative improvement of the metamodel is necessary to obtain a more accurate prediction of the process response specifically around the
optimum and consequently obtain a more accurate robust optimum. To reduce the metamodel error near the optimum, the metamodel is updated using the $EI$ criterion expressed in Section (2.12). In this chapter, $\bar{\omega} = 0.5$ is selected to balance between local and global search. Figure 4.7 shows the improvement of prediction of optimum design and objective function value by subsequent iterative improvement steps. Each marker shows the optimum design and the objective function value after adding one DOE point in each iterative improvement step. To follow the sequence of the improvements, the smallest markers indicate the beginning of the iterative improvement stage using the initial metamodel. As the iterative improvement progresses, those markers become larger in size. The star mark in Figure 4.7 is the reference optimum design and the reference objective function value.

The capability of the analytical approach in predicting the robust optimum is apparent from Figure 4.7. Even though the algorithm detects distant designs for optimum, e.g. $x = -1.24$ and $x = -1.05$, subsequent iterative improvement steps lead to the reference robust optimum successfully.

The MC method using 100 random samples has quite large deviations in the prediction of both optimum design and objective function value even after iterative improvement. In this case, the search for a robust design converges in a distant design point, showing that even improving the metamodel does not help to find the robust optimum design for a small sample size. The prediction error decreases by increasing the sample size to 1000. It is interesting to see that at some point the predicted optimum arrives at the vicinity of the reference optimum. However, by continuing the iterative improvement, the predicted optimum moves away from the reference optimum and converges in a more distant design point.

The error in prediction of optimum design and objective function value after iterative improvement is shown in Table 4.2. Fewer iterations are required to find the robust optimum using the analytical method than when using the MC method. As the predictions of the mean, the standard deviation and $\hat{s}$ are more accurate than those obtained by MC, the search for the robust optimum using analytical method is more efficient. By eliminating both sampling error and the metamodel error near the optimum, the analytically-obtained robust optimum has around 0.9% error in predicting $x_{opt}$ and around 0.02% error in predicting $f_{opt}$ compared to the reference optimum.
4.5. Robust optimization based on analytical approach

**Figure 4.7:** Improving the prediction of the optimum design and objective function value by iterative improvement using a Kriging metamodel of the Branin function

**Table 4.2:** Comparison of the accuracy of the analytical and MC methods for predicting the optimum design and objective function value using a Kriging metamodel of the Branin function

<table>
<thead>
<tr>
<th>Reference value</th>
<th>Analytical</th>
<th>MC-Rand100</th>
<th>MC-Rand1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>-1.12</td>
<td>-1.13</td>
<td>-1.39</td>
</tr>
<tr>
<td>f</td>
<td>47.97</td>
<td>47.96</td>
<td>44.92</td>
</tr>
<tr>
<td>Number of steps</td>
<td>-</td>
<td>11</td>
<td>14</td>
</tr>
</tbody>
</table>

In this section, only the mean and the standard deviation are used to predict the robust optimum design. From Figure 4.5 it is apparent that at $x_{\text{ref}} = -1.12$ the skewness and kurtosis of the response is much higher than other design points. The nonlinearity of the response and the convexity of the metamodel around the optimum are the main reasons for this observation. The standard deviation is emphasized in the objective function by using $w = 3$ in Equation (4.2) and therefore the search for
minimum objective function is mainly influenced by the search for minimum standard deviation. A small value for the standard deviation leads to a large skewness and kurtosis values as those statistical moments are normalized by division to $\sigma^3_r$ and $\sigma^4_r$, respectively. It will be shown in Chapter 5 that the higher order statistical moments of the response can be relevant in evaluation of the robust optimum.
4.6 Mean and standard deviation for Gaussian RBFs

Figure 4.8 shows the mean and the standard deviation of the response as a function of $x$ for the metamodel of the Branin function built using Gaussian RBFs. For comparison purposes MC predictions are also included. The mean and the standard deviation obtained using the MC method with various samples of the same size drawn from a normal distribution show variations around the results obtained analytically. As discussed earlier, a bigger sample size increases the accuracy of the prediction, but it increases the computational cost greatly.

It is apparent that the predictions of RBF are different from those of Kriging (4.1) even though both the Kriging and RBF metamodels are representing the same function. However, they are essentially different due to dissimilar parametrizations during the fitting, as mentioned in Section 3.5. These differences influence the evaluation of the robust optimum.

Figure 4.9 shows the gradient of the response mean and the gradient of the response standard deviation for the RBF model of the Branin function. Similarly to mean and standard deviation, significant differences are observed in comparison with the gradients of response mean and the standard deviation for the Kriging model presented in Figure 4.3. These differences result in a different solution for the optimization problem which is expressed in Table 4.3. Again, increasing the sample size reduces the variation around the analytically-obtained robust design.
Chapter 4. Validation of the analytical approach

Figure 4.8: Comparison of the mean and the standard deviation of the response on design points obtained using the analytical and MC method for a Gaussian RBF metamodel of the Branin function.
Figure 4.9: Comparison of the gradient of mean of the response and the gradient of standard deviation of the response on design points obtained using the analytical and MC method for a Gaussian RBF metamodel of the Branin function.
4.7 Influence of the sampling method in MC

In the previous sections, the results of the analytical method were compared with the results obtained from MC using random sampling. The sampling method from a probability distribution in MC can significantly affect the prediction of the variation of the characteristics of the response distribution. In this section, the random sampling and LHS in the MC method are compared.

To show the differences of random sampling and LHS in the MC method, 75 samples are generated using each method. Two sample sizes of 100 and 1000 are used for comparative purposes. These samples are then used to propagate the noise through a Kriging metamodel of the Branin function. Figure 4.10 shows various characteristics of the response distribution obtained using 75 random sample sets and 75 LHS sample sets. The results that are obtained analytically are also shown using dashed lines.

To a large extent, MC using LHS has less variations than using random sampling, when both of those methods have equal sample size. It is shown that LHS sampling from a normally-distributed noise leads to a very small deviation from analytical calculations of the response mean, the response standard deviation, and the uncertainty of the objective function. However, the variation increases when both methods are used to predict the higher order statistical moments. Therefore, the analy-

Table 4.3: Comparison of the objective function value and the robust design using the Gaussian RBF model for various approaches without iterative improvement

<table>
<thead>
<tr>
<th></th>
<th>$x_{opt}$</th>
<th>$f_{opt}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td>-1.12</td>
<td>47.97</td>
</tr>
<tr>
<td>Analytical</td>
<td>-1.10</td>
<td>51.13</td>
</tr>
<tr>
<td>MC-Rand100 #1</td>
<td>-1.71</td>
<td>47.45</td>
</tr>
<tr>
<td>MC-Rand100 #2</td>
<td>-0.98</td>
<td>45.69</td>
</tr>
<tr>
<td>MC-Rand100 #3</td>
<td>-0.66</td>
<td>50.35</td>
</tr>
<tr>
<td>MC-Rand1000 #1</td>
<td>-1.06</td>
<td>51.83</td>
</tr>
<tr>
<td>MC-Rand1000 #2</td>
<td>-1.02</td>
<td>52.26</td>
</tr>
<tr>
<td>MC-Rand1000 #3</td>
<td>-1.19</td>
<td>47.41</td>
</tr>
</tbody>
</table>
4.7. Influence of the sampling method in MC

Figure 4.10: The comparison of the prediction of various sampling methods with the analytical approach
tical approach is the preferred method for considering the higher order statistical moments of the response during robust optimization (Chapter 5).

Throughout this chapter, the Branin function with only one design variable and one noise variable was used to demonstrate the potential of using the analytical method in robust optimization. For a problem with more design variables and more noise variables the reader is referred to the article by Nejadseyfi et al. (2019) in which a basketball free throw in windy weather conditions is optimized.

4.8 Conclusions and remarks

The analytical approach to evaluating response characteristics and objective function uncertainty is used to show the advantages of using it in robust optimization. A robust optimization technique is studied using the Branin function. A robust design in the presence of uncertainties is obtained for Kriging and RBF metamodels and the results obtained with the analytical method are compared with those obtained by the Monte Carlo method in terms of accuracy and efficiency.

It is shown that an analytical evaluation of statistical moments used in robust optimization is capable of predicting the uncertainty propagation more accurately and consistently with minimal computational effort. In addition, analytical evaluation provides the analytical gradients which is a big advantage when using gradient-based optimization. Moreover, employing the analytical approach for iterative improvement of the Kriging metamodels leads to an accurate prediction of the optimum and requires fewer improvement steps than using numerical derivatives and MC analysis.

It is shown that the MC method with LHS sampling can improve the predictions of the characteristics of the response distribution compared to the random sampling in MC. However, for higher order statistical moments the predictions are not accurate enough with small sample size.
Chapter 5

Non-normal response distribution

If a noise variable which is normally distributed propagates through a linear process, the response will also follow a normal distribution. However, the propagation of a noise variable which is normally distributed via a nonlinear function leads to a non-normal response distribution. This chapter deals with the non-normal distribution of response and introduces a method of evaluating the robustness of the process and the satisfaction of constraints.

To improve the description of the response, the mean, standard deviation and skewness of the response are calculated by applying the analytical approach. A robustness criterion that accounts for skewness of response is presented for use during robust optimization. The goal is to get a better description of response probability distribution to improve the calculation of reliability of satisfying the constraints. Moreover, the sigma quality levels and the probability of the response falling into $\pm n\sigma$ from the mean introduced in Chapter 2 are based on the assumption that the distribution is normal. For a non-normal response those calculations are not accurate and therefore the link between the reliability and $\sigma$ quality level is lost. In this chapter, it is shown how to link the reliability and $\sigma$ quality level for a non-normal response.

To show the applicability of the proposed method, it is applied to

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This chapter contains content from:

the optimization of a metal forming process. The optimization is defined by an objective and a constraint, which are both nonlinear functions of design and noise variables. Kriging is used as a nonlinear model of that forming process. The results demonstrate that taking into account the skewness of the response helps to satisfy the reliability constraints at the desired level accurately while minimizing the variation of response. It is shown that this method can be extended to account for higher order statistical moments of the response during robust optimization.

5.1 Normal input and normal output, a general assumption in robust optimization

To consider the variation of response and evaluation of constraints during robust optimization, only mean and standard deviation are used in literature. (Cui et al., 2014; Du et al., 2008; Havinga et al., 2017; Zhao et al., 2015). The evaluation of the reliability of constraint satisfaction from Figure 2.5 and the sigma design quality level from Figure 2.6 are based on the normal probability distribution. Assuming that a normally-distributed noise leads to a normally-distributed response is correct when the relationship between input and output is linear as shown in Figure 5.1(a). A nonlinear relation between input and output leads to a non-normal distribution even if the input is normally distributed. For instance, concavity or convexity of the function might lead to an asymmetrical distribution of the response. This effect is shown in Figure 5.1(b). Additionally, a highly nonlinear response will give rise to higher order statistical moments of response (Mekid and Vaja, 2008). It is shown schematically in Figure 5.1(c) that by increasing nonlinearity of the process, kurtosis can be used to accurately describe the response distribution.

For a non-normal distribution of response, considering only the mean and the standard deviation induces errors in calculation of the reliability of constraint satisfaction and the sigma quality level. This is related to the shift of the tails of the response distribution. The term *tail of a distribution* refers to a particular quantile of the response.

There have been attempts to capture the non-normality of the response by applying various methods and to include it in the optimization in the presence of uncertainty. For instance, Mekid and Vaja (2008) performed higher order uncertainty propagation using Taylor expansions and compared their approach with other methods that included MC.
sampling from a Gaussian input distribution. It was concluded that the necessity of considering higher order statistical moments depends on the nonlinearity of the response and other input factors.

In this chapter, a new approach is introduced for robust optimization that takes the skewness of the response into accounts. Skewness is used for evaluation of the robustness measure and constraints. The analytical method developed in Chapter 3 is used to calculate the mean, standard deviation, and skewness of the response by propagating a normally-distributed noise through a Kriging metamodel. The analytical method is used since it is fast and accurate.

This chapter is organized as follows: Section 5.2 introduces the new robustness measure and the method of applying the constraints at a desired level of reliability. Section 5.3 discusses the finite element (FE) simulation of a stretch-bending process as a case study. In that section, the optimization problem is formulated on the basis of the proposed approach. The results are presented and then discussed in Section 5.4.

5.2 Robust optimization including skewness

Once the mean, standard deviation and skewness of the response have been calculated, they can be used to evaluate the robustness measure and the constraints. In this section, a new approach is proposed to include the skewness measure during robust optimization. Even though the preferred method of calculating the statistical moments of the response in this chapter is by following an analytical approach, any other method for calculation of noise propagation (e.g. MC) can be used to evaluate those statistical moments and include them during the robust
optimization.

5.2.1 A probability distribution with skewness

A skew-normal distribution (SND) is considered with location-scale-shape parameters (\(\xi, \eta, \) and \(\lambda\) respectively) and it is denoted by \(\phi_D(\mathbf{r}; \xi, \eta, \lambda)\). The subscript D indicates the use of the direct parametrization in the work of Azzalini (1985). The density function is:

\[
\phi_D(\mathbf{r}; \xi, \eta, \lambda) = \frac{2}{\eta} \phi \left( \frac{r - \xi}{\eta} \right) \Phi \left( \lambda \frac{r - \xi}{\eta} \right)
\]

where \(\phi\) is the probability density function (PDF) of a standardized normal distribution (ND) and \(\Phi\) is the cumulative distribution function (CDF) of a standardized ND. This equation can be used to describe the probability distribution; however, the evaluation as given in Section 3.1 yields so-called centred parameters \((\mu, \sigma, \gamma)\) rather than location, scale and shape parameters. Therefore, it is necessary to make a connection between these two sets of parameters. Azzalini (1985) calculated \(\mu, \sigma, \) and \(\gamma\) for the above-mentioned distribution:

\[
\begin{align*}
\mu &= \xi + \eta \left( \sqrt{\frac{2}{\pi}} \frac{\lambda}{\sqrt{1 + \lambda^2}} \right) \\
\sigma^2 &= \eta^2 \left( 1 - \frac{2}{\pi} \frac{\lambda^2}{1 + \lambda^2} \right) \\
\gamma &= 4 - \pi \left( \sqrt{\frac{2}{\pi}} \frac{\lambda}{\sqrt{1 + \lambda^2}} \right)^3 \left( 1 - \frac{2}{\pi} \frac{\lambda^2}{1 + \lambda^2} \right)^{3/2}
\end{align*}
\]

By inverting these equations, once the statistical moments of a given distribution are known, location-scale-shape parameters can be obtained and used for further calculation (Pérez-Rodríguez et al., 2017):

\[
\begin{align*}
\xi &= \mu - \sigma \left( \frac{2\gamma}{4 - \pi} \right)^{1/3} \\
\eta^2 &= \sigma^2 \left( 1 + \left( \frac{2\gamma}{4 - \pi} \right)^{2/3} \right) \\
\lambda &= \left( \frac{2\gamma}{4 - \pi} \right)^{1/3 \left( \frac{2}{\pi} + \left( \frac{2\gamma}{4 - \pi} \right)^{2/3} \left( \frac{2}{\pi} - 1 \right) \right)^{-1/2}}
\end{align*}
\]
5.2. Robust optimization including skewness

Equation (5.1) is used as a mathematical description of the response during the optimization to calculate the reliabilities. The skewness parameter calculated for the density function, $\gamma$, is confined to a range of $-0.99527 < \gamma < 0.99527$, whereas the skewness of response, $\gamma_1$, based on (3.15) can vary infinitely, $-\infty < \gamma_1 < \infty$. Therefore, a connection is needed between these two parameters. Since both $\gamma = 0.99527$ in mathematical description and $\gamma_1 = \infty$ in Equation (3.15) lead to a half normal distribution, the following relation between these two parameters is used:

$$\gamma = 0.99527 \times \frac{\gamma_1}{\sqrt{1 + \gamma_1^2}}$$

(5.4)

Figure 5.2 shows SNDs of various $\gamma$ values. For all these distributions, $\mu = 0$ and $\sigma = 1$, while the left and right tails are shifting due to change in $\gamma$. The impact of tails shift on satisfying constraints; the reliability of a process and robustness are discussed in the following section.

5.2.2 Including skewness in robust optimization

In a design for a six sigma or three sigma process, the calculation of the probability of performance falling in a particular range is based on the assumption that the response is normally distributed (Koch et al., 2004).
Chapter 5. Non-normal response distribution

For an \( n\sigma \) process, the Sigma quality level is estimated via integration of PDF of an ND from \(-n\sigma\) to \(n\sigma\) (or \( \Phi(n\sigma) - \Phi(-n\sigma) \)). This quality level is valid only if the response distribution follows a normal distribution. In addition, the handling of constraints in robust optimization is based on requirements on the reliability of constraints satisfaction. If the response is not normally distributed, the reliability changes due to shift of the tails of the distribution, as shown in Figure 5.2.

When there is an upper bound, the reliability constraints are generally defined by:

\[
\mu_{rc}(x) + n\sigma_{rc}(x) < C_{rc}
\]  
(5.5)

and in the case of a lower bound:

\[
\mu_{rc}(x) - n\sigma_{rc}(x) > C_{rc}
\]  
(5.6)

For a robustness measure that minimizes the response variation in addition to the difference between mean and target value, \( C_r \), several expressions are proposed in the literature such as (Koch et al., 2004):

\[
\text{minimize } (\mu_{r}(x) - C_{r})^2 + w\sigma_{r}^2(x)
\]  
(5.7)

or (Havinga et al., 2017; Wiebenga et al., 2012):

\[
\text{minimize } (|\mu_{r}(x) - C_{r}| + w\sigma_{r}(x))
\]  
(5.8)

In equations (5.5) and (5.6), the choice of \( n \) is related to the desired reliability level in a normal distribution while in equations (5.7) and (5.8), \( w \) is a weighting factor to adjust the optimization objective between mean on target and response variation.

As mentioned previously, the response might not follow a normal distribution and therefore the constraints and robustness measure must be redefined properly. Functions \( L \) and \( U \) are defined to account for lower tail and upper tail shift, as shown in Figure 5.3.

To account for skewness in the evaluation of upper bound constraints one can use:

\[
\mu_{rc}(x) + U(\gamma; n)\sigma_{rc}(x) < C_{rc}
\]  
(5.9)

and in the case of lower bound:

\[
\mu_{rc}(x) + L(\gamma; n)\sigma_{rc}(x) > C_{rc}
\]  
(5.10)

In these equations, \( L(\gamma; n) < 0 \) and \( U(\gamma; n) > 0 \) and they are a function of skewness for a desired reliability level of \( n\sigma \). For a normal distribution,
5.2. Robust optimization including skewness

$$\text{SND} \mu = 0, \sigma = 1, \gamma = 0$$

$$\text{SND} \mu = 0, \sigma = 1, \gamma = 0.95$$

$$\bar{L} = L(0.95; 3), \bar{U} = L(0.95; 3)$$

$$L(\gamma; n) = -n \text{ and } U(\gamma; n) = +n.$$ Then equations (5.9) and (5.10) reduce to (5.5) and (5.6). For the robustness measure, a similar approach is used to account for the effect of the shift of the tails on the variation of the response. By modifying Equation (5.8):

$$\min \left| \mu_r(x) + \frac{U(\gamma; n) + L(\gamma; n)}{2} \sigma_r(x) - C_r \right|$$

$$+ \frac{w}{n} \times \frac{U(\gamma; n) - L(\gamma; n)}{2} \sigma_r(x)$$

(5.11)

It can be seen that for ND the robustness measure reduces to (5.8). As shown in Figure 5.3, the new criterion sets the centre of distribution \( (\mu_r(x) + (U(\gamma; n) + L(\gamma; n))/2)\sigma_r(x) \) on target and minimizes \((w/n)((U(\gamma; n) - L(\gamma; n))/2)\sigma_r(x)\).

Now the task is to obtain the functions \( L(\gamma; n) \) and \( U(\gamma; n) \). To achieve this, the quantiles of SND which lead to the same reliability as \( n\sigma \) for an ND are approximated. When, for example, a reliability of 3\( \sigma \) is required, \( L(\gamma; 3) \) is defined as the 0.0013 quantile of the cumulative SND and \( U(\gamma; 3) \) is defined as the 0.9987 quantile of the cumulative SND:

$$L(\gamma; 3) = \Phi_{\text{SND}}^{-1}(\Phi(-3\sigma); \mu, \sigma, \gamma) = \Phi_{\text{SND}}^{-1}(0.0013; \mu, \sigma, \gamma)$$

$$U(\gamma; 3) = \Phi_{\text{SND}}^{-1}(\Phi(3\sigma); \mu, \sigma, \gamma) = \Phi_{\text{SND}}^{-1}(0.9987; \mu, \sigma, \gamma)$$

(5.12)
Chapter 5. Non-normal response distribution

It is evident that for $\gamma = 0$, $L(\gamma; 3) = -3$ and $U(\gamma; 3) = +3$. As $\gamma$ increases or decreases, $L(\gamma; n)$ and $U(\gamma; n)$ change asymmetrically. To illustrate the approach to finding $L(\gamma; n)$ and $U(\gamma; n)$ in detail, Figure 5.4 shows the CDF of five SNDs with various $\gamma$ parameters. A horizontal line on this graph represents a specific reliability level or a specific quantile. A dashed line on the 0.0013 quantile shown in Figure 5.4 intersects with SND on $l_1 = -3$. The intersection of that line with CDFs of SNDs with different $\gamma$ values is at different points, namely $l_2$ to $l_5$. Similarly for the 0.9987 quantile, the dashed line intersects with SND CDFs on $u_2$ to $u_5$. Functions $L(\gamma; n)$ and $U(\gamma; n)$ are evaluated for various $\gamma$ values in the case of a 3$\sigma$ level and the results are plotted in Figure 5.5. $l_1$ to $l_5$ and $u_1$ to $u_5$ in Figure 5.4 are also shown on the plot of Figure 5.5.

For other values of $n$, Figure 5.6 shows $L(\gamma; n)$ and $U(\gamma; n)$. For a negative $\gamma$, due to symmetry, one can use:

$$L(-\gamma; n) = -U(\gamma; n), \quad U(-\gamma; n) = -L(\gamma; n),$$

(5.13)

One can pre-evaluate those functions for various skewness values to find a closed-form expression. In this section third order polynomials are fitted to those curves. Table 5.1 shows the fitting parameters for 3$\sigma$ and 6$\sigma$ reliability levels. During the robust optimization procedure, one can calculate $\gamma$ using the analytical method or by MC and evaluate $L(\gamma; n)$ and $U(\gamma; n)$ calculated by using the formulas listed in Table 5.1. Then
5.2. Robust optimization including skewness

Figure 5.5: $L(\gamma; 3)$ and $U(\gamma; 3)$ to obtain the reliability levels similar to $\pm 3\sigma$ in an ND
Chapter 5. Non-normal response distribution

Table 5.1: The fitted curves and the accuracy of the fits for \( L(\gamma;n) \) and \( U(\gamma;n) \)

<table>
<thead>
<tr>
<th>Coefficients of fit ((a\gamma^3 + b\gamma^2 + c\gamma + d))</th>
<th>( R^2 )</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L(\gamma;3) )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a = 1.31, b = -1.06, c = 1.29, d = -3 )</td>
<td>0.998</td>
<td>0.017</td>
</tr>
<tr>
<td>( U(\gamma;3) )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a = 0.29, b = -0.85, c = 1.55, d = 3 )</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>( L(\gamma;6) )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a = 4.05, b = -3.94, c = 4.08, d = -6 )</td>
<td>0.998</td>
<td>0.047</td>
</tr>
<tr>
<td>( U(\gamma;6) )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a = 2.31, b = -5.08, c = 5.64, d = 6 )</td>
<td>0.999</td>
<td>0.022</td>
</tr>
</tbody>
</table>

The robustness measure and satisfaction of constraints can be evaluated using equations (5.9) to (5.11) to find the robust optimum incorporating the non-normality of the response.

5.3 A case study: stretch-bending of dual-phase (DP) steel sheet

In this section, a demonstration case is presented to investigate the significance of accounting for skewness of the response during robust optimization. The stretch-bending process of DP800 steel sheet is chosen. During this process, a steel sheet is simultaneously stretched and bent to a desired curvature. After bending of the sheet material, the final bend angle will differ from the applied angle due to elastic spring-back. The amount of spring-back depends on the mechanical properties of the sheet material. By applying simultaneous stretching, the amount of spring back may be diminished and the accuracy of the process, in terms of the deviation of the final bend angle from the desired one, can be improved. On the other hand, applied stretching causes thickness reduction of the sheet, which should be limited.

Normally-distributed noise variables are defined for the material morphology and the sheet thickness. The resulting material model and the stretch-bending process are nonlinear and give rise to non-normally distributed results.
5.3. A case study: stretch-bending of dual-phase (DP) steel sheet

Figure 5.6: $L(\gamma; n)$ and $U(\gamma; n)$ for different $n$
5.3.1 The finite element model

A one-dimensional finite element model, as shown in Figure 5.7, is used to simulate this process. In this model, each through-thickness element has two nodes in the Z direction and five degrees of freedom. Nodal displacement increments for one element are shown in Figure 5.7(b) as $du_1$ and $du_2$. Additionally, three other degrees of freedom, the curvature ($\kappa$) and the membrane strains in circumferential ($\varepsilon_m$) and transverse ($\varepsilon_t$) direction are specified. Then, the local strain increments are determined using:

$$
\begin{bmatrix}
    d\varepsilon_{XX} \\
    d\varepsilon_{YY} \\
    d\varepsilon_{ZZ}
\end{bmatrix} = 
\begin{bmatrix}
    d\varepsilon_m - Zd\kappa - \frac{du_2}{r} \\
    \frac{d\varepsilon_t}{\partial du_z} \\
    \frac{\partial d\varepsilon_t}{\partial z}
\end{bmatrix}
$$

(5.14)

![Figure 5.7: (a) Finite element model and (b) one dimensional generalized plane-strain element](image)

5.3.2 A noisy material model

To model the material behaviour, a micro/macro approach using mean-field homogenization is implemented. In this approach, the rule of mixture is applied to a representative volume element (RVE) and the overall properties are obtained by weighted averaging of the respective properties of the constitutive phases in the material. This method is appropriate for composites or materials consisting of more than one phase, like DP steels. This method was developed by among others (Hashin and Shtrikman, 1963; Hill, 1965), and is based on the inclusion model proposed by Eshelby (1957). Any other material model can also be used.
5.3. A case study: stretch-bending of dual-phase (DP) steel sheet

More details about modelling the material behaviour using mean-field homogenization can be found in Appendix D.

To find the average properties, the Lielens interpolation method (Hori and Nemat-Nasser, 1993; Perdahcoğlu and Geijselaers, 2011) is used in this chapter. This method was proposed to improve the accuracy of the Mori-Tanaka method (Tanaka and Mori, 1970) and is also known as the double inclusion model. Using mean-field homogenization, it is possible to consider the variations in microstructural features of DP steel sheet.

Several microstructural aspects contribute to the steel’s mechanical properties. The volume fraction of the martensite distributed in the ferrite matrix plays a key role in controlling the mechanical properties. Additionally, it is known that DP steel often shows a banded martensite structure that is mostly concentrated at the centre of the sheet (Niazi et al., 2013). This depends on the cooling rate during hot rolling, the intercritical annealing temperatures, and the soaking time (Caballero et al., 2006). Another microstructural feature is the shape of martensite grains. Grains tend to elongate during the rolling process. It is assumed that, as a consequence, the martensite grains are not perfectly spherical but have an elongated shape. These three microstructural features are combined with thickness variations of the sheet and are considered as noise parameters during optimization. Figure 5.8 shows the variations in these parameters schematically.

5.3.3 The optimization problem

After developing the finite element model and defining the material model, the optimization problem can be set up by defining the inputs, outputs, objective function and constraints. As described in Table 5.2, in the stretch-bending process, there are two design parameters: $x_1$, applied curvature and $x_2$, stretch. It should be noted that the final curvature is different from applied curvature because of spring-back.

In this process, there are four noise variables that are stated in Table 5.3. Martensite volume fraction ($F_v$) and shape factor ($F_s$) are taken into account by applying Eshelby’s solution as described in Appendix D. To take into account the concentration of martensite in the middle layer of the material, a banding parameter ($F_b$) is introduced. This parameter is defined as the ratio of martensite volume fraction from $0.4t$ to $0.6t$ to the martensite volume fraction in the rest of the through-thickness region, $0$ to $0.4t$ and $0.6t$ to $t$. A sensitivity analysis step showed that
Figure 5.8: Variations in material thickness and martensite phase morphology

Table 5.2: Design parameters, x, in the stretch-bending process

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forming curvature (m(^{-1}))</td>
<td>50</td>
<td>55</td>
</tr>
<tr>
<td>Stretch (%)</td>
<td>2</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 5.3: Noise variables in the stretch-bending process

<table>
<thead>
<tr>
<th>Noise variable</th>
<th>Mean (\mu_x)</th>
<th>St. dev. (\sigma_z)</th>
<th>(\mu_x - 3\sigma_z)</th>
<th>(\mu_x + 3\sigma_z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sheet thickness, (t) (mm)</td>
<td>1</td>
<td>0.1/6</td>
<td>0.95</td>
<td>1.05</td>
</tr>
<tr>
<td>Volume fraction, (F_v) (%)</td>
<td>35</td>
<td>10/6</td>
<td>30</td>
<td>40</td>
</tr>
<tr>
<td>Shape factor, (F_s) (-)</td>
<td>0.7</td>
<td>0.1</td>
<td>0.4</td>
<td>1</td>
</tr>
<tr>
<td>Banding factor, (F_b) (-)</td>
<td>1.5</td>
<td>1/6</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>
these noise parameters have sufficient influence on the response to justify keeping them in the optimization procedure.

The output of the simulation is the final curvature and the percentage thickness reduction of the sheet. The percentage thickness reduction of the sheet is defined by:

$$\delta = -\frac{t_{\text{fin}} - t_{\text{init}}}{t_{\text{init}}} \times 100$$

(5.15)

In which, $t_{\text{fin}}$ and $t_{\text{init}}$ are the final and initial thickness of the sheet. For robust optimization, the aim is to obtain a target curvature, $C_r = 50m^{-1}$, and a constraint is defined on the thinning percentage, $C_{rc} = 2.5\%$. Design variables are set by defining upper and lower bounds, noise variables are taken into account through a normal probability distribution and the constraint is expressed using an inequality expression.

The objective function and the constraint are:

$$\min_{x} \left| \mu_r(x) + \frac{U(\gamma; n) + L(\gamma; n)}{2} \sigma_r(x) - C_r \right|
+ \frac{w}{n} \times \frac{U(\gamma; n) - L(\gamma; n)}{2} \sigma_r(x)$$

subject to

$$\mu_{rc}(x) + U(\gamma; n)\sigma_{rc}(x) - C_{rc} \leq 0$$

$$lb \leq x \leq ub$$

$$z \sim N(\mu_z, \sigma_z)$$

(5.16)

After defining the input, output, objective function and constraints, the optimization steps are followed according to Chapter 2. First, a DOE of 793 points is generated on the six-dimensional design-noise input space based on the combination of a Latin hypercube design (LHS) and a full-factorial design (FFD). Responses (final curvature and thinning) are evaluated by FE analysis as explained in Section 5.3.1. Kriging metamodels are fitted to both the final curvature and the final sheet thickness. Mean, standard deviation and skewness of the response are calculated using the analytical approach described in Chapter 3. Equation (5.16) is used as objective function and constraint by choosing $w = n = 3$ and the optimization is solved using an SQP algorithm.
Chapter 5. Non-normal response distribution

5.4 Results and discussion

To observe the influence of skewness in the robust optimization procedure, the proposed criterion of Equation (5.11) is used and is compared with formulation of Equation (5.8).

The robust optimum design obtained taking the 3 sigma approach and applying the new criterion is presented in Table 5.4. For comparative purposes, MC sampling is used to show the variation of response at the robust optimum design which is obtained using the analytical approach. Figure 5.9 shows the variation of response at the robust optimum found by assuming a normally-distributed response. MC sampling shows that the response distribution at the robust optimum does not follow an ND. The presence of multiple samples outside the ±3σ range for final curvature makes the robustness of the optimum obtained with a normally-distributed response questionable. Moreover, the goal to reduce the deviation of response by setting the mean on target is not achieved due to a shift of the mean as a result of the skewness of the output. In addition, the overestimation of the right tail for thinning causes a too conservative constraint. If one switches to a six sigma reliability design to be able to reduce the scrap rate (Koch et al., 2004), the influence of this conservative constraint will be significant. Nevertheless, as long as skewness exists the expected nσ reliability for the process will not be accurate. Therefore, the use of skewness in the robust optimum evaluation is essential.

Using the criterion proposed in Equation (5.11), a different robust optimum design is obtained that has a lower objective function value. To analyze the differences in detail, the variation of output around this optimum is evaluated and is shown in Figure 5.10. The SND shows an improved prediction of tails shift for each output and maintains the desired reliability for constraints. The new method shifts \( \mu + (U(\gamma; n) + L(\gamma; n))\sigma/2 \) to the target curvature, 50m\(^{-1}\), and successfully reduces the deviation from that target value. It can be seen that as a result of using this objective function the population is centred on the specified target.

It should be noted that the higher order statistical moments of the distribution are ignored. Even though a better estimation of robust optimum is expected using SND, a slight deviation of the percentage variation within the lower and upper tails is inevitable.

Another important aspect about the new criterion is the treatment of the constraint, which is more accurate than for the conventional method. If the reliability of the constraint is considered using Equation (5.5)
(shown by dashed ND in Figure 5.10(b)), there is a big difference between the upper specification limit on thinning and the actual upper limit of the response population. This difference, which originates from the skewness of the response distribution, implies that there is room for improvement. In other words, considering the reliability of constraint using an ND fit to the population shown using bar plot in the background of Figure 5.10(b) shows the inaccuracy of the conventional approach. Thus, the new criterion can considerably improve the search for the

\[ C_r - 3\sigma \]
\[ C_r \]
\[ C_r + 3\sigma \]

\[ N(\text{Final curvature})(1E-3) \]
\[ N(\text{Thinning})(1E-3) \]

\[ 49.4 \ 49.5 \ 49.6 \ 49.7 \ 49.8 \ 49.9 \ 50 \ 50.1 \ 50.2 \ 50.3 \]

\[ 1.7 \ 1.8 \ 1.9 \ 2 \ 2.1 \ 2.2 \ 2.3 \ 2.4 \ 2.5 \ 2.6 \]

**Figure 5.9:** Variation of response at the robust optimum found by the conventional method (The bars in the background are results from MC)
robust optimum by proper predictions of the tails of the distribution.

### 5.5 Using kurtosis during robust optimization

In the previous section, only the skewness of the response was used to account for non-normality of the output. However, the methodology of Section 5.2.2 can be extended to account for kurtosis in the calculations of the robustness measure and evaluation of constraints. Equations (5.9) to (5.11) were based on skew-normal distribution and the goal was to maintain the \( n\sigma \) reliability level as for normal distributions. In that case, the reliability was calculated from the definition of a skew-normal distribution and the parameters were obtained from the statistical moments of the response as expressed in Equation (5.1).

In Section 5.2.2 the estimation of the tails of the distribution to maintain the \( n\sigma \) reliability level was used to modify the constraint and objective function considering first three statistical moments. A number of methods exists to estimate the reliability based on the first four statistical moments without defining a probability distribution. Using those methods, the reliabilities can be estimated without obtaining a probability distribution from the first four statistical moments. In this section, the Edgeworth series (Kendall et al., 1987) is employed to obtain the reliabilities based on the first four statistical moments of the output.

The second-order Edgeworth series approximation to the CDF of a
5.5. Using kurtosis during robust optimization

Figure 5.10: Variation of response at the robust optimum found by including skewness (The bars in the background are the results from MC)

random variable using its first four statistical moments is:

$$\Phi_{\text{Edgeworth}}(r) = \Phi(r) - \phi(r) \left( \frac{\gamma_1(r^2 - 1)}{6} + \frac{(\gamma_2 - 3)(r^3 - 3r)}{24} + \frac{\gamma_2(r^5 - 10r^3 + 15r)}{72} \right)$$  \hspace{1cm} (5.17)

In this equation, it is assumed that the mean is zero and the standard deviation is 1. $\gamma_1$ and $\gamma_2$ are expressed in Equations (3.15) and (3.18).
Figure 5.11: $L(\gamma_1, \gamma_2; 3)$ and $U(\gamma_1, \gamma_2; 3)$
5.5. Using kurtosis during robust optimization

Table 5.5: The fitted curves and the accuracy of the fits for $L(\gamma_1, \gamma_2; 3)$ and $U(\gamma_1, \gamma_2; 3)$

<table>
<thead>
<tr>
<th>Coefficients of fit</th>
<th>$R^2$</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(a_{30} \gamma_1^3 + a_{03} (\gamma_2 - 3)^3 + a_{21} \gamma_1^2 (\gamma_2 - 3))$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$+ a_{12} \gamma_1 (\gamma_2 - 3)^2 + a_{20} \gamma_1^2 + a_{02} (\gamma_2 - 3)^2$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$+ a_{11} \gamma_1 (\gamma_2 - 3) + a_{10} \gamma_1 + a_{01} (\gamma_2 - 3)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(a_{00})$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$L(\gamma_1, \gamma_2; 3)$</td>
<td>$\begin{array}{c} a_{30} = 1.31, \ a_{03} = -0.02, \ a_{21} = -0.34 \ a_{12} = 0.35, \ a_{20} = -1.06, \ a_{02} = -0.17 \ a_{11} = -0.67, \ a_{10} = 1.29, \ a_{01} = 0.69 \ a_{00} = -3 \end{array}$</td>
<td>0.983</td>
</tr>
<tr>
<td>$U(\gamma_1, \gamma_2; 3)$</td>
<td>$\begin{array}{c} a_{30} = 0.29, \ a_{03} = -0.10, \ a_{21} = 0.11 \ a_{12} = -0.23, \ a_{20} = -0.85, \ a_{02} = 0.84 \ a_{11} = 0.61, \ a_{10} = 1.55, \ a_{01} = -1.60 \ a_{00} = 3 \end{array}$</td>
<td>0.999</td>
</tr>
</tbody>
</table>

The approach described in Section 5.2, can be extended to account for the kurtosis of the response during robust optimization. In this case, the definition of robustness measure and the constraints does not change. The only difference is that $L$ and $U$ will be not only a function of $\gamma_1$, but also of $\gamma_2$. For a $3\sigma$ quality level the bounds $L$ and $U$ are:

$$L(\gamma_1, \gamma_2; 3) = \Phi_{\text{Edgeworth}}^{-1}(\Phi(-3\sigma); \mu, \sigma, \gamma_1, \gamma_2)$$
$$U(\gamma_1, \gamma_2; 3) = \Phi_{\text{Edgeworth}}^{-1}(\Phi(3\sigma); \mu, \sigma, \gamma_1, \gamma_2)$$

(5.18)

During robust optimization it is possible to implicitly evaluate $L(\gamma_1, \gamma_2; n)$ and $U(\gamma_1, \gamma_2; n)$ for each evaluation of objective function and constraints. To speed up the calculations during the robust optimization, $L(\gamma_1, \gamma_2; n)$ and $U(\gamma_1, \gamma_2; n)$ can be pre-evaluated for different $n$. Then, the closed-form expressions for $L(\gamma_1, \gamma_2; n)$ and $U(\gamma_1, \gamma_2; n)$ can be employed during each function evaluation. Figure 5.11 shows the surfaces which have been fitted to different values of $\gamma_1$ and $\gamma_2$ and the fitting constants are expressed in Table 5.5. For a normal distribution $\gamma_1 = 0$ and $\gamma_2 = 3$ lead to $L(0, 3; 3) = -3$ and $U(0, 3; 3) = 3$. In addition, in the case of $\gamma_2 = 3$,
the constants of fitting for both $L(\gamma_1, 3; 3) = -3$ and $U(\gamma_1, 3; 3) = 3$ are equal to the constants obtained in Section 5.2.2. Once $L(\gamma_1, \gamma_2; n)$ and $U(\gamma_1, \gamma_2; n)$ are obtained during each evaluation of objective function and constraints using the first four statistical moments, Equation (5.16) can be used to evaluate the robust optimum.

5.6 Conclusions and remarks

When a normally distributed input parameter is subjected to a nonlinear process, the resulting output will be characterized by higher order statistical moments. The mean, standard deviation and skewness of the output distribution can be calculated analytically when the process is modelled by Kriging. The skewness parameter is then used to calculate the shift of the tails of the distributions of the objective function and the constraints. The shift of the tails is embedded in the definition of the robustness measure as well as in the evaluation of constraints during robust optimization.

Application of this approach for objective function and evaluation of constraints shows that the variation of output is successfully reduced and the constraints are handled more accurately than in robust optimum evaluation using only mean and standard deviation. In addition, accounting for higher order moments changes the optimum design setting. Moreover, it is shown how kurtosis can be included during robust optimization in a very similar manner using a proper definition of the shift of the tails of the distribution.
Chapter 6

Non-normal and correlated input

Numerical simulation is an essential tool for predicting the outcome of a metal forming process and for optimizing the process. Building, running and validating a model need to be accompanied by accurate characterization of the input parameters. Material properties are some of the main inputs to such models. These vary not only from coil to coil, but also within the same coil (de Souza and Rolfe, 2010; Mukhopadhyay and Iqbal, 2005). Therefore, a detailed stochastic description of the material parameters is required for application in the optimization of forming processes. Characterizing both the in coil variation and the coil-to-coil variation is a tedious task. It is therefore not straightforward to obtain a statistically-significant input. Moreover, the characterization methods are often limited to simple mechanical tests such as uniaxial tensile tests.

In this chapter, 49 coils of DP800 steel are characterized using tensile tests at $0^\circ$, $45^\circ$ and $90^\circ$ to rolling direction to find the variation of material behaviour. Moreover, the correlations between those material parameters are investigated and the correlated parameters are transformed to linearly uncorrelated principal components. A design of experiments

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This chapter contains content from:
(DOE) for varying material parameters is made to perform finite element simulations using AutoForm. Then, a metamodel of the response is built using Kriging method. This metamodel is used to represent the process in robust optimization, considering the non-normality of input and its influence on the output. The analytical approach, described in Chapter 3, is modified to be used for propagating the input uncertainty. Finally, the results of correlations between noise parameters and the influence of their variation on springback and thinning during a metal forming process are presented and discussed.

6.1 Variability of material properties

There have been some efforts to investigate the influence of variable input in metal forming processes. For example, de Souza and Rolfe (2010) investigated in-coil variation for DP600 and used it to predict the springback robustness for a sheet metal forming process. They performed 36 tensile tests at different locations in the same coil. It was found that the yield stress and the ultimate tensile stress were linearly correlated and that the strain hardening exponent, $n$, remained constant. They concluded that the variation of the material’s flow behaviour has a larger influence on springback than the variation of process parameters.

Marretta and Di Lorenzo (2010) investigated the influence of coil-to-coil variation of an aluminium alloy for a metal forming process. They included anisotropy effects of the sheets to address the thinning and springback accurately. It was shown that the effect of material variation was different at various operative conditions. In particular, it was more relevant within regions characterized by higher restraining force levels.

Wiebenga et al. (2014) studied the effect of coil-to-coil variation using 41 coils of a forming steel DX54D+Z (EN 10327:2004) collected from multiple casts. They performed extensive mechanical testing and texture analysis to achieve the stochastic material behaviour. Vegter yield locus (Vegter and van den Boogaard, 2006) was used to fit the data points from a crystal plasticity model (An et al., 2011). They validated their numerical approach by forming 41 hemispherical cup products. It was shown that the experimental scatter can be reproduced accurately using FE simulations and metamodels, demonstrating the potential of both the modelling approach and the robustness analysis.
6.1. Variability of material properties

6.1.1 The complexity of the material model

In literature, the material behaviour is considered using different models, from very simple ones to complicated ones. For a simple material model less effort is required to collect the variation data. On the other hand, complex material modelling requires a large number of characterization tests. This is a trade-off between the accuracy of the model and the effort to characterize the material.

Research on the material properties variation in metal forming processes generally ignores the effects of anisotropy (de Souza and Rolfe, 2010; Prates et al., 2018). It was shown by Gomes et al. (2005) that anisotropy has a considerable effect on springback and therefore, for an accurate prediction, anisotropy cannot be ignored. Recently, Abspoel et al. (2017) introduced an easy to use advanced yield locus that is able to describe the anisotropy accurately using only parameters of standard uniaxial tests. They demonstrated that for a wide range of materials the stress points in biaxial, plane strain and shear modes can be predicted using the flow curves and R-values obtained from uniaxial tensile tests at $0^\circ$, $45^\circ$ and $90^\circ$ to rolling direction. This method is employed in this chapter to measure the material anisotropy and to use it in the simulations.

6.1.2 Non-normality of input parameters

It is commonly assumed that the input probability distribution follows a normal distribution (Atzema et al., 2009; de Souza and Rolfe, 2010; Marretta and Di Lorenzo, 2010; Wiebenga et al., 2012). However, in practice non-normal input probability distributions are encountered. For example, in steel production, steel grades are manufactured from different batches and over different production lines. In addition to that, downgrading or upgrading of a product after characterization leads to a multimodal distribution of material properties.

To see these effects, a large number of tests are required. For example, Hora et al. (2011) showed after testing about 6000 samples that the ultimate tensile strength of DC06 steel grade follows a multimodal distribution. A method of efficiently capturing the influence of non-normal input probability distributions must be considered in robust optimization. In this case, the response probability distribution after noise propagation will not follow a normal distribution. A non-normal input distribution leads to a non-normal response distribution which can be
handled analytically, as described in Chapter 3. The handling of non-normal distributions of the input material parameters is addressed in this chapter.

6.2 Material characterization

Material characterization was performed on 49 samples obtained from 49 coils of DP800 steel sheet. Those coils were collected from various production lines. For each sample, the thickness of the sheet, $t$, was measured. Then the tensile properties in $0^\circ$, $45^\circ$ and $90^\circ$ were obtained as shown in Figure 6.1. The Swift hardening law is fitted to the results of the tensile test in rolling direction. The hardening is described using two parameters, $K$ and $n$ and it is assumed that $\varepsilon_0 = 0.002$.

To account for anisotropy, the method presented by Abspoel et al. (2017) is used. In that method, the anisotropy is described accurately using only parameters of standard uniaxial tests. Vegter yield locus (Vegter and van den Boogaard, 2006) is used, and therefore all measured stresses are normalized to the uniaxial stress in the rolling direction providing the stress factors, such that:

\begin{align}
F_{00} &= S_{00}/S_{00} = 1 \\
F_{45} &= S_{45}/S_{00} \\
F_{90} &= S_{90}/S_{00}
\end{align}

in which $S_{00}$, $S_{45}$ and $S_{90}$ are the ultimate tensile strength, $Rm$, divided by uniform elongation, $Ag$ in each direction (Abspoel et al., 2017).
6.2. Material characterization

Figure 6.2: Variation of material parameters
Chapter 6. Non-normal and correlated input

The parameters $r_{00}$, $r_{45}$, and $r_{90}$ are defined as the plastic strain in thickness direction, $\varepsilon_t$, divided by the plastic strain in width direction, $\varepsilon_w$, in uniaxial tensile tests.

Figure 6.2 shows the variations of the above-mentioned parameters around their mean value which are measured for 49 coils. The fitted normal distribution to each data set is shown in this figure. It is apparent that for some parameters the deviation of the fit from the underlying population is significant. In addition, there might be some correlations between the parameters that must be considered.

6.2.1 Correlations between the parameters

The correlations among noise parameters are evaluated for a better description of the input noise. For this purpose, the covariance principal component analysis (PCA) is used to find the principal components (PCs) of the noise parameters as described by Wiebenga et al. (2014). The purpose of PCA analysis is to get uncorrelated subspace, to possibly reduce the parameter space and to avoid sampling of physically-unlikely parameter combinations when the DOE is created.

The orthogonal transformation from the correlated data to linearly uncorrelated PCs is shown schematically in Figures 6.3(a) and 6.3(b). The DOE is then created in the PC space (Figure 6.3(c)) avoiding physically-unlikely parameters sets, the hashed area shown in Figure 6.3(d). A set of physically-unlikely parameters can lead to an overestimation of the response scatter during the robust optimization (Wiebenga et al., 2014). For finite element simulations, a back transformation from the PC domain to the physical parameter domain is required. The mutual linear correlation coefficient for various material parameters are
calculated by:
\[ \rho_{X,Y} = \frac{\text{Cov}(X, Y)}{\sigma_X \sigma_Y} \]  
(6.2)

where \( X \) and \( Y \) are two random variables centred about their mean, \( \sigma_X \) and \( \sigma_Y \) are their standard deviations, and \( \text{Cov}(X, Y) \) is the covariance, the degree of linear relationship between \( X \) and \( Y \). The value for the correlation coefficient ranges from -1 to 1 and it indicates the amount of correlation between two parameters.

The results of the material characterization for the samples obtained from 49 different coils are shown in Figure 6.4. The scatter plots in the top triangle of Figure 6.4 show the material properties variation and possible correlations between them. The parameter names are on the diagonal and the bottom triangle shows the mutual linear correlation coefficients for various material parameters calculated by (6.2). In this figure, a thicker box around the scatter plot in the upper triangle and a larger font in the bottom triangle indicate a higher mutual linear correlation among the parameters.

Inspection of Figure 6.4 reveals that strong correlations are present between \( F_{45} \) and \( F_{90} \), \( K \) and \( r_{90} \), \( K \) and \( r_{00} \), and between \( K \) and \( t \).

### 6.3 Setting up the optimization problem

DP800 steel is being used in car body to make the pillars between windows and/or doors which are designated alphabetically from the front: A-, B-, C-pillar, etc. The B-pillar is located between front and rear doors and contributes to the protection of the passengers against side impact crash. In the lower part of the B-pillar there are many potential forming problems, thus this geometry represents a critical test case; therefore, the lab-type B-pillar geometry (Abspoel et al., 2016) is chosen to investigate the effects of material variation.

#### 6.3.1 Finite element simulations

The FE model of this process is built in AutoForm R7 software as shown in Figure 6.5(a). In this process, a DP800 steel sheet is simultaneously stretched and bent over the die using a punch. The metal sheet is placed on the die and the blank holder is then moved towards the metal to clamp the sheet. The punch stroke forms the part and the part is removed from the die. Due to spring-back, the final shape of the part does not exactly match the shape of the die.
Chapter 6. Non-normal and correlated input

Figure 6.4: The variation of material properties within ±3σ box for 49 coils after subtracting their mean value (top triangle), the parameter names (diagonal), and mutual linear correlation coefficients (bottom triangle)
6.3. Setting up the optimization problem

The Swift hardening law is used to describe the work hardening behaviour and Vegter yield locus is used as an anisotropic yield function. The parameters for these models are obtained as described in the previous section. The sheet is discretized using shell elements with 11 integration points in the thickness direction (EPS-11).

A result of this simulation is shown in Figure 6.5(b). There are many outputs from such simulations. For instance, the final geometry of the product, force-displacement curves, and stresses and strains in different regions of the part can be evaluated. In this chapter, the main output of the model is the final angle of the profile ($\theta$) shown in Figure 6.5(b).

It is customary to use forming limit curve (FLC) as shown in Figure 6.6 as a fracture constraint in the optimization of sheet metal forming processes (Wiebenga et al., 2014). The constraints in forming processes are set using the critical forming regions that can be predicted from an FLC curve based on major and minor strains. Alternatively, major and minor strains can be used to evaluate a single parameter, the maximum percentage thinning ($\delta$) which is shown in Figure 6.6. Handling the constraint based on $\delta$ is easier than accounting for major and minor
strains during optimization.

6.3.2 Formulating the robust optimization problem

The relevant responses of the model are the final angle of the profile ($\theta$) and the maximum percentage thinning ($\delta$). The goal of the optimization problem is to minimize the variation of $\theta$, $\sigma_\theta$, while setting the mean, $\mu_\theta$, on a given target value, $C_\theta$. A constraint is also defined for maximum thinning. The optimization problem is defined using:

\[
\begin{align*}
\text{minimize} & \quad \left( (\mu_\theta(x) - C_\theta)^2 + w\sigma_\theta^2(x) \right) \\
\text{subject to} & \quad \mu_\delta(x) + n\sigma_\delta(x) - C_\delta \leq 0 \\
& \quad lb \leq x \leq ub \\
& \quad z \sim p(z) \\
& \quad C_\theta = 22^\circ \\
& \quad C_\delta = 15\% \quad (6.3)
\end{align*}
\]

where $x$ is the vector of design parameters, $z$ is the vector of noise parameters, $w$ is a weighting factor to adjust the optimization objective between mean on target and response variation, and $n$ adjusts the desired reliability level of the constraint.
6.3. Setting up the optimization problem

### Table 6.1: The ranges of the design parameters

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_{bh}$ (kN)</td>
<td>150</td>
<td>200</td>
</tr>
<tr>
<td>$R$ (mm)</td>
<td>60</td>
<td>90</td>
</tr>
</tbody>
</table>

The ranges of the design parameters are specified in Table 6.1. The design parameters are blank-holder force ($F_{bh}$) and blank corner radius ($R$) as shown in Figure 6.5. They are specified using their upper and lower bounds and they can be adjusted in that range. The noise parameters originate from the material as specified in Section 6.2.

After principal component analysis, the distribution of individuals in each PC is obtained. Before proceeding with the metamodeling, a screening step is performed to decide which PCs have significant influence on the response.

For robust optimization, the Latin hypercube sampling (LHS) technique is used to create a DOE in PC space. The responses, $\theta$ and $\delta$, are calculated using FE simulations which are considered as black-box function evaluations. Then, a Kriging metamodel is built using the response values to account for nonlinear relationships between input and output (Bonte et al., 2008). The metamodel of this process is used for robust optimization including non-normal input.

#### 6.3.3 Noise propagation for multimodal input

When the input parameters do not follow a normal distribution, the general form of $C_{1iq}$ and $C_{2ijq}$ coefficients presented in Chapter 3 can be used to find the normalized statistical moments of the response. In that chapter, those expressions are evaluated for the combination of Kriging and normal probability distribution. In this section, $C_{1iq}$ and $C_{2ijq}$ are adapted for a bimodal normal input. The method presented here can be generalized for multimodal input distributions.

A bimodal distribution is expressed by a sum of two unimodal distributions:

$$p(z_q) = \omega_q p_1(z_q) + (1 - \omega_q) p_2(z_q) \quad 0 \leq \omega_q \leq 1 \quad (6.4)$$

where $p_1$ and $p_2$ are two probability distributions and $\omega_q$ is a weighting factor. If it is assumed that $p_1$ and $p_2$ are two normal distributions which are characterized by parameters $\mu_q^{[1]}$, $\sigma_q^{[1]}$, $\mu_q^{[2]}$ and $\sigma_q^{[2]}$, the probability
density function (PDF) and the cumulative distribution function (CDF) of a bimodal normal distribution ($\mathcal{B}$) are defined by:

$$\text{PDF}^{\mathcal{B}}(z_q) = \omega_q \mathcal{N}_1(z_q; \mu_q^{[1]}, \sigma_q^{[1]}) + (1 - \omega_q) \mathcal{N}_2(z_q; \mu_q^{[2]}, \sigma_q^{[2]})$$

(6.5)

$$\text{CDF}^{\mathcal{B}}(z_q) = \omega_q \text{CDF}^{\mathcal{N}_1}(z_q; \mu_q^{[1]}, \sigma_q^{[1]}) + (1 - \omega_q) \text{CDF}^{\mathcal{N}_2}(z_q; \mu_q^{[2]}, \sigma_q^{[2]})$$

(6.6)

where $\mathcal{N}_1$ and $\mathcal{N}_2$ are two normal probability distributions. Figure 6.7 shows schematically the probability distribution and cumulative distribution of a bimodal input. The underlying normal distributions that are used to build this distribution are shown by superscripts, [1] and [2]. The superscripts are related to each mode of the input and they are put in brackets to distinguish them from exponents. For the sake of brevity, throughout this chapter, we use the term bimodal distribution to refer to bimodal normal distribution, $\mathcal{B}$. By substituting Equation (6.5) into Equations (3.9) and (3.11):

$$C_{1iq}^{\text{Krig,}\mathcal{B}} = \int_{z_q} b_{iq}(z_q) \left( \omega_q \mathcal{N}_1(z_q; \mu_q^{[1]}, \sigma_q^{[1]}) + (1 - \omega_q) \mathcal{N}_2(z_q; \mu_q^{[2]}, \sigma_q^{[2]}) \right) dz_q$$

$$= \omega_q C_{1iq}^{\text{Krig,}\mathcal{N}_1} + (1 - \omega_q) C_{1iq}^{\text{Krig,}\mathcal{N}_2}$$

(6.7)

$$C_{2ijq}^{\text{Krig,}\mathcal{B}} = \int_{z_q} b_{iq}(z_q) b_{jq}(z_q) \times$$

$$\left( \omega_q \mathcal{N}_1(z_q; \mu_q^{[1]}, \sigma_q^{[1]}) + (1 - \omega_q) \mathcal{N}_2(z_q; \mu_q^{[2]}, \sigma_q^{[2]}) \right) dz_q$$

(6.8)

$$= \omega_q C_{2ijq}^{\text{Krig,}\mathcal{N}_1} + (1 - \omega_q) C_{2ijq}^{\text{Krig,}\mathcal{N}_2}$$

In these equations $C_{1iq}^{\text{Krig,}\mathcal{N}_1}$, $C_{1iq}^{\text{Krig,}\mathcal{N}_2}$, $C_{2ijq}^{\text{Krig,}\mathcal{N}_1}$ and $C_{2ijq}^{\text{Krig,}\mathcal{N}_2}$ are the coefficients for the combination of Kriging basis functions and each input mode. When $C_{1iq}$ and $C_{2ijq}$ for a normal distribution and a specific metamodel are known, it is feasible to extend the analytical calculation of uncertainty for a bimodal or multimodal distribution in a straightforward manner for that metamodel.

The propagation of a bimodal input will lead to a multimodal response. Considering $n_z$ noise variables and assuming that each noise variable follows a bimodal distribution, the response consists of $2^n_z$ modes. As an example, assume there are two bimodal noise parameters as $z_1$ with a parameter set of $([\mu_1^{[1]}, \sigma_1^{[1]}], [\mu_1^{[2]}, \sigma_1^{[2]}], \omega_1)$ and $z_2$ with
6.3. Setting up the optimization problem

a parameter set of $([\mu_1^1, \sigma_1^1], [\mu_2^1, \sigma_2^1], \omega_2)$. The response consists of four modes which are obtained from propagation of the combinations of the modes of the noise. The combinations of the modes of the noise are $([\mu_1^1, \sigma_1^1], [\mu_2^1, \sigma_2^1]); ([\mu_1^2, \sigma_1^2], [\mu_2^2, \sigma_2^2]); ([\mu_1^2, \sigma_1^2], [\mu_2^1, \sigma_2^1]);$ and $([\mu_1^2, \sigma_1^2], [\mu_2^2, \sigma_2^2])$.

The modes of the response are denoted using $[\mu_r^1, \sigma_r^1], [\mu_r^2, \sigma_r^2], [\mu_r^3, \sigma_r^3], [\mu_r^4, \sigma_r^4]$. The weights of the response modes are $\omega_1\omega_2$, $\omega_1(1-\omega_2)$, $(1-\omega_1)\omega_2$, and $(1-\omega_1)(1-\omega_2)$, respectively. These response modes can be also referred using vector of means, $\mu_r$, vector of standard deviations, $\sigma_r$, and vector of weights, $\omega_r$. For constraints, these modes are denoted by $\mu_{rc}$, $\sigma_{rc}$, and $\omega_{rc}$. The combination of all response modes must be considered in the definition of objective function and the analysis of constraints.

6.3.4 Multimodality of the response as a result of the multimodal input

To illustrate the importance of accounting for a multimodal input, Figure 6.8 shows the propagation of a one-dimensional dataset, $z$, that follows a bimodal normal distribution. The input data set is shown using a bar plot and it is propagated to obtain the response bar plot. As mentioned earlier, the input dataset is usually treated as a normal distribution and a normal distribution fit to the input dataset (dashed curve) is propagated through the function, to achieve the response distribution. This leads to the response distribution shown using dashed curve and...
Chapter 6. Non-normal and correlated input

it has a large deviation from the underlying response distribution. It is shown in this figure that if a bimodal distribution is fitted to the data and then propagated through the metamodel, the resulting bimodal response closely follows the underlying dataset. This observation confirms the significance of accounting for a non-normal input distribution to find the response distribution.

Figure 6.8: Propagation of a bimodal normal distributions and the resulting response

In Chapter 5 a method was implemented to adjust the value of $n$ when the response does not follow a normal distribution, such that the response preserves the required reliability. In that method, the functions $U$ and $L$ were introduced to replace $\pm n$ in an $n\sigma$ method to account for the non-symmetry of the response distribution. In this section, a similar approach is used to account for bimodal or multimodal response.

If there is an upper bound, the constraints are generally defined by:

$$\mu_{rc}(\mathbf{x}) + n\sigma_{rc}(\mathbf{x}) < C_{rc} \quad (6.9)$$
or if there is a lower bound:

\[ \mu_{rc}(x) - n\sigma_{rc}(x) > C_{rc} \]  

(6.10)

where \( C_{rc} \) is the constraint specification limit. In this equation the choice of \( n \) is related to the required reliability level for a constraint if it follows a normal distribution. The superscript \( rc \) indicates the response of the constraint. For a robustness measure which minimizes the variation of response and reduces the difference between mean and target value, \( C_r \), the objective function can be formulated as (Koch et al., 2004):

\[
\text{minimize } \left( \left( \mu_r(x) - C_r \right)^2 + w\sigma_r^2(x) \right)
\]

(6.11)

In this equation \( w \) is a weighting factor to adjust the optimization objective function between mean on target and minimal response variation. The superscript \( r \) indicates the main response.

Similar to Chapter 5, functions \( U \) and \( L \) are defined to correct the \( n\sigma \) method considering the shift of upper tail and lower tail. The term tail of a distribution refers to a particular quantile of the response. Figure 6.9 shows the PDF and CDF of a dataset which follows a bimodal distribution. In this figure, the dashed line represents the equivalent normal distribution of the response. It is apparent that relying on the equivalent normal distribution of the response leads to a big deviation in the prediction of the tails of the distribution. Hence, it is necessary to re-define the objective function and the constraints.

Figure 6.9: Schematic of shift of the tails for a bimodal distribution compared to equivalent normal distribution (a) and the difference between cumulative distribution of equivalent normal and bimodal probability distribution functions (b)
Based on this explanation, functions $U$ and $L$ are implemented in evaluating the upper bound constraints using:

$$
\mu_{rc}^{eq}(x) + U(\mu_{rc}, \sigma_{rc}, \omega_{rc}; n)\sigma_{rc}^{eq}(x) < C_{rc}
$$

(6.12)

and in the case of lower bound:

$$
\mu_{rc}^{eq}(x) - L(\mu_{r}, \sigma_{r}, \omega_{r}; n)\sigma_{rc}^{eq}(x) > C_{rc}
$$

(6.13)

In these equations, the superscript $\text{eq}$ indicates the equivalent values for mean and standard deviation of the response and $L$ and $U$ are the functions that can be evaluated using means, standard deviations, and weights of each mode of the response to obtain a desired reliability level equivalent to $n\sigma$. For a normal distribution $L(\mu_{r}, \sigma_{r}, \omega_{r}; n) = -n$ and $U(\mu_{r}, \sigma_{r}, \omega_{r}; n) = +n$. Similarly, the robustness measure is obtained by:

$$
\left(\mu_{r}^{eq}(x) + \frac{U(\mu_{r}, \sigma_{r}, \omega_{r}; n) + L(\mu_{r}, \sigma_{r}, \omega_{r}; n)}{2}\sigma_{r}^{eq}(x) - C_{r}\right)^2
$$

$$
+ \frac{w U(\mu_{r}, \sigma_{r}, \omega_{r}; n) - L(\mu_{r}, \sigma_{r}, \omega_{r}; n)}{2}\left(\sigma_{r}^{eq}(x)\right)^2
$$

(6.14)

To obtain $L(\mu_{r}, \sigma_{r}, \omega_{r}; n)$ and $U(\mu_{r}, \sigma_{r}, \omega_{r}; n)$ based on maintaining the same level of reliability as for $n\sigma$ with a normal distribution, the quantiles of bimodal distribution which lead to the same reliability as $n\sigma$ for a normal distribution are calculated. When, for example, a reliability according to a $3\sigma$ process is required, this is expressed by:

$$
L(\mu_{r}, \sigma_{r}, \omega_{r}; 3) = (\text{CDF}^B)^{-1}(\mu_{r}, \sigma_{r}, \omega; \text{CDF}^N(-3\sigma))
$$

$$
U(\mu_{r}, \sigma_{r}, \omega_{r}; 3) = (\text{CDF}^B)^{-1}(\mu_{r}, \sigma_{r}, \omega; \text{CDF}^N(3\sigma))
$$

(6.15)

The intersection of the two horizontal lines drawn in Figure 6.9(b) with CDFs of bimodal distribution is at $\bar{U}$ and $\bar{L}$ points. During the robust optimization procedure, after the modes of response have been evaluated by uncertainty propagation, $U$ in $L$ are used to evaluate the objective function value and the reliability constraints.

### 6.4 Results and discussion

#### 6.4.1 Describing input distribution

PCA is performed on the correlated data and the distributions of projection of experiments on the PCs are shown in Figure 6.10. It can be seen
that some of the distributions deviate significantly from a normal distribution. Bimodal distribution is used to describe those distributions due to the fact that it inherently has the advantage of the normal probability distribution (Titterington et al., 1985). It is flexible, tractable, and scalable to any problem size and can be handled analytically. As the number of measurements is not very large, each distribution is described using either unimodal or bimodal distribution. If one is willing to use more than two modes of the normal distribution to describe the noise, the method described in Section 6.3.3 is still valid.

The histograms shown in Figure 6.10 are bin-size dependent and the choice of the number of bins influences their appearance, many authors have suggested various techniques to choose an optimal bin size. For instance, Scott (1979) proposed a formula for the optimal histogram bin width based on minimization of the integrated mean squared error. Knuth (2006) introduced a data-based method of determining the optimal number of bins. In this section, to avoid the bin-size dependent fit over the histograms, the fitting is performed on the CDF and using the parameters obtained from the fitting, the probability distributions shown in Figure 6.10 are plotted. To decide whether a PC should be considered a normal distribution or a bimodal distribution, the five parameters of the bimodal distribution in Equation (6.6) are fitted to the cumulative probability distribution of each PC. Then a unimodality test is performed according to Eisenberger (1964) by evaluating the separation of the two components of the bimodal distribution:

$$
\Delta_q = \mu_q^{[2]} - \mu_q^{[1]}
$$

$$
v_q = \frac{27(\sigma_q^{[1]})^2(\sigma_q^{[2]})^2}{4\left((\sigma_q^{[1]})^2 + (\sigma_q^{[2]})^2\right)}
$$

if \(\Delta_q^2 < v_q \rightarrow p(z) \sim N(z)\)

where \(\Delta_q\) is the difference between means of two modes of the distribution and \(v_q\) is a function of standard deviations of two modes of the distribution. This equation is used to decide whether the input is unimodal or bimodal. The values of \(\Delta^2\) and \(v\) and the fitted curves to the projection of experiments on the PCs are shown in Figure 6.10.

6.4.2 Screening

Screening step is done for dimension reduction. Figure 6.11 shows the Pareto plots of the responses. As can be seen in this figure, most PCs
Figure 6.10: Variation of material parameters after PCA
6.4. Results and discussion

Effects on springback ($\theta$)

<table>
<thead>
<tr>
<th>PC1</th>
<th>PC2</th>
<th>PC3</th>
<th>PC4</th>
<th>PC5</th>
<th>PC6</th>
<th>PC7</th>
<th>PC8</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
</tbody>
</table>

$0\%$ $25\%$ $50\%$ $75\%$ $100\%$

Effects on thinning ($\delta$)

<table>
<thead>
<tr>
<th>PC1</th>
<th>PC2</th>
<th>PC3</th>
<th>PC4</th>
<th>PC5</th>
<th>PC6</th>
<th>PC7</th>
<th>PC8</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
</tbody>
</table>

$0\%$ $25\%$ $50\%$ $75\%$ $100\%$

Figure 6.11: Pareto plots of the springback and thinning

make a major contribution to at least one of the responses. PC1, PC4, and PC5, are among the least important ones. Considering the influence of PCs on both parameters, PC4 is eliminated because it has a total contribution of less than 10% for both responses, thus over 90% control on the process is retained. Eliminating one more PC (e.g. PC1 or PC 5) is not recommended as the total control over the responses will fall below 80% (Wiebenga et al., 2014).

The distributions of the projection of the experiments on the PCs, shown in Figure 6.10, are used after eliminating PC4. The remaining seven PCs that represent the noise space are used for generating the metamodel of the process. Table 6.2 shows the parameters of the noise distribution according to Figure 6.10. PC1, PC3 and PC6 are considered as bimodal distributions and the other PCs are assumed to follow a normal distribution. The PCs that are described using a normal distribution have a zero mean due to subtracting their mean values, and they have the same standard deviation due to normalization. For comparison purposes, the results of the robust optimization assuming that all noise parameters are normally distributed is also presented.

6.4.3 Optimization based on non-normal input and output

A Kriging metamodel is built on the nine-dimensional space of two design variables and seven PCs that represent the noise space. This metamodel is used during the robust optimization. The analytical method presented in Chapter 3 and Section 6.3.3 is employed to propagate the independent noise parameters and to find the output modes. Those output modes are then incorporated in both robustness analysis and constraint evaluation as described in Section 6.3.4. While calculating objective function value and constraints, $L$ and $U$ are evaluated implic-
Chapter 6. Non-normal and correlated input

Table 6.2: The variation of principal components used in robust optimization

<table>
<thead>
<tr>
<th>Distribution type</th>
<th>PC</th>
<th>$\mu_q^{[1]}$</th>
<th>$\sigma_q^{[1]}$</th>
<th>$\mu_q^{[2]}$</th>
<th>$\sigma_q^{[2]}$</th>
<th>$\omega_q$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PC1</td>
<td>0.144</td>
<td>0.08</td>
<td>-0.116</td>
<td>0.08</td>
<td>0.429</td>
</tr>
<tr>
<td></td>
<td>PC3</td>
<td>0.212</td>
<td>0.1</td>
<td>-0.044</td>
<td>0.103</td>
<td>0.158</td>
</tr>
<tr>
<td></td>
<td>PC6</td>
<td>0.057</td>
<td>0.1</td>
<td>-0.147</td>
<td>0.1</td>
<td>0.73</td>
</tr>
<tr>
<td>Bimodal</td>
<td>PC2</td>
<td>0</td>
<td>0.144</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>PC5</td>
<td>0</td>
<td>0.144</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>PC7</td>
<td>0</td>
<td>0.144</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>PC8</td>
<td>0</td>
<td>0.144</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

itly during each evaluation of objective function and constraints. This is different from the approach presented in Chapter 5 in which the values of $L$ and $U$ were pre-evaluated for different skewness values and the fitted curves were used during each evaluation of objective function and constraints.

According to Table 6.2, three input parameters are considered as bimodal distribution and therefore eight modes in the responses are expected as explained in Section 6.3.3. This is referred to as Case 1. For comparison purposes, the results of the robust optimization assuming that all noise parameters are normally distributed are also presented as Case 2.

Figure 6.12 shows the modes of each response multiplied by its respective weight as a result of considering PC1, PC3 and PC5 as bimodal distributions. It is apparent from this figure that each mode of both responses has a different contribution to the objective of the optimization. Some modes have bigger variations while others have larger deviation from the target values. The magnitude of the contribution of each mode is also different due to different weights. Figure 6.13 shows the overall PDF and CDF of each output considering the bimodal input expressed in Table 6.2. For comparison purposes, the same results are obtained for an equivalent normal distribution of PCs. It must be noted, that the resultant distribution for the bimodal input case, which is plotted in Figure 6.13, is the superposition of the eight modes of the output, as presented in Figure 6.12. Although the superposition of those eight modes resembles a normal distribution due to interfering modes, the resulting distribution has clear deviations from a normal distribution, specifically at the tails of the distribution. This emphasizes the impor-
6.4. Results and discussion

Figure 6.12: The modes of each response

Table 6.3: Robust optimum design for different cases

<table>
<thead>
<tr>
<th>Case</th>
<th>$R_{\text{robust}} \text{[mm]}$</th>
<th>$F_{\text{bh}}^{\text{robust}} \text{[KN]}$</th>
<th>Objective value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1: Bimodal distributions</td>
<td>64.9</td>
<td>155.4</td>
<td>0.128</td>
</tr>
<tr>
<td>Case 2: Normal distributions</td>
<td>66.6</td>
<td>153.0</td>
<td>0.178</td>
</tr>
</tbody>
</table>

tance of accounting for the bimodal input to increase the accuracy of constrained robust optimization.

As mentioned earlier, considering the effect of non-normal input and the resulting output, can significantly affect the objective function of the robust optimization and the evaluation of constraints. It is apparent from Figure 6.13, that considering all modes of input has a significant influence on prediction of the variation of output and mean value which are used to evaluate robustness. Additionally, the tails of both distributions, which affect the satisfaction of constraints, change and they lead to a different robust optimum design. Therefore, assuming a simple normal distribution for input imposes big deviations in the prediction of output distribution. Consequently, errors in the search for a robust optimum design is expected. Table 6.3 compares the robust optimum obtained for case 1 and case 2. This slight adjustment of the design parameters as a result of a more accurate noise input leads to a more robust process and less scrap rate.

It is notable that instead of analyzing the bimodality of the output, the equivalent moments of the multimodal response could be calculated using the method described in (Cohen, 1967) and then used to evaluate the robustness and evaluation of constraints as discussed in Chapter 5. In that case, the higher order moments of each response can be used
Figure 6.13: The comparison of output probability and cumulative distribution considering bimodality of input (Case 1) and neglecting bimodality of input (Case 2)

to analyze the robustness and to evaluate the constraints. Nevertheless, for a bimodal input, the current method shows a great applicability and improves the prediction of the robust optimum by enabling a better prediction of the tails of the output distributions.

There are many advantages by using the methods presented in this chapter. First, accounting for the material scatter is done by using only parameters of standard uniaxial tests in three directions as proposed by (Abspoel et al., 2017). Therefore, the stochastic description of the input scatter data is simple to obtain. Second, analyzing the correlations between those parameters helps to obtain the uncorrelated description of parameters and avoids unnecessary sampling in infeasible parameter domain. Third, the handling of the optimization procedures is performed using the analytical approach; the noise is propagated using the analytical method which is fast and accurate compared to other approaches such as Monte Carlo analysis. Last but not least, the new formulations for evaluation of robustness and constraints consider the shift of the tails of the response due to non-normal input, and consequently, they lead to a more accurate prediction of the robust optimum.
6.5 Conclusions

DP800 steel has been characterized via mechanical testing for 49 different coils to account for the material scatter in a metal forming process, forming a lab-type B-pillar part. Accounting for the material scatter is done by using only parameters of standard uniaxial tests in three directions. Therefore, the stochastic description of the input scatter data is simple to obtain. Principal component analysis is employed to describe the variation of material parameters using linearly uncorrelated principal components. It is shown that the distribution of individuals in some PCs deviates significantly from a normal probability distribution. In that case, a bimodal normal probability distribution is considered and propagated using an analytical method through the metamodel of the metal forming process. Consequently, a multimodal response is obtained and both the robustness criterion and the reliability formulation are altered to achieve an accurate robust optimum design. The results are compared with a simplified case in which all input parameters are assumed to follow a normal probability distribution. It is shown that using bimodal material scatter changes the robust optimum design by improved estimation of the robustness measure and the constraints reliability.
Chapter 7

Tailoring of scatter

Performing robust optimization, which is referred to in this chapter as a forward problem, allows a minimum variation around the target mean to be achieved. If the minimum variation does not have a satisfactory level and further reduction of variation is required, the tolerance on the noise variables must be tightened. Since it is expensive to suppress all noise variables, the variation of noise up to a certain level can be accepted as long as the response is within a required tolerance.

The goal of this chapter is to develop a method determine the acceptable material and process scatter from the specified product tolerance by inverting the robust optimization method. This problem is regarded as the reverse process of a robust optimization problem and is referred to as tailoring of scatter. The nonlinearity of the process and the presence of multiple noise variables are the main challenges to address in tailoring of scatter.

To solve inverse problems in forming-related processes, various methods have been implemented. These methods are divided into two categories: derivative-free and gradient-based methods. Derivative-free methods such as brute force strategy (Cardozo and Aanonsen, 2009) and Genetic Algorithm (GA) (António et al., 2005) are easy to implement.

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but computationally expensive. These methods require the evaluation of the forward problem many times. Therefore, they are not efficient for inverting the robust optimization method. Gradient-based methods (Ponthot and Kleinermann, 2006) used to solve inverse methods are more efficient in terms of computational effort. Most of these studies consider deterministic inverse approaches, which means that the effects of variation of input and output are ignored.

In this chapter, a gradient-based reverse approach is applied to a forming process. A metamodel of this process is used and the analytical approach developed in Chapter 3 is used to perform the inverse analysis efficiently. To the best of the author’s knowledge, tailoring the noise scatter has not been addressed in the literature. The only similar approach is the work by Chassein et al. (2019). In their work, they analyze how optimal robust solutions change when the size of the uncertainty set increases and they apply their method to variable-sized minmax robust optimization.

This Chapter is structured as follows. In Section 7.1, the robust optimization approach and tailoring noise scatter is introduced and formulated. In Section 7.2, the numerical simulation of a lab-type B-pillar which was presented in Chapter 6 is used and the input and output of the process for both the forward and the inverse method are defined. The results are presented and discussed in Section 7.3.

7.1 The concept of tailoring of scatter

7.1.1 Robust optimization

Figure 7.1(a) shows the robust optimization approach, schematically. In this figure, \( x \) represents a design parameter and \( z \) represents a noise parameter that has a known probability distribution. The response can be evaluated using a metamodel, \( r = r(x, z) \). In the robust optimization method the search for an optimum design, \( x_{opt} \), is performed based on the propagation of the given noise parameter through the metamodel. An objective function is then defined in terms of statistical parameters and the goal is to minimize it based on the propagation of noise parameter.

In a general case, the vector of design variables, \( x \), and the vector of noise variables, \( z \), are used to evaluate the response of the process, \( r(x, z) \). As mentioned in Chapter 2, the objective function aims to
7.1. The concept of tailoring of scatter

minimize the variation of the response \( \sigma_r(x) \) while setting the mean value of the response \( \mu_r(x) \) on the target value \( C_r \):

\[
\begin{align*}
\text{minimize} \quad & f(x) = (\mu_r(x) - C_r)^2 + w\sigma_r^2(x) \\
\text{subject to} \quad & \mu_{rc}(x) + n\sigma_{rc}(x) - C_{rc} \leq 0 \\
& \text{lb} \leq x \leq \text{ub} \\
& z \sim \mathcal{N}(\mu_z, \sigma_z)
\end{align*}
\]

where \( w \) is a weighting factor to adjust the optimization objective between mean on target and response variation, \( \mu_{rc} \) are the means of the responses of constraints and \( \sigma_{rc} \) are their standard deviations. The choice of \( n \) for constraints is related to the desired reliability level assuming that the responses of constraints follow a normal distribution.

It is generally assumed that the noise input follows a known normal distribution that has a fixed or nominal mean and standard deviation (Bonte et al., 2010). A change in the input mean and standard deviation leads to a different robust optimum. Therefore, mean and standard deviation can be assumed as variables while in a robust optimization formulation they are predefined constants. Therefore, Equation (7.1)

\[\text{Figure 7.1: (a) Finding robust optimum based on uncertainty propagation from a given input noise (b) Finding an acceptable noise variation from a specified tolerance}\]
can be written as:

\[
\begin{align*}
\text{minimize} & \quad f(x, \mu_z, \sigma_z) = (\mu_r(x, \mu_z, \sigma_z) - C_r)^2 + w\sigma_r^2(x, \mu_z, \sigma_z) \\
\text{subject to} & \quad \mu_r(x, \mu_z, \sigma_z) + n\sigma_r(x, \mu_z, \sigma_z) - C_r \leq 0 \\
& \quad lb \leq x \leq ub \\
& \quad z \sim N(\mu_z, \sigma_z) \\
& \quad \mu_z = \mu_z^{\text{nom}} \\
& \quad \sigma_z = \sigma_z^{\text{nom}}
\end{align*}
\]

Equation (7.2) reflects the fact that the objective function and constraints are functions of the input mean and standard deviation while in robust optimization they are evaluated using nominal values.

### 7.1.2 Tailoring of scatter

The concept of tailoring input scatter is illustrated in Figure 7.1(b). In this approach, one works back from the specified response variation to the acceptable input noise. Ideally, the input noise must be zero to achieve zero variation in the response. However, a tighter control of a noise parameter incurs additional costs. Therefore, to minimize costs, the variation of the input noise parameters can be accepted up to a certain level where the response meets the specified tolerance. A weighted sum formulation is used as it is often employed to provide feasible solutions by varying the weighting factors (Marler and Arora, 2005; Proos et al., 2001). The inverse approach for tailoring the noise scatter is then formulated as:

\[
\begin{align*}
\text{maximize} & \quad \Sigma(\omega\bar{\sigma}_z) \\
\text{subject to} & \quad \left( (\mu_r(x, \mu_z, \sigma_z) - C_r)^2 + w\sigma_r^2(x, \mu_z, \sigma_z) \right) - C_{tol} \leq 0 \\
& \quad \mu_r(x, \mu_z, \sigma_z) + n\sigma_r(x, \mu_z, \sigma_z) - C_r \leq 0 \\
& \quad lb \leq x \leq ub \\
& \quad z \sim N(\mu_z, \sigma_z) \\
& \quad \mu_z = \mu_z^{\text{nom}} \\
& \quad \sigma_z = \sigma_z^{\text{nom}}
\end{align*}
\]

where \( \bar{\sigma}_z \) are defined as \( \sigma_z/\sigma_z^{\text{nom}} \). The objective is to find a set of \( (\sigma_z, x) \) that maximizes the weighted sum of the normalized noise variation. Besides, the constraints are assessing the feasibility of the obtained solution.
7.2 Application in a forming process

The objective function in Equation (7.3) handles the following requirements simultaneously. Maximizing noise variation leads to less tight control of that variable. Various noise parameters can have different dimensions, and therefore each noise parameter is normalized using its nominal value. The weighting factors are associated with the relative cost for controlling each noise variable. If a noise parameter is more expensive to control than other parameters, it gains a bigger weight; thus the maximization problem concentrates more on maximizing the variation of that noise parameter.

Based on these explanations, the weights are non-dimensional coefficients that are obtained using the costs of controlling each noise parameter. As an example, assume that $z_1$ and $z_2$ are two noise parameters. If reducing $\sigma_{z_1}$ and $\sigma_{z_2}$ by 50% cost 50€ and 100€, respectively, the weight factors are $\omega_1 \propto (50€)$ and $\omega_2 \propto (100€)$. When they are normalized such that $\sum \omega_i = 1$, $\omega_1 = 1/3$ and $\omega_2 = 2/3$ are obtained.

It must be noted that the objective function in Equation (7.3) can be formulated using other expressions, and the choice of objective function is not limited to the above-mentioned expression. Moreover, the constraints in Equation (7.3) handle the feasibility of satisfying the specified tolerance. It can be seen that the objective of the robust optimization in Equation (7.2) becomes the constraint of the inverse problem in Equation (7.3). It is assumed that the noise mean is fixed on the nominal value and the focus is on the effect of the variation of noise parameters.

Compared to Equation (7.1) in which the search for the robust optimum design is performed only on $x$, the proposed method is computationally more expensive as the optimization is performed on combined $(x, \sigma_z)$ parameters space. Therefore, the analytical method developed in Chapter 3 is employed to calculate the uncertainty propagation in each step of inverse analysis. It is shown in Chapter 3 that using the analytical method during robust optimization procedure improves the speed and accuracy of the calculations compared to existing approaches.

7.2 Application in a forming process

7.2.1 Finite element simulations

The B-pillar model, introduced in Chapter 6, is used in this chapter to perform the forward and the inverse analysis. The simulation results of the FE model are used to make a metamodel of the process. The noise inputs to the FE model in the previous chapter comprise only
material parameters. In this chapter two material inputs and one process parameter are used as noise input to that model.

The design and noise parameters of the optimization problem are specified in Table 7.1. Recalling from Chapter 6 the design parameters which can be adjusted during forming are blank-holder force ($F_{bh}$) and blank corner radius ($R$). These parameters can vary between their lower and their upper bound. The Noise parameters are the strength coefficient in the Swift hardening law ($K$), the friction coefficient ($m$) in the Coulomb model and the thickness of the sheet ($t$).

To use equations (3.8) and (3.10), it is assumed that the noise variables are statistically independent. The input $K$ depends on the processing history and the elemental composition of the material, $t$ is usually controlled in the last rolling step during sheet production stage, and $m$ originates from the surface texture and lubrication condition during the process. The deformation in the last rolling step is so small that the influence of thickness reduction on hardening behaviour can be ignored. Therefore, it is a rational assumption that the three input parameters can vary independently of each other. Moreover, it is assumed that the noise parameters have a normal probability distribution.

The main response of the FE simulations is the final angle of the profile ($\theta$), and a constraint is defined on the percentage thinning ($\delta$) in the corner as described in Chapter 6, Section 6.3.1.

### 7.2.2 Sampling and constructing a metamodel

The Latin hypercube sampling (LHS) technique is used to create a DOE consisting of 90 points in the five-dimensional parameter domain. The responses, $\theta$ and $\delta$, are calculated using the FE simulations similar to Chapter 6. Figure 7.2 shows the final shapes of the profiles and the variation of $\theta$, on DOE points obtained using FE simulations. The Kriging method is used to model the nonlinear relationship between
7.2. Application in a forming process

20

\[ \theta \]

\[ y \]

\[ z \]

-40

-40

-30

-20

-10

0

10

40

60

80

100

Figure 7.2: The profiles shapes after springback and the variation of \( \theta \) obtained from simulations on the initial DOE points

input and output (Dang et al., 2018).

7.2.3 The forward problem

Based on Equation (7.1), the robust optimization problem (forward problem) is defined as:

\[
\begin{align*}
\text{minimize } & \quad (\mu_{\theta}(F_{bh}, R) - \theta_{\text{trgt}})^2 + 3\sigma_{\theta}^2(F_{bh}, R) \\
\text{subject to } & \quad \mu_{\delta}(F_{bh}, R) + 3\sigma_{\delta}(F_{bh}, R) - \delta_{\text{max}} \leq 0 \\
& \quad 150 \leq F_{bh} \leq 200 \\
& \quad 60 \leq R \leq 90 \\
& \quad K \sim \mathcal{N}(\mu_{K}^{\text{nom}}, \sigma_{K}^{\text{nom}}) = \mathcal{N}(1000, 10) \\
& \quad t \sim \mathcal{N}(\mu_{t}^{\text{nom}}, \sigma_{t}^{\text{nom}}) = \mathcal{N}(1, 0.01) \\
& \quad m \sim \mathcal{N}(\mu_{m}^{\text{nom}}, \sigma_{m}^{\text{nom}}) = \mathcal{N}(0.081, 0.003) \\
& \quad \theta_{\text{trgt}} = 23^\circ \\
& \quad \delta_{\text{max}} = 15\% 
\end{align*}
\]  

(7.4)

Throughout this chapter, the minimum objective function of the forward problem is referred to as the process quality indicator. A forward analysis is performed using a nominal set of noise parameters to find the nominal process quality indicator which is denoted by \( C_{\text{nom}} \).
7.2.4 The inverse problem

In the inverse method, the required objective function value is reduced and the goal is to find the maximum variation in the input noise that satisfies the requirements of the response. The inverse approach is expressed by:

$$\text{maximize } [F_{bh}, R, \sigma_K, \sigma_t, \sigma_m]$$

subject to

$$\left(\mu_{\theta}(F_{bh}, R, \sigma_K, \sigma_t, \sigma_m) - \theta_{\text{trgt}}\right)^2 + 3\sigma_{\theta}^2(F_{bh}, R, \sigma_K, \sigma_t, \sigma_m) - C_{\text{tol}} \leq 0$$

$$\mu_{\delta}(F_{bh}, R, \sigma_K, \sigma_t, \sigma_m) + 3\sigma_{\delta}^2(F_{bh}, R, \sigma_K, \sigma_t, \sigma_m) - \delta_{\text{max}} \leq 0$$

$$150 \leq F_{bh} \leq 200$$

$$60 \leq R \leq 90$$

$$K \sim \mathcal{N}(1000, \sigma_K)$$

$$t \sim \mathcal{N}(1, \sigma_t)$$

$$m \sim \mathcal{N}(0.081, \sigma_m)$$

$$0 \leq \sigma_K \leq \sigma_K^{\text{nom}}$$

$$0 \leq \sigma_t \leq \sigma_t^{\text{nom}}$$

$$0 \leq \sigma_m \leq \sigma_m^{\text{nom}}$$

$$\theta_{\text{trgt}} = 23^\circ$$

$$\delta_{\text{max}} = 15\%$$

(7.5)

Using this formulation, different requirements on response can be set using parameter $C_{\text{tol}}$, and a single objective function is defined using weighting factors, $\omega_i$, for each noise parameter. The presence of the upper bounds for $\sigma_K$, $\sigma_t$, and $\sigma_m$ in Equation (7.5) are due to the range of these parameters while making the DOE on which the metamodel is based. When one of those becomes active, it means that the DOE must be extended in that direction. This is discussed in Section 7.3.2.
7.3 Results and discussion

The result of robust optimization using nominal noise variations is obtained based on the analytical approach presented in Chapter 3 and the results are presented in Table 7.2. At the robust optimum design, the variations of $\theta$ are shown using a normal distribution in Figure 7.3. This figure represents the minimum scatter at the optimum design setting, in which the weighted sum of the deviation of mean from target and response variation is minimum. The process quality indicator is obtained at that specific design setting and is presented in Table 7.2. For comparative purposes, the results of an MC sampling method are also shown in Figure 7.3 in a bar plot.

For tailoring the scatter two scenarios are defined. First, the process quality indicator is set to a lower value than the nominal process quality indicator, $C_{tol} < C_{nom}$, and the inverse problem is solved to find the acceptable variation of noise variables which will be less than nominal values. In the second scenario, the process quality indicator remains intact, $C_{tol} = C_{nom}$, and the inverse problem is solved to relax the variation of noise variables. These scenarios are addressed in the following sections.

Table 7.2: Robust optimum design and the objective function value for forward problem

<table>
<thead>
<tr>
<th>$F_{bh}$ (kN)</th>
<th>$R$ (mm)</th>
<th>$(\mu_\theta(F_{bh}, R) - 23)^2 + 3\sigma_\theta^2(F_{bh}, R)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>184.3</td>
<td>90</td>
<td>$C_{nom} = 0.52$</td>
</tr>
</tbody>
</table>

7.3.1 Tighter response tolerance, tighter specifications

As a starting point, one can set the required process quality indicator on $C_{tol} < C_{nom}$ and solve the inverse problem. The results of an inverse analysis for various values of $C_{tol}$ are shown in Figure 7.4. In all cases, the weighting factors are equal to $[1/3, 1/3, 1/3]$, meaning all noise factors are considered equally expensive to control. This figure shows how reducing the value of $C_{tol}$ decreases the acceptable variation of each parameter. For the majority of the range of $C_{tol}$, the required standard deviation of the friction coefficient remains at its specified upper limit. In this case, it is not required to tighten the control on $m$ and $\sigma_m = 1$
which means that $m$ varies within the nominal range. This means, that a relaxation of this upper limit would give a cheaper optimum. In addition, the acceptable variation of each parameter does not proportionally decrease by reducing $C_{tol}$ due to the nonlinear response to the variation of the parameters and the differences in sensitivities.
Table 7.3: The acceptable noise variation and the optimum design for various weighting factors

<table>
<thead>
<tr>
<th>$C_{tol}$</th>
<th>$[\omega_K, \omega_t, \omega_m]$</th>
<th>$[\bar{\sigma}_K, \bar{\sigma}_t, \bar{\sigma}_m]$</th>
<th>$F_{bh}^{opt}$ (kN)</th>
<th>$R_{opt}^{opt}$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1$C_{nom}$</td>
<td>1/3 1/3 1/3</td>
<td>0.06 0.22 0.87</td>
<td>193.4</td>
<td>90</td>
</tr>
<tr>
<td>0.1$C_{nom}$</td>
<td>1/5 2/5 2/5</td>
<td>0.03 0.23 0.90</td>
<td>193.5</td>
<td>90</td>
</tr>
<tr>
<td>0.1$C_{nom}$</td>
<td>2/5 2/5 1/5</td>
<td>0.10 0.37 0.62</td>
<td>192.4</td>
<td>90</td>
</tr>
<tr>
<td>0.1$C_{nom}$</td>
<td>2/5 1/5 2/5</td>
<td>0.06 0.09 0.97</td>
<td>194.2</td>
<td>68.4</td>
</tr>
<tr>
<td>0.1$C_{nom}$</td>
<td>1/4 1/2 1/4</td>
<td>0.05 0.38 0.63</td>
<td>192.6</td>
<td>90</td>
</tr>
<tr>
<td>0.1$C_{nom}$</td>
<td>1/4 1/4 1/2</td>
<td>0.03 0.09 1.00</td>
<td>194.2</td>
<td>68.3</td>
</tr>
<tr>
<td>0.1$C_{nom}$</td>
<td>1/2 1/4 1/4</td>
<td>0.11 0.22 0.81</td>
<td>193.1</td>
<td>90</td>
</tr>
</tbody>
</table>

Figure 7.5 shows the acceptable variation of noise parameters for $C_{tol} = 0.1C_{nom}$ and various weighting factors. This figure shows that if a parameter is more expensive to control than the other ones, the accepted variation for that parameter increases, however, to achieve the specified tolerance another parameter should be controlled tighter. Table 7.3 shows the optimum settings for different weighting factors. This table shows that, depending on the settings in the inverse approach, different process design parameters are obtained than when to the forward approach is used.

Pareto optimal solution sets can be obtained for multi-objective optimization problems to show the trade-off between the objectives (Wang et al., 2018). Although in this chapter only one objective function is used, comprising the weighted sum of the variation of various parameters. Therefore, a range of optimal solutions can be found by modifying weighting factors to meet the constraints.

Figure 7.6 shows the optimum acceptable variation of noise when $C_{tol} = 0.5C_{nom}$. As $\sigma_m = 1$ and does not vary; the Pareto front is plotted only in 2D. Despite the weighting factors being selected at equal intervals, the points on the Pareto front are not evenly distributed. The uneven distribution of points on the Pareto front is observed in most studies and the reasons are addressed in (Das and Dennis, 1997). Since the shape of the Pareto front is not known in advance, it is not feasible to determine the values of $\omega$ that lead to a uniform distribution of the points on the Pareto front.

As mentioned earlier, when $C_{tol}$ is reduced to $0.1C_{nom}$, all three
noise parameters must be controlled tighter. Then, a 3D Pareto front is plotted and shown in Figure 7.7. This surface represents the fit over 55 solution sets and demonstrates the trade-off among the variation of noise parameters.

### 7.3.2 Intact response tolerance, wider specifications

In the previous section, $C_{\text{tol}}$ was set lower than the minimum objective function in robust optimum, $C_{\text{nom}}$, meaning that a tighter tolerance of the response is required. In this section the aim is to achieve a cheaper process specification that results in the same process quality indicator by setting $C_{\text{tol}} = C_{\text{nom}}$. This usually means that $\sigma$ exceeds the bounds in Equation (7.5).

Theoretically, the noise variation can be increased outside of those given bounds since a material or process with wider specifications is cheaper. However, these bounds are present to avoid using the meta-model of the metal forming process beyond those bounds. As there are no DOE points outside the $\pm 3\sigma_{\text{nom}}$ bounds, the metamodel of the process is less accurate in those regions. Therefore, those regions are omitted to avoid inaccurate predictions occurring by extrapolating the
7.3. Results and discussion

Figure 7.6: Pareto front for $C_{tol} = 0.5 C_{nom}$

Figure 7.7: Fitted Pareto front for $C_{tol} = 0.1 C_{nom}$
results. Nevertheless, the possible solution is to add new DOE points to improve the prediction of the metamodel in those regions.

First of all, it is required to realize which noise bounds will be violated in the case of $C_{\text{tol}} = C_{\text{nom}}$. For this purpose, the initial metamodel, despite being not accurate outside the bounds, is used to estimate the required extension of noise bounds. An inverse analysis using equal weights for all noise parameters considering Equation (7.5) is performed without including the bounds for $\sigma$. The results of the preliminary analysis are shown in the first row of Table 7.4. As expressed in this table, $\sigma_K$ and $\sigma_t$ are within the initial noise variation, but $\sigma_m$ exceeds the initial limit. Since there are no DOE points from $3\sigma_m$ to $3.8 \times 3\sigma_m$ and from $-3.8 \times 3\sigma_m$ to $-3\sigma_m$, the results of the robust optimization and inverse analysis is inaccurate. As observed in other studies (Bolstad et al., 1998), a more complete sampling, around the periphery and within the study region is required to obtain an accurate metamodel. Therefore, new DOE points are added to the regions without sampling points.

The strategy of adding new DOE points is explained using Figure 7.8. An initial 2D DOE, in which $z_1$ and $z_2$ represent two noise variables, is shown schematically in Figure 7.8(a). Assuming that an inverse approach using the initial metamodel finds a solution in which $\sigma_{z_2}$ exceeds $\sigma^\text{hom}_{z_2}$ ($\sigma_{z_2} > 1$), the DOE can then be extended using infill points in that direction. A larger variation of one noise will lead to a smaller variation of another noise. This has been shown in Figure 7.8(b) using the dashed lines. Therefore, the new infill points are confined in the range of $\pm 3\sigma_{z_1}$ in $z_1$ direction. The new infill points are shown by circles in Figure 7.8(b).

According to the first row of Table 7.4, the DOE should be extended in $m$ variable direction. The initial DOE is enriched by adding six infill points. The LHS method is used to generate 5000 sets of the new infill points in the expanded region, from which a set having the maximum sum of the distances from initial DOE points is selected. The FE simulation is then performed on those newly added points and the procedure of inverse analysis is repeated using the metamodel built on the updated DOE.

Table 7.4 shows the results of using the updated metamodel in the inverse approach. In this table, adding only six infill points changes the results of the inverse analysis significantly.
Table 7.4: The acceptable noise variation and the optimum design outside the initial noise limits using improved metamodel

<table>
<thead>
<tr>
<th>$C_{tol}$</th>
<th>DOE</th>
<th>$[\omega_K, \omega_t, \omega_m]$</th>
<th>$[\bar{\sigma}_K, \bar{\sigma}_t, \bar{\sigma}_m]$</th>
<th>$F_{bh}^{opt}$ (kN)</th>
<th>$R_{opt}$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{nom}$ Initial</td>
<td>1/3 1/3 1/3</td>
<td>0.16 0.74 3.8</td>
<td>195.7</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>$C_{nom}$ Updated</td>
<td>1/3 1/3 1/3</td>
<td>0.33 0.87 2.23</td>
<td>190.6</td>
<td>90</td>
<td></td>
</tr>
</tbody>
</table>

Figure 7.8: The strategy of adding infill points

7.3.3 Outlook

In this chapter, a general method for tailoring of scatter is presented and implemented. This method is flexible and it can be modified to be applied in other engineering problems. It can also be combined with the other approaches presented in the previous chapters.

First, the objective function is chosen to maximize the weighted sum of normalized sigma. In this chapter, the objective function is normalized using the nominal variation of noise. Using this method, the percentage acceptable variation is obtained for each parameter during tailoring material scatter. The normalization can be performed using various methods (Haftka and Gürdal, 1992). Nevertheless, normalization is an important step to set the weights such that they are significant relative to each other and relative to the objectives (Marler and Arora, 2010).

Second, in Equation (7.3), the material scatter is tailored considering a fixed mean value for all noise parameters. When the mean value for
some applications needs to be adjusted, a new objective function must be
defined to take into account the costs of the deviation of the mean value
of each noise parameter from the nominal mean. Then, the objective
function must be able to handle not only the variation of noise, but also
the deviation of noise mean from the nominal mean.

Third, the first inequality constraint can be considered as an equal-
ity constraint meaning that it is always active within the computational
accuracy. This is due to the fact that inactivity of this constraint means
that there is still room for increasing the variation of the noise param-
eters. It originates from the fact that a material with tighter tolerance
could not be cheaper to produce than a material with larger variations.

Fourth, the constraint in Equation (7.3) which is the objective func-
tion of the forward problem in (7.2) includes only the mean and the
standard deviation of the response. Recalling from Chapter 5, in the
case of a non-normal response distribution the constraint in Equation
(7.3) can be altered to account for the non-normality of the response.
For a non-normal input, which was the topic of Chapter 6, the objec-
tive function in Equation (7.3) must be selected in such a way that it
accounts for the non-normality of each input.

Last but not least, the objective function in the inverse method is
a linear combination of noise variations to be maximized. Determining
a set of weights for the relative importance of objectives is only locally
valid (Marler and Arora, 2010) and they cannot reflect the relative im-
portance of objectives in the whole domain. For instance, reducing the
scatter of a noise parameter by 50% can be relatively cheap, whereas it
might be expensive to reduce it by 25% due to the nonlinear nature of
controlling a noise parameter. Therefore, the weights and their appli-
cable domain must be selected carefully or a nonlinear weighting factor
must be generated.

7.4 Conclusions

An inverse robust optimization approach is presented and implemented
to tailor the variation of material and process noise parameters based on
the specified product tolerance. This method has been successfully ap-
plicated to the forming process of a lab-type B-pillar. The results show how
the acceptable material scatter varies by setting a tighter product tol-
erance or setting various weighting factors. This approach is flexible in
terms of adjusting weighting factors which are related to the costs of con-
trolling each noise parameter. Not all parameters need to be controlled up to a certain reduction of the product tolerance. However, further reduction of the product tolerance, requires more control on all noise parameters. For these cases, the Pareto fronts are presented to show the influence of employing various weighting factors and demonstrate the trade-off between controlling the parameters to minimize costs. Additionally, the developed method could equally be used to relax material specifications when a process meets the initial tolerance by a large margin. This, however, requires a re-construction of the metamodel on a wider (noise) space to ensure that it is sufficiently accurate.
Conclusions and recommendations

The following conclusions are drawn based on the presented results in this thesis:

- For efficient robust process optimization, the black-box process model must be replaced by an approximating metamodel (Chapters 3 and 4).

- For some metamodels calculation of response statistics can be done analytically (Chapters 3 and 4).

- Analytical calculation of response statistics is fast and accurate within the accuracy of the metamodel (Chapters 3 and 4).

- The convergence by iterative improvement of the metamodel requires fewer iterations using analytical calculation of the uncertainty of the objective function value (Chapters 3 and 4).

- The analytical derivatives of the response statistical moments with respect to each design variable improves the search for robust optimum design (Chapters 3 and 4).

- Analytical calculation of response statistics allows efficient modelling of non-normal noise and non-normal response (Chapters 5 and 6).

- Taking higher order statistical moments into account changes the optimum design (Chapter 5).

- For a non-normal response probability distribution, the robust optimization problem must be redefined properly (Chapter 5).
For correlated input parameters, principal component analysis can be used to describe the variation of parameters using linearly uncorrelated principal components (Chapter 6).

Using analytical calculation of response statistics it is possible to efficiently specify optimal material and process tolerances to obtain a required process robustness (Chapter 7).

A re-construction of the metamodel on a wider (noise) space is required to relax material specifications when a process meets the initial tolerance by a large margin (Chapter 7).

The following recommendations are given based on the achievements in this thesis:

- The feasibility of using other metamodeling techniques such as co-Kriging in both robust optimization and tailoring the scatter can be investigated.

- Other families of probability distributions can be used in analytical calculation of response statistics.

- For tailoring the scatter, it is recommended to consider different classes of non-normal or truncated distributions.

- It is recommended to study the real-time parameter estimation to control forming processes based on the analytical noise propagation and metamodels.

- The adjoint method can be used to obtain the derivatives of the output with respect to design variables in FE simulations and it is recommended to include those derivatives in robust optimization method.
## Nomenclature

- **b**: univariate basis function
- **f**: objective function value
- **f_{opt}**: objective function value at the robust optimum design
- **f_{ref}**: objective function value at the reference robust optimum design
- **m**: friction coefficient
- **n**: the weight in constraint evaluation
- **n**: hardening exponent in the Swift law
- **n_v**: number of variables
- **n_x**: number of design variables
- **n_z**: number of noise variables
- **p**: probability density function
- **r**: response
- **r**: r-values in tensile test (the ratio of strains)
- **r_c**: constraint response
- **\hat{s}_f**: uncertainty of the objective function value
- **t**: thickness
- **u**: displacement
- **v**: input variable
- **v_q**: measure of unimodality
- **w**: weighting factor in robustness measure
- **x**: design variable
- **x_{opt}**: robust optimum design
- **x_{ref}**: reference robust optimum design
- **z**: noise variable
Nomenclature

\( \mathbf{r} \) \hspace{1cm} vector of responses
\( \mathbf{v} \) \hspace{1cm} vector of input variables
\( \mathbf{x} \) \hspace{1cm} vector of design variables
\( \mathbf{z} \) \hspace{1cm} vector of noise variables

\( \mathbf{Ag} \) \hspace{1cm} uniform elongation
\( B \) \hspace{1cm} tensor-product basis functions
\( \mathbf{B} \) \hspace{1cm} bimodal distribution
\( \mathbf{C}_{\text{nom}} \) \hspace{1cm} nominal objective function obtained from robust optimization
\( \mathbf{C}_r \) \hspace{1cm} the target value for mean of a process
\( \mathbf{C}_{c} \) \hspace{1cm} specification limit for constraint
\( \mathbf{C}_{\text{tol}} \) \hspace{1cm} specified value for output objective function
\( \mathbf{C}_1 \) \hspace{1cm} two-dimensional array used for analytical noise propagation
\( \mathbf{C}_2 \) \hspace{1cm} three-dimensional array used for analytical noise propagation
\( \mathbf{C}_3 \) \hspace{1cm} four-dimensional array used for analytical noise propagation
\( \mathbf{C}_4 \) \hspace{1cm} five-dimensional array used for analytical noise propagation
\( \mathbf{F} \) \hspace{1cm} stress factors
\( \mathbf{F}_b \) \hspace{1cm} banding of Martensite
\( \mathbf{F}_{bh} \) \hspace{1cm} blank-holder force
\( \mathbf{F}_s \) \hspace{1cm} shape factor of Martensite
\( \mathbf{F}_v \) \hspace{1cm} volume fraction of Martensite
\( \mathbf{K} \) \hspace{1cm} hardening parameter in the Swift law
\( \mathbf{L} \) \hspace{1cm} parameter related to lower tail shift for non-normal response
\( \mathbf{N}_{\text{mc}} \) \hspace{1cm} number of MC samples
\( \mathbf{N} \) \hspace{1cm} normal probability distribution
\( \mathbf{R} \) \hspace{1cm} corner radius
\( \mathbf{Rm} \) \hspace{1cm} tensile strength
\( \mathbf{S} \) \hspace{1cm} the ratio of tensile strength to uniform elongation
\( \mathbf{T} \) \hspace{1cm} calculation time
\( \mathbf{U} \) \hspace{1cm} parameter related to upper tail shift for non-normal response
\( \mathbf{X} \) \hspace{1cm} random variable
\( \mathbf{Y} \) \hspace{1cm} random variable
\(\gamma\) skewness calculated using Azzalini (1985) equation
\(\gamma_1\) skewness
\(\gamma_2\) kurtosis
\(\delta\) percentage thinning
\(\Delta_q\) separation of two components of a bimodal distribution
\(\varepsilon\) strain
\(\zeta\) interpolation function in the Lielens homogenization method
\(\eta\) scale parameter in skew-normal distribution
\(\theta\) coefficients of fitting the Kriging model
\(\theta_f\) final angle of the profile
\(\kappa\) curvature
\(\lambda\) shape parameter in skew-normal distribution
\(\mu\) mean
\(\xi\) location parameter in skew-normal distribution
\(\rho\) coefficients of fitting the RBF model
\(\rho_{X,Y}\) mutual linear correlation coefficients
\(\sigma\) standard deviation
\(\overline{\sigma}\) normalized variation
\(\tau\) coefficients of fitting the RBF model
\(\phi\) probability density function of a standardized normal distribution
\(\Phi\) cumulative distribution function of a standardized normal distribution
\(\omega\) weighting factor in tailoring scatter
## Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CDF</td>
<td>cumulative distribution function</td>
</tr>
<tr>
<td>DOE</td>
<td>design of experiments</td>
</tr>
<tr>
<td>DP</td>
<td>dual-phase</td>
</tr>
<tr>
<td>EI</td>
<td>expected improvement</td>
</tr>
<tr>
<td>FE</td>
<td>finite element</td>
</tr>
<tr>
<td>FORM</td>
<td>first-order reliability method</td>
</tr>
<tr>
<td>FLC</td>
<td>forming limit curve</td>
</tr>
<tr>
<td>FFD</td>
<td>full factorial design</td>
</tr>
<tr>
<td>GA</td>
<td>genetic algorithm</td>
</tr>
<tr>
<td>GQ</td>
<td>Gaussian quadrature</td>
</tr>
<tr>
<td>LHS</td>
<td>Latin hypercube sampling</td>
</tr>
<tr>
<td>MSE</td>
<td>mean squared error</td>
</tr>
<tr>
<td>MC</td>
<td>Monte Carlo</td>
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<tr>
<td>ND</td>
<td>normal distribution</td>
</tr>
<tr>
<td>PC</td>
<td>principal component</td>
</tr>
<tr>
<td>PCA</td>
<td>principal component analysis</td>
</tr>
<tr>
<td>PDF</td>
<td>probability density function</td>
</tr>
<tr>
<td>RBF</td>
<td>radial basis function</td>
</tr>
<tr>
<td>RMSE</td>
<td>root mean square error</td>
</tr>
<tr>
<td>RVE</td>
<td>representative volume element</td>
</tr>
<tr>
<td>SORM</td>
<td>second-order reliability method</td>
</tr>
<tr>
<td>SQP</td>
<td>sequential quadratic programming</td>
</tr>
<tr>
<td>SND</td>
<td>skew-normal distribution</td>
</tr>
</tbody>
</table>
Appendix A

Evaluations of normalized output moments

Assume a process that has \( n_v \) inputs and one response. The vector of input variables is considered as \( v \in \mathbb{R}^{n_v} \) which includes design parameters, \( x \in \mathbb{R}^{n_x} \), and noise variables, \( z \in \mathbb{R}^{n_z} \). If a response function, \( r(v) \) can be defined using linear expansion of multivariate basis functions, it also can be re-written in terms of univariate basis functions as follows:

\[
    r(v) = r(x, z) = a_0 + \sum_{i=1}^{N} a_i B_i(v) = a_0 + \sum_{i=1}^{N} \left\{ a_i \prod_{t=1}^{n_v} b_{it}(v_t) \right\}
\]

where \( B_i(v) \) are multivariate basis functions and \( b_{it}(v_t) \) are univariate basis functions. To obtain the response mean, the integral of the multiplication of the metamodel and noise probability distribution is calculated using:
\[
\mu_r(x) = \int r(x, z)p(z)dz = \int r(x, z) \prod_{q=1}^{n_z} [p(z_q)dz_q]
\]

\[
= \int \left\{ a_0 + \sum_{i=1}^{N} \left[ a_i \prod_{t=1}^{n_x} b_{it}(v_t) \right] \right\} \prod_{q=1}^{n_z} [p(z_q)dz_q]
\]

\[
= \int \left\{ a_0 + \sum_{i=1}^{N} \left[ a_i \prod_{p=1}^{n_x} b_{ip}(x_p) \prod_{q=1}^{n_z} b_{iq}(z_q) \right] \right\} \prod_{q=1}^{n_z} [p(z_q)dz_q] \quad (A.2)
\]

\[
= a_0 + \sum_{i=1}^{N} \left\{ a_i \prod_{p=1}^{n_x} b_{ip}(x_p) \prod_{q=1}^{n_z} \left[ \int b_{iq}(z_q)p(z_q)dz_q \right] \right\}
\]

\[
= a_0 + \sum_{i=1}^{N} \left\{ a_i \prod_{p=1}^{n_x} b_{ip}(x_p) \prod_{q=1}^{n_z} C_{1iq} \right\}
\]
For the standard deviation of the response:

\[ \sigma^2_r(x) = \int \left( r(x, z) - \mu_r(x) \right)^2 p(z) dz \]

\[ = \int r(x, z)^2 p(z) dz - 2\mu_r(x) \int r(x, z) p(z) dz + \mu_r^2(x) \int p(z) dz \]

\[ = \int r(x, z)^2 p(z) dz - \mu_r^2(x) \]

\[ = \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_x+n_z} b_{it}(v_t) \right)^2 \prod_{q=1}^{n_z} (p(z_q) dz_q) \]

\[ - \left( \sum_{i=1}^{N} a_i \prod_{p=1}^{n_x} \prod_{q=1}^{n_z} C1_{iq} \right)^2 \]

\[ = \int \left( \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \prod_{t=1}^{n_x+n_z} b_{it}(v_t) b_{jt}(v_t) \right) \prod_{q=1}^{n_z} (p(z_q) dz_q) \]

\[ - \sum_{i=1}^{N} \sum_{j=1}^{N} \left( a_i a_j \prod_{p=1}^{n_x} b_{ip}(x_p) b_{jp}(x_p) \prod_{q=1}^{n_z} C1_{iq} C1_{jq} \right) \]

\[ = \sum_{i=1}^{N} \sum_{j=1}^{N} \left\{ a_i a_j \prod_{p=1}^{n_x} b_{ip}(x_p) b_{jp}(x_p) \right. \]

\[ \times \left( \prod_{q=1}^{n_z} \int b_{iq}(z_q) b_{jq}(z_q) p(z_q) dz_q - \prod_{q=1}^{n_z} C1_{iq} C1_{jq} \right) \left\} \right. \]

\[ = \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \left\{ \prod_{p=1}^{n_x} b_{ip}(x_p) b_{jp}(x_p) \left( \prod_{q=1}^{n_z} C2_{ijq} - \prod_{q=1}^{n_z} C1_{iq} C1_{jq} \right) \right\} \]

(A.3)
Appendix A. Evaluations of normalized output moments

For skewness:

\[
\gamma_1(x) = \frac{1}{\sigma_x^3} \int (f(x, z) - \mu_x(x, z))^3 p(z) \, dz \\
= \frac{1}{\sigma_x^3} \int \left\{ \phi^3 + \sum_{i=1}^{N} \left( a_i \prod_{t=1}^{n_x} b_{lt}(v_t) \right)^3 \sigma_x - \sum_{i=1}^{N} \left( a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right)^3 \right\} \\
\times \prod_{q=1}^{n_x} \left( p(z_q) \, dz_q \right) \\
= \frac{1}{\sigma_x^3} \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_x+n_z} b_{lt}(v_t) \right)^3 \prod_{q=1}^{n_x} \left( p(z_q) \, dz_q \right) \\
- 3 \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_x+n_z} b_{lt}(v_t) \right)^2 \left( \sum_{i=1}^{N} \left( a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right) \right) \prod_{q=1}^{n_x} \left( p(z_q) \, dz_q \right) \\
+ 3 \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_x+n_z} b_{lt}(v_t) \right) \left( \sum_{i=1}^{N} a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right)^2 \prod_{q=1}^{n_x} \left( p(z_q) \, dz_q \right) \\
- \int \left( \sum_{i=1}^{N} a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right)^3 \prod_{q=1}^{n_x} \left( p(z_q) \, dz_q \right) \\
= \frac{1}{\sigma_x^3} \int \left\{ \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \left( a_i a_j a_k \prod_{p=1}^{n_x} b_{ip}(x_p) b_{jp}(x_p) b_{kp}(x_p) \right) \right. \\
\times \left( \prod_{q=1}^{n_x} b_{iq}(z_q) b_{jq}(z_q) b_{kq}(z_q) p(z_q) \, dz_q \right) \\
- 3 \int \left( \prod_{q=1}^{n_x} b_{iq}(z_q) b_{jq}(z_q) p(z_q) \, dz_q \right) C_{1kq} \\
+ 3 \int \left( \prod_{q=1}^{n_x} b_{iq}(z_q) p(z_q) \, dz_q \right) C_{1jq} C_{1kq} - \left( \prod_{q=1}^{n_x} C_{1iq} C_{1jq} C_{1kq} \right) \right\} \\
= \frac{1}{\sigma_x^3} \int \left\{ \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \left( a_i a_j a_k \prod_{p=1}^{n_x} b_{ip}(x_p) b_{jp}(x_p) b_{kp}(x_p) \right) \right. \\
\times \left( C_{3ijkq} - 3C_{2ijq} C_{1kq} + 3C_{1iq} C_{1jq} C_{1kq} - C_{1iq} C_{1jq} C_{1kq} \right) \\
\left. \prod_{q=1}^{n_x} \left( C_{3ijkq} - 3C_{2ijq} C_{1kq} + 2C_{1iq} C_{1jq} C_{1kq} \right) \right\} \\
(A.4)
And for kurtosis:

\[
\gamma_2(x) = \frac{1}{\sigma^4(x)} \int (f(x, z) - \mu(x, z))^4 p(z) dz
\]

\[
= \frac{1}{\sigma^4(x)} \int \left\{ \sigma^2 + \sum_{i=1}^{N} \left( a_i \prod_{t=1}^{n_z} b_{it}(v_t) \right) \sigma^2 - \sum_{i=1}^{N} \left( a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right) \right\}^4
\]

\[
\times \prod_{t=1}^{n_z} (p(z_q)dz_q)
\]

\[
= \frac{1}{\sigma^4(x)} \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_z+n_z} b_{it}(v_t) \right)^4 \prod_{q=1}^{n_z} (p(z_q)dz_q)
\]

\[
- 4 \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_z+n_z} b_{it}(v_t) \right)^3 \left( \sum_{i=1}^{N} a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right) \prod_{q=1}^{n_x} [p(z_q)dz_q]
\]

\[
+ 6 \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_z+n_z} b_{it}(v_t) \right)^2 \left( \sum_{i=1}^{N} a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right)^2 \prod_{q=1}^{n_x} [p(z_q)dz_q]
\]

\[
- 4 \int \left( \sum_{i=1}^{N} a_i \prod_{t=1}^{n_z+n_z} b_{it}(v_t) \right) \left( \sum_{i=1}^{N} a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right)^3 \prod_{q=1}^{n_x} [p(z_q)dz_q]
\]

\[
+ \int \left( \sum_{i=1}^{N} a_i \prod_{q=1}^{n_x} C_{1iq} \prod_{p=1}^{n_x} b_{ip}(x_p) \right)^4 \prod_{q=1}^{n_x} [p(z_q)dz_q]
\]

\[
\text{(A.5)}
\]

\[
\frac{1}{\sigma^4(x)} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} \left\{ a_{i} a_{j} a_{k} a_{l} \prod_{q=1}^{n_z+n_z} b_{ip}(x_p)b_{jp}(x_p)b_{kp}(x_p)b_{lp}(x_p)
\right\}
\]

\[
\times \int \left( \prod_{q=1}^{n_z} b_{iq}(z_q) b_{jq}(z_q) b_{kp}(z_q) b_{lp}(z_q) p(z_q) dz_q \right)
\]

\[
- 4 \prod_{q=1}^{n_z} \left( b_{iq}(z_q) b_{jq}(z_q) b_{kp}(z_q) p(z_q) dz_q \right) C_{1iq} t_{q}
\]

\[
+ 6 \prod_{q=1}^{n_z} \left( b_{iq}(z_q) b_{jq}(z_q) p(z_q) dz_q \right) C_{1iq} C_{1iq} t_{q}
\]

\[
- 4 \prod_{q=1}^{n_z} \left( b_{iq}(z_q) p(z_q) dz_q \right) C_{1iq} C_{1iq} C_{1iq} t_{q} + \prod_{q=1}^{n_z} C_{1iq} C_{1iq} C_{1iq} C_{1iq} t_{q}
\]

\[
= \frac{1}{\sigma^4(x)} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} a_{i} a_{j} a_{k} a_{l} \prod_{p=1}^{n_x} b_{ip}(x_p)b_{jp}(x_p)b_{kp}(x_p)b_{lp}(x_p)
\]

\[
\times \prod_{q=1}^{n_z} \left[ C_{4ijkl} - 4 C_{3ijkl} C_{1iq} + 6 C_{2ijkl} C_{1iq} C_{1iq} t_{q}
\right.
\]

\[
- 3 C_{1iq} C_{1iq} C_{1iq} C_{1iq} t_{q}]
\]
Appendix A. Evaluations of normalized output moments

Note that:

\[
\left( \sum_{i=1}^{N} a_i \right) \left( \sum_{j=1}^{N} a_j \right) = \left( \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \right) = \left( \sum_{k=1}^{N} a_k \right)^2 \quad (A.6)
\]

In Equations (A.2) to (A.5):

\[
C_{1iq} = \int_{z_q} b_{iq}(z_q)p(z_q)dz_q \quad (A.7)
\]

\[
C_{2ijq} = \int_{z_q} b_{iq}(z_q)b_{jq}(z_q)p(z_q)dz_q \quad (A.8)
\]

\[
C_{3ijkq} = \int_{z_q} b_{iq}(z_q)b_{jq}(z_q)b_{kj}(z_q)p(z_q)dz_q \quad (A.9)
\]

\[
C_{4ijklq} = \int_{z_q} b_{iq}(z_q)b_{jq}(z_q)b_{kj}(z_q)b_{lk}(z_q)p(z_q)dz_q \quad (A.10)
\]
Appendix B

Derivations for Kriging

Equations (A.7) to (A.10) are written in a general form and for a specific metamodel combined with a specific description of the noise distribution, those integrals can be evaluated. For an ordinary Kriging metamodel:

\[ r(x) = a_0 + r(v) \mathbf{T}_R^{-1}(y_0 - a_0 \mathbf{1}) \]

\[ = a_0 + r(v) \mathbf{T}_\kappa \]

\[ = a_0 + \sum_{i=1}^{N} \kappa_i \prod_{t=1}^{n_v} b_{it}(v_t) \]

\[ (B.1) \]

In this equation, \( \mathbf{R} \) contains the correlations between all DOE points. This equation is in the form of equation (A.1).

Considering univariate basis functions of Kriging metamodel as:

\[ b_{it}(v_t) = e^{-\theta_t^2(v_t - v_{it})^2} \]

\[ (B.2) \]

and assuming that the noise parameters are normally distributed:

\[ \mathcal{N}(z_q) = \frac{1}{\sigma_q \sqrt{2\pi}} e^{-\frac{(z_q - \mu_q)^2}{2\sigma_q^2}} \]

\[ (B.3) \]
Then $C_{1iq}^{\text{Krig},N}$ is calculated as follows:

$$C_{1iq}^{\text{Krig},N} = \int b_{iq}(z_q)N(z_q)dz_q$$

$$= \int e^{-\theta_q^2(z_q-z_{iq})^2}\left(\frac{1}{\sigma_q \sqrt{2\pi}}e^{-\frac{(z_q-\mu_q)^2}{2\sigma_q^2}}\right)dz_q$$

$$= \frac{1}{\sigma_q \sqrt{2\pi}} \int e^{-\left(\theta_q^2 z_q^2 - 2\theta_q z_q z_{iq} + \theta_q^2 z_{iq}^2 + z_q^2 \frac{\sigma_q^2}{2\sigma_q^2} - 2z_q \mu_q \frac{\sigma_q^2}{2\sigma_q^2} + \mu_q^2 \frac{\sigma_q^2}{2\sigma_q^2}\right)}dz_q$$

$$= \frac{1}{\sigma_q \sqrt{2\pi}} \int e^{-\left(\frac{2\theta_q^2}{\sigma_q^2} z_q^2 + \frac{4\theta_q^2 z_q \sigma_q^2 + 2\mu_q}{2\sigma_q^2} z_q - (\theta_q^2 z_{iq}^2 + \frac{\mu_q^2}{2\sigma_q^2})\right)}dz_q$$

$$= \frac{1}{\sigma_q \sqrt{2\pi}} \left[\frac{\pi}{\left(\frac{2\sigma_q^2 \theta_q^2 + 1}{2\sigma_q^2}\right)^\frac{3}{2}} e^{-\left(\theta_q^2 z_{iq}^2 + \frac{\mu_q^2}{2\sigma_q^2}\right)}\right]$$

$$= \sqrt{\frac{1}{2\sigma_q^2 \theta_q^2 + 1}} e^{-\left(\frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} - \frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)}\right)}$$

$$= \sqrt{\frac{1}{2\sigma_q^2 \theta_q^2 + 1}} e^{-\left(\frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} - \frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)}\right)}$$

$$= \frac{\theta_q^2}{\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} e^{-\left(\frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} - \frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)}\right)}$$

$$= \frac{\theta_q^2}{\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} e^{-\left(\frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} - \frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)}\right)}$$

$$= \frac{\theta_q^2}{\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} e^{-\left(\frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} - \frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)}\right)}$$

$$= \sqrt{\frac{\theta_q^2}{2\sigma_q^2 \theta_q^2 + 1}} e^{-\left(\frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)} - \frac{2\theta_q^2 z_{iq}^2 + \mu_q^2}{2\sigma_q^2(2\sigma_q^2 \theta_q^2 + 1)}\right)}$$

Note that:

$$\int_{-\infty}^{\infty} e^{-ax^2 \pm bx - c} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a} - c} \quad a > 0 \quad (B.4)$$
Similarly for \( C_{ijq}^{Krig,N} \), \( C_{ijq}^{Krig,N} \), and \( C_{ijklq}^{Krig,N} \):

\[
C_{ijq}^{Krig,N} = \int b_{iq}(z_q)b_{jq}(z_q)N(z_q)\,dz_q
\]

\[
= \int e^{-\frac{\theta^2 q (z_q - z_{iq})^2}{2}} e^{-\frac{\theta^2 q (z_q - z_{jq})^2}{2}} \left( \frac{1}{\sigma_q \sqrt{2\pi}} e^{-\frac{(z_q - \mu_q)^2}{2\sigma_q^2}} \right) \,dz_q
\]

\[
= \frac{1}{\sigma_q \sqrt{2\pi}} \int e^{-\left(\frac{4\sigma^2 q \theta^2 q + 1}{2\sigma_q^2}\right)z_q^2 + \left(\frac{4\theta^2 q \sigma^2 q + 4\theta^2 q \sigma^2 q + 2\mu_q}{2\sigma_q^2}\right)z_q} \left(\frac{1}{\sigma_q^2 \theta^2 q + 1}\right) \,dz_q
\]

\[
= \frac{1}{\sigma_q \sqrt{2\pi}} \sqrt{\frac{\pi}{\left(\frac{4\sigma^2 q \theta^2 q + 1}{2\sigma_q^2}\right)}} e^{-\left(\frac{4\sigma^2 q \theta^2 q + 1}{2\sigma_q^2}\right)z_q^2 - \left(\frac{4\theta^2 q \sigma^2 q + 4\theta^2 q \sigma^2 q + 2\mu_q}{2\sigma_q^2}\right)z_q}
\]

\[
= \frac{1}{\sqrt{4\sigma^2 q \theta^2 q + 1}} e^{-\left(\frac{4\sigma^2 q \theta^2 q + 1}{2\sigma_q^2}\right)z_q^2 - \left(\frac{4\theta^2 q \sigma^2 q + 4\theta^2 q \sigma^2 q + 2\mu_q}{2\sigma_q^2}\right)z_q}
\]

\[
= \frac{1}{\sqrt{4\sigma^2 q \theta^2 q + 1}} e^{-\left(\frac{4\sigma^2 q \theta^2 q + 1}{2\sigma_q^2}\right)z_q^2 - \left(\frac{4\theta^2 q \sigma^2 q + 4\theta^2 q \sigma^2 q + 2\mu_q}{2\sigma_q^2}\right)z_q}
\]

\[
= \frac{1}{\sqrt{4\sigma^2 q \theta^2 q + 1}} e^{-\left(\frac{4\sigma^2 q \theta^2 q + 1}{2\sigma_q^2}\right)(z_{iq} - z_{jq})^2 + (\mu_q - z_{iq})^2 + (\mu_q - z_{jq})^2}
\]

(B.6)
\[ C_{\text{N}ijkq} = \int b_{iq}(z_q) b_{jq}(z_q) b_{pq}(z_q) p(z_q) \, dz_q \]

\[ = \int e^{-\theta^2_q(z_q-z_{iq})^2} e^{-\theta^2_q(z_q-z_{jq})^2} e^{-\theta^2_q(z_q-z_{kq})^2} \frac{1}{\sigma_q \sqrt{2\pi}} \frac{(x_q - \mu_q)^2}{2\sigma_q^2} \, dz_q \]

\[ = \frac{1}{\sigma_q \sqrt{2\pi}} \int \exp \left\{ -\left( \theta^2_q - 2 \theta_q z_q z_{iq} + \theta^2_q z_{iq}^2 + \theta^2_q z_{jq}^2 - 2 \theta_q z_q z_{jq} \right. \right. \]

\[ \left. + \theta^2_q z_{jq}^2 + \theta^2_q z_{kq}^2 - 2 \theta_q z_q z_{kq} + \theta^2_q z_{kq}^2 \right. \left. + \frac{z_q^2}{2\sigma_q^2} - \frac{2z_q \mu_q}{2\sigma_q^2} + \frac{\mu^2_q}{2\sigma_q^2} \right\} \, dz_q \]

\[ = \frac{1}{\sigma_q \sqrt{2\pi}} \int \exp \left\{ -\left( \frac{6\sigma^2_q \theta^2_q + 1}{2\sigma_q^2} \right) z_q^2 + \left( \frac{4\theta^2_q z_{iq} \sigma^2_q + 4\theta^2_q z_{jq} \sigma^2_q + 4\theta^2_q z_{kq} \sigma^2_q + 2\mu^2_q}{2\sigma_q^2} \right) \right. \]

\[ \left. - \left( \theta^2_q z_{iq}^2 + \theta^2_q z_{jq}^2 + \frac{\mu^2_q}{2\sigma_q^2} \right) \right\} \, dz_q \]

\[ = \sqrt{\frac{1}{6\sigma^2_q \theta_q + 1}} \exp \left\{ \frac{-\theta^2_q}{6\sigma^2_q \theta^2_q + 1} \left( \frac{4\sigma^2_q \theta^2_q + 1}{\sigma^2_q \theta^2_q + \frac{\mu^2_q}{2\sigma^2_q}} \right) \right. \]

\[ \left. - \left( \frac{\mu^2_q}{2\sigma^2_q} \right) \right\} \left( -2 \theta_q z_{iq} \sigma^2_q + 6 \theta^2_q \sigma^2_q + 2 \theta_q z_{jq} \sigma^2_q + 2 \theta_q z_{kq} \sigma^2_q + 2 \mu^2_q \right) \}

\[ = \sqrt{\frac{1}{6\sigma^2_q \theta_q + 1}} \exp \left\{ \frac{-\theta^2_q}{6\sigma^2_q \theta^2_q + 1} \left( \frac{4\sigma^2_q \theta^2_q + 1}{\sigma^2_q \theta^2_q + \frac{\mu^2_q}{2\sigma^2_q}} \right) \right. \]

\[ \left. + 4 \theta^2_q z_{jq} \theta^2_q - 2z_{iq} \mu_q - 4z_{jq} \theta^2_q z_{kq} \sigma^2_q \right\} \}

\[ = \sqrt{\frac{1}{6\sigma^2_q \theta_q + 1}} \exp \left\{ \frac{-\theta^2_q}{6\sigma^2_q \theta^2_q + 1} \left( \frac{\mu^2_q - z_{iq}^2 + \mu^2_q - z_{jq}^2 + \mu^2_q - z_{kq}^2}{2\sigma^2_q \theta^2_q + 1} \right) \right. \]

\[ \left. + 2\sigma^2_q \theta^2_q \left( z_{iq}^2 + z_{jq}^2 + z_{kq}^2 \right) \right\} \}

(B.7)
\[ C_{ijklq}^{Kiij,N} = \int b_{iq}(z_q)b_{jq}(z_q)b_{kq}(z_q)b_{lq}(z_q)p(z_q)dz_q \]

\[ = \int e^{-(z_q-z_{iq})^2}e^{-\frac{\theta^2_q(z_q-z_{jq})^2}{2\sigma_q^2}}e^{-\frac{\theta^2_q(z_q-z_{kq})^2}{2\sigma_q^2}}e^{-\frac{\theta^2_q(z_q-z_{lq})^2}{2\sigma_q^2}} \frac{1}{\sigma_q\sqrt{2\pi}}e^{-\frac{(z_q-\mu_q)^2}{2\sigma_q^2}}dz_q \]

\[ = \frac{1}{\sigma_q\sqrt{2\pi}} \int \exp \left\{ -\frac{\theta^2_q z_q^2 - 2\theta_q z_q z_{iq} + \theta^2_q z_{iq}^2 + \theta^2_q z_{iq}^2 - 2\theta_q z_q z_{jq} + \theta^2_q z_{jq}^2}{2\sigma_q^2} + \frac{z_q^2}{2\sigma_q^2} - \frac{z_q^2 z_{iq}^2}{2\sigma_q^2} + \frac{\mu_q^2}{2\sigma_q^2} \right\} dz_q \]

\[ = \frac{1}{\sigma_q\sqrt{2\pi}} \int \exp \left\{ -\frac{(2\theta^2_q z_{iq}^2 + 4\theta^2_q z_{jq}^2 + 4\theta^2_q z_{kq}^2 + 4\theta^2_q z_{lq}^2 + 2\mu_q^2)}{2\sigma_q^2} \right\} dz_q \]

\[ = \frac{1}{\sigma_q\sqrt{2\pi}} \int \exp \left\{ \frac{\theta^2_q z_{iq}^2 + \theta^2_q z_{jq}^2 + \theta^2_q z_{kq}^2 + \theta^2_q z_{lq}^2 + \mu_q^2}{2\sigma_q^2} \right\} dz_q \]

\[ = \sqrt{\frac{1}{8\sigma_q^2\theta_q^2 + 1}} \left\{ \frac{1}{8\sigma_q^2\theta_q^2 + 1} \left( 6z_{iq}^2\theta_q^2 + z_{iq}^2 + 6z_{jq}^2\theta_q^2 + z_{jq}^2 + 6z_{kq}^2\theta_q^2 + z_{kq}^2 \right) \right\} \]

\[ = \sqrt{\frac{1}{8\sigma_q^2\theta_q^2 + 1}} \left\{ \frac{1}{8\sigma_q^2\theta_q^2 + 1} \left( 6z_{iq}^2\theta_q^2 + z_{iq}^2 + 6z_{jq}^2\theta_q^2 + z_{jq}^2 + 6z_{kq}^2\theta_q^2 + z_{kq}^2 \right) \right\} \]

\[ = \sqrt{\frac{1}{8\sigma_q^2\theta_q^2 + 1}} \left\{ \frac{1}{8\sigma_q^2\theta_q^2 + 1} \left( 6z_{iq}^2\theta_q^2 + z_{iq}^2 + 6z_{jq}^2\theta_q^2 + z_{jq}^2 + 6z_{kq}^2\theta_q^2 + z_{kq}^2 \right) \right\} \]

\[ = \sqrt{\frac{1}{8\sigma_q^2\theta_q^2 + 1}} \left\{ \frac{1}{8\sigma_q^2\theta_q^2 + 1} \left( 6z_{iq}^2\theta_q^2 + z_{iq}^2 + 6z_{jq}^2\theta_q^2 + z_{jq}^2 + 6z_{kq}^2\theta_q^2 + z_{kq}^2 \right) \right\} \]

\[ = \sqrt{\frac{1}{8\sigma_q^2\theta_q^2 + 1}} \left\{ \frac{1}{8\sigma_q^2\theta_q^2 + 1} \left( 6z_{iq}^2\theta_q^2 + z_{iq}^2 + 6z_{jq}^2\theta_q^2 + z_{jq}^2 + 6z_{kq}^2\theta_q^2 + z_{kq}^2 \right) \right\} \]
Uncertainty of objective function for Kriging can be obtained as follows:

\[ s_{\text{obj}}^2 = \int s^2(x, z)N(z)dz \]

\[ = \int \hat{s}^2(1 - r(x, z)^T R^{-1}r(x, z))N(z)dz \]

\[ = \int \hat{s}^2 \left( 1 - \left( \sum_{i=1}^{N} \prod_{t=1}^{n_v} b_{it} \right)^T R^{-1} \left( \sum_{i=1}^{N} \prod_{t=1}^{n_v} b_{it} \right) \right) N(z)dz \]

\[ = \hat{s}^2 - \hat{s}^2 \left( \sum_{i=1}^{N} \sum_{j=1}^{N} R_{ij}^{-1} \prod_{p=1}^{n_x} b_{ip} b_{jp} \right) \int \left( \sum_{i=1}^{N} \sum_{j=1}^{N} \prod_{q=1}^{n_z} b_{iq} b_{jq} \right) N(z)dz \]

\[ = \hat{s}^2 \left( \sum_{i=1}^{N} \prod_{p=1}^{n_x} b_{ip} b_{jp} \right) \left( \sum_{q=1}^{n_z} \prod_{q=1}^{n_z} C_{2ijq} \right) \]

In case of Kriging with polynomial trend, one can separate the integral of equations (A.2) and (A.3) to two parts. One for a general polynomial trend model and the other one for weighted sum of residual random function. For example, for the universal Kriging with a linear trend:

\[ r(v) = a_0 + \sum_{i=1}^{N} b_i \prod_{t=1}^{n_v} b_{it}(v_t) + \sum_{i=1}^{N} \kappa_i \prod_{t=1}^{n_v} b_{it}(v_t) \]

This can be directly substituted in equations (A.2) and (A.3). Univariate basis functions for linear trend, \( b_{it}(v_t) \), are defined as follows:

\[ b_{it} = \begin{cases} 1 & i \neq t \\ v_t & i = t \end{cases} \]

and design and noise parameters can be separated for the linear part:

\[ r(v)_{\text{linear}} = a_0 + \sum_{i=1}^{N} b_i \prod_{p=1}^{n_x} b_{ip}(x_p) \prod_{q=1}^{n_z} b_{iq}(z_q) \]

By replacing these basis functions and normal distribution in equation (B.4):

\[ C_{1iq}^{\text{linear,N}} = \begin{cases} \int N(z_q)dz_q = 1 & i \neq q \\ \int z_q N(z_q)dz_q = \mu_q & i = q \end{cases} \]
similarly for standard deviation:

\begin{equation}
C_{ijq}^{2,\text{linear},\mathcal{N}} = \begin{cases} 
\int N(z_q)dz_q = 1 & i \neq q \text{ and } j \neq q \\
\int z_q N(z_q)dz_q = \mu_q & (i = q \text{ or } j = q) \text{ and } i \neq j \\
\int z_q^2 N(z_q)dz_q = \mu_q^2 + \sigma_q^2 & i = j = q 
\end{cases}
\end{equation}

(B.14)

and by substituting (B.13) and (B.14) in (A.2) and (A.3)

\begin{equation}
\mu_{r,\text{linear}}(x) = a_0 + \sum_{q=1}^{n_z} b_q \mu_q + \sum_{p=n_z+1}^{n_z+n_x} (b_p x_p) \tag{B.15}
\end{equation}

\begin{equation}
\sigma_{r,\text{linear}}^2(x) = \sum_{q=1}^{n_z} (b_q^2 \sigma_q^2) \tag{B.16}
\end{equation}

This means that the linear expressions, \( \mu_{r,\text{linear}} \) and \( \sigma_{r,\text{linear}}^2 \), are added to the original expression given by (A.2) and (A.3). The analytical integration can be extended for polynomials of higher orders. For example for second order polynomials, \( \mu_{r,\text{second order}}(x) \) is expressed using:

\begin{equation}
\mu_{r,\text{second order}}(x) = a_0 + \sum_{q=1}^{n_z} b_q \mu_q + \sum_{q=1}^{n_z} b_{qq} \sigma_q^2 + \sum_{q=1}^{n_z} \sum_{q \geq q} b_{qq} \mu_q \mu_q \\
+ \sum_{p=n_z+1}^{n_z+n_x} \left( b_p + \sum_{q=1}^{n_z} b_{pq} \mu_q \right) x_p + \sum_{p=n_z+1}^{n_z+n_x} \sum_{p \geq p} b_{pp} x_p x_p \tag{B.17}
\end{equation}

and for \( \sigma_{r,\text{second order}}^2(x) \):

\begin{equation}
\sigma_{r,\text{second order}}^2(x) = \sum_{q=1}^{n_z} b_{qq}^2 \sigma_q^4 + \sum_{q=1}^{n_z} \sum_{q \geq q} b_{qq}^2 \sigma_q^2 \sigma_q^2 \\
+ \sum_{q=1}^{n_z} \left( b_q + b_{qq} \mu_q + \sum_{q=1}^{n_z} b_{qq} \mu_q \right) \left( \sum_{p=n_z+1}^{n_z+n_x} b_{pp} x_p x_p \right) \sigma_q^2 \tag{B.18}
\end{equation}
Appendix C

Derivations for RBFs

For Gaussian RBF the same approach as in Appendix B can be used:

\[ r(v) = a_0 + \psi(v)^T \Psi^{-1}(y_0 - a_0 1) \]

\[ = a_0 + \psi(v)^T \omega \]

\[ = a_0 + \sum_{i=1}^{N} \omega_i \prod_{t=1}^{n_v} b_{it}(v_t) \]

The following basis functions are selected for RBFs:

\[ b_{it}(v_t) = e^{-\frac{\rho_i^2}{2 \tau^2} (v_t - v_{it})^2} \]

The derivations of the coefficients \( C1 \) and \( C2 \) are very similar to Kriging. The difference is that the fitting coefficients in RBF are assigned to each basis function and variables instead of being assigned to each variable.
only. Therefore:

\[
C_{1_{iq}}^{RBF,N} = \int b_{iq}(z_q)N(z_q)dz_q
\]

\[
= \int e^{-\frac{\rho_q^2}{2\tau_i^2}(z_q-z_{iq})^2}\left(\frac{1}{\sigma_q\sqrt{2\pi}}e^{-\frac{(z_q-\mu_q)^2}{2\sigma_q^2}}\right)dz_q
\]

\[
= \frac{1}{\sigma_q\sqrt{2\pi}} \int e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 - \frac{\rho_q^2}{2\tau_i^2}z_{iq}z_q^2 + \frac{z_q^2}{2\sigma_q^2} - 2z_q\mu_q + \mu_q^2} dz_q
\]

\[
= \frac{1}{\sigma_q\sqrt{2\pi}} \int e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}} - \frac{\rho_q^2}{2\tau_i^2}z_{iq}^2 + \frac{\mu_q}{\sigma_q^2}} dz_q
\]

\[
= \frac{1}{\sigma_q\sqrt{2\pi}} \int e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}} dz_q
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= \frac{1}{\sqrt{\sigma_q^2\frac{\rho_q^2}{\tau_i^2} + 1}} e^{-\frac{\rho_q^2}{2\tau_i^2}z_q^2 + \frac{\mu_q}{\sigma_q^2}}
\]

\[
= 1
\]

(C.3)
\[ C_{ijq}^{\text{RBF},N} = \int b_{i}(z_q)b_{j}(z_q)N(z_q)dz_q \]

\[
= \int e^{-\frac{x_q^2}{2\tau_i^2} - \frac{y_q^2}{2\tau_j^2}}(z_q-z_{iq})^2 \frac{1}{\sigma_q \sqrt{2\pi}} \exp \left( \frac{(z_q - z_{jq})^2}{2\sigma_q^2} \right) dz_q \\
= \frac{1}{\sigma_q \sqrt{2\pi}} \int \left( 2\frac{\rho_q^2 2^2 + 2\mu_q^2 2^2 + 2\mu_q^2 2^2}{\tau_i^2 + \frac{\sigma_q^2}{2\tau_j^2} + 1} - e^{-\frac{2\rho_q^2 2^2 + 2\mu_q^2 2^2 + 2\mu_q^2 2^2}{\tau_i^2 + \frac{\sigma_q^2}{2\tau_j^2} + 1}} \right) \\
= \frac{1}{\tau_i \tau_j} \sqrt{\frac{\rho_q^2 \sigma_q^2 2^2 + \rho_q^2 \sigma_q^2 2^2 + \tau_i^2 \tau_j^2}{\tau_i^2 + \frac{\sigma_q^2}{2\tau_j^2} + 1}} \\
\times \frac{-\rho_q^2 2^2 - \rho_q^2 \sigma_q^2 2^2 - \mu_q^2 2^2 - \mu_q^2 \sigma_q^2 2^2 - \mu_q^2 \sigma_q^2 2^2 - \mu_q^2 \sigma_q^2 2^2 + 2\rho_q^2 \sigma_q^2 \sigma_q^2 + 2\mu_q^2 \sigma_q^2 \sigma_q^2 + 2\mu_q^2 \sigma_q^2 \sigma_q^2}{(2\rho_q^2 \sigma_q^2 2^2 + \rho_q^2 \sigma_q^2 2^2 + \tau_i^2 \tau_j^2)} \\
= \frac{1}{\tau_i \tau_j} \sqrt{\frac{\rho_q^2 \sigma_q^2 2^2 + \rho_q^2 \sigma_q^2 2^2 + \tau_i^2 \tau_j^2}{\tau_i^2 + \frac{\sigma_q^2}{2\tau_j^2} + 1}} \\
\times \frac{-\rho_q^2}{e^{-\frac{2\rho_q^2 \sigma_q^2 2^2 + \rho_q^2 \sigma_q^2 2^2 + \tau_i^2 \tau_j^2}{\tau_i^2 + \frac{\sigma_q^2}{2\tau_j^2} + 1}}} \left( \tau_j^2 (\mu_q - z_{jq})^2 + \tau_i^2 (\mu_q - z_{iq})^2 + \rho_q^2 \sigma_q^2 (z_{iq} - z_{jq})^2 \right) \\
\text{(C.4)}
Appendix D

Material model for heterogeneous materials

Choosing a proper material model to account for uncertainty of the material noise is an important step in both robust optimization and tailoring the scatter. The choice of the material model dictates the characterization methods to be used to identify the variation in the material parameters. Simplified models usually require less effort and cost to collect the variation data, however, complicated ones require a detailed characterization techniques. This is a trade-off between the accuracy of modelling and the costs of material characterization based on available resources. In this section, homogenization approach to model the materials that are comprised of more than one phase is discussed.

D.1 Mean-field homogenization

Mean-Field homogenization employs the rule of mixture and calculates the overall properties by averaging over the respective properties of the constitutive phases in the material. This method is appropriate for composites or materials consisting of more than one phase. This method was developed by among others (Hashin and Shtrikman, 1963; Hill, 1965), and is based on the inclusion model proposed by Eshelby (Eshelby, 1957). In this method, the average material properties is obtained via solving a boundary value problem by means of analytical (or semi-analytical) methods. Therefore, compared to full-filed homogenization, this method is less expensive in terms of computational cost.

In micro-macro approach, on each material point the macro-strain
is known and the macro stress should be calculated. It was shown that in case of applying linear boundary conditions to the RVE, the problem of relating strain and stress in macro level can be translated into the relation between average stress and average strain in the RVE (Nemat-Nasser and Hori, 2013). If \( x \) is considered as micro-coordinate, \( \tau \) as macro-coordinate, \( \omega \) as RVE domain, \( v \) as volume fraction, \( I \) as subscript for inclusion, and \( M \) as subscript for matrix, then the average of any function (here strain) over the RVE can be expressed as:

\[
\langle \epsilon \rangle = v_M \langle \epsilon \rangle_{\omega M} + v_I \langle \epsilon \rangle_{\omega I} \tag{D.1}
\]

Then the average strain in different phases can be related using strain concentration tensor \( H \):

\[
\langle \epsilon \rangle_{\omega I} = H_I : \langle \epsilon \rangle_{\omega M} \tag{D.2}
\]

In order to correlate the average strain in each phase to the macro-strain:

\[
\langle \epsilon \rangle_{\omega M} = [v_I H_I + v_M I]^{-1} : \langle \epsilon \rangle \tag{D.3}
\]

In which \( I \) is the fourth order unit tensor. One can consider changing the subscripts in Equation (D.2) to obtain the relation among inclusion strain and total average strain:

\[
\langle \epsilon \rangle_{\omega M} = H_M : \langle \epsilon \rangle_{\omega I} = H_I^{-1} : \langle \epsilon \rangle_{\omega I} \tag{D.4}
\]

\[
\langle \epsilon \rangle_{\omega I} = [v_M H_M + v_I I]^{-1} : \langle \epsilon \rangle = [v_M H_I^{-1} + v_I I]^{-1} : \langle \epsilon \rangle \tag{D.5}
\]

\( A \) is called strain concentration tensor which describes the strain in inclusion with respect to the overall average. The expression for \( H \) determines the homogenization method which are briefly presented in the following sections.

## D.2 Mori-Tanaka

In Mori-Tanaka (MT) method the \( H \) tensor is presented as (Tanaka and Mori, 1970):

\[
H = [I - S : (I - C_M^{-1} : C_I)]^{-1} \tag{D.6}
\]
where $S$ is the Eshelby tensor for the inclusion and $C$ is the isotropic stiffness. The explicit nature of this homogenization method makes it appropriate for numerical implementation. This method is accurate for the low volume fraction of the second phase. The validity of this method for the intermediate volume fraction of the inclusion is questionable. It should be noted that this method is also valid for high volume fractions because the definition of matrix and of inclusion are interchangeable.

### D.3 Lielens interpolation method

The Lielens interpolation method, also called the double inclusion (DI) model, was proposed to improve the accuracy of the MT method (Hori and Nemat-Nasser, 1993) for the intermediate volume fraction of the inclusion. This method is based on the interpolation of the MT model. In this approach, the strain concentration tensor is calculated by interpolation between the forward and reverse MT approach:

$$ A = \{(1 - \zeta) \overrightarrow{H}^{-1} + \zeta \overleftarrow{H}\}^{-1} \quad (D.7) $$

where:

$$ \overrightarrow{H} = [\overline{I} - S : (\overline{I} - C_M^{-1} : C_I)]^{-1} \quad (D.8) $$

$$ \overleftarrow{H} = [\overline{I} - S : (\overline{I} - C_I^{-1} : C_M)]^{-1} \quad (D.8) $$

In these equations, $\overrightarrow{H}$ is for forward MT approach, $\overleftarrow{H}$ is for reverse MT approach (Matrix and inclusion interchanged), and $\zeta$ is an interpolation function. The upper and lower bounds of $\zeta$ are 0 and 1 when $\nu_I$ approaches 0 and 1 respectively.

For numerical implementations $\overrightarrow{H}$ can be written as:

$$ \overrightarrow{H} = (C_M : S^{-1} - C_M + C_I)^{-1} : C_M : S^{-1} \quad (D.9) $$

It is also worth mentioning that the interpolation method is arbitrary, and one can modify the strain concentration tensor in Equation (D.7) in different ways such as:

$$ A = \{(1 - \zeta) \overrightarrow{H} + \zeta \overleftarrow{H}^{-1}\} \quad (D.10) $$

### D.4 Self-consistent

The main idea behind MT and DI methods is that they consider an
Appendix D. Material model for heterogeneous materials

Figure D.1: Spherical, oblate spheroid and prolate spheroid inclusions

Inclusion in an infinite matrix. In contrast, self-consistent (SC) method considers an inclusion in the overall RVE (Hill, 1965). In this homogenization scheme, the strain concentration tensor can be expressed by:

\[ A = (I - S : (I - C^{-1} : C))^{-1} \]  \hspace{1cm} (D.11)

This equation is very similar to Equation (D.6) but the isotropic stiffness tensor of the matrix is replaced with that of the RVE. It means that this method has an implicit nature which requires numerical algorithms to be solved.

D.5 Eshelby

The methods proposed in the previous sections are all based on the solution of Eshelby for an inclusion. The Eshelby’s solution for the relevant shapes in this thesis is presented in this section. Three cases are considered in this section: spherical inclusion, oblate spheroid and prolate spheroid. Oblate spheroids \((a < b = c)\) have an aspect ratio of \(\alpha = a/b < 1\) and prolate spheroids \((a > b = c)\) have an aspect ratio of \(\alpha = a/b > 1\) as shown in figure D.1 For an spheroidal inclusion, the components of the Eshelby tensor is written as follows:

\[
S_{1111} = S_{2222} = S_{3333} = \frac{7 - 5\nu_M}{15(1 - \nu_M)} \\
S_{1122} = S_{2211} = S_{2233} = \frac{5\nu_M - 1}{15(1 - \nu_M)} \\
S_{1212} = S_{2323} = S_{1313} = \frac{4 - 5\nu_M}{15(1 - \nu_M)}
\]  \hspace{1cm} (D.12)
in which \( \nu_M \) is Matrix Poisson’s ratio. In indicial notation one can write these components in compact form:

\[
S = \frac{1 + \nu_M}{3(1 + \nu_M)} I^v + \frac{2(4 - 5\nu_M)}{15(1 - \nu_M)} I^d
\]  

(D.13)

This equation can be re-written in terms of bulk modulus (\( \kappa \)) and shear modulus (\( \mu \)):

\[
S = \frac{3\kappa_M}{3\kappa_M + 4\mu_M} I^v + \frac{6(\kappa_M + 2\mu_M)}{5(3\kappa_M + 4\mu_M)} I^d
\]

(D.14)

where \( I^v \) and \( I^d \) are fourth order unit volumetric and deviatoric tensors, respectively, that are the decomposition of the fourth order unit tensor (\( I \)):

\[
I^v = \frac{1}{3} 1 \otimes 1
\]

\[
I^d = I - I^v
\]  

(D.15)

or:

\[
I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})
\]

\[
I^v_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}
\]  

(D.16)

\[
I^d_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - \frac{1}{3}\delta_{ij}\delta_{kl}
\]

Eshelby’s solution for general spheroid \((a \neq b \neq c)\) has an implicit nature. To make it simpler for numerical implementations in this thesis, it is supposed that two out of three radii of the spheroid are equal\((a \neq b = c)\). In this case, the Eshelby tensor can be expressed explicitly and \( S \) depends only on the aspect ratio of the inclusion and Poisson’s ratio (Doghri and Ouaar, 2003; Mura, 1987). The components of the Eshelby tensor for an ellipsoid \((a \neq b = c)\) with an aspect ratio of \( \alpha = a/b \) for which the axis of length 2a is parallel to the 1 direction are (Clyne and
Appendix D. Material model for heterogeneous materials

Withers, 1995; Pierard et al., 2007):

\[
S_{1111} = \frac{1}{2(1-\nu_M)} \left\{ \frac{4\alpha^2 - 2}{\alpha^2 - 1} - u(\alpha) \left[ 1 - 2\nu_M + \frac{3\alpha^2}{\alpha^2 - 1} \right] - 2\nu_M \right\}
\]

\[
S_{2222} = S_{3333} = \frac{1}{4(1-\nu_M)} \left\{ \frac{3\alpha^2}{2(\alpha^2 - 1)} + u(\alpha) \left[ 1 - 2\nu_M - \frac{9}{4(\alpha^2 - 1)} \right] \right\}
\]

\[
S_{1122} = S_{1133} = \frac{1}{2(1-\nu_M)} \left\{ \frac{-\alpha^2}{\alpha^2 - 1} + u(\alpha) \left[ 1 + 2\nu_M + \frac{3}{2(\alpha^2 - 1)} \right] + 2\nu_M \right\}
\]

\[
S_{2211} = S_{3311} = \frac{1}{4(1-\nu_M)} \left\{ \frac{-2\alpha^2}{\alpha^2 - 1} - u(\alpha) \left[ 1 - 2\nu_M - \frac{3\alpha^2}{\alpha^2 - 1} \right] \right\}
\]

\[
S_{2233} = S_{3322} = \frac{1}{4(1-\nu_M)} \left\{ \frac{\alpha^2}{2(\alpha^2 - 1)} - u(\alpha) \left[ 1 - 2\nu_M + \frac{3}{4(\alpha^2 - 1)} \right] \right\}
\]

\[
S_{1212} = S_{1313} = \frac{1}{8(1-\nu_M)} \left\{ \frac{-4}{\alpha^2 - 1} - u(\alpha) \left[ 1 - 2\nu_M - \frac{3(\alpha^2 + 1)}{\alpha^2 - 1} \right] - 4\nu_M \right\}
\]

\[
S_{2323} = \frac{1}{4(1-\nu_M)} \left\{ \frac{\alpha^2}{2(\alpha^2 - 1)} + u(\alpha) \left[ 1 - 2\nu_M - \frac{3}{4(\alpha^2 - 1)} \right] \right\}
\]

(D.17)

The function \(u(\alpha)\) depends on the aspect ratio of the ellipsoid and is calculated for oblate \((\alpha < 1)\) and prolate \((\alpha > 1)\) as follows:

\[
u(\alpha) = \frac{\alpha}{(\alpha^2 - 1)^{\frac{3}{2}}} \left[ \alpha(\alpha^2 - 1)^{\frac{1}{2}} - \cosh^{-1}\alpha \right] \quad \alpha > 1
\]

\[
u(\alpha) = \frac{\alpha}{(1 - \alpha^2)^{\frac{3}{2}}} \left[ \cos^{-1}\alpha - \alpha(1 - \alpha^2)^{\frac{1}{2}} \right] \quad \alpha < 1
\]

(D.18)

For the limit case of \(\alpha \to 1\), the calculated Eshelby tensors for both oblate and prolate spheroids approach the tensor for spherical inclusion (Equation (D.12)). For a comprehensive solution of Eshelby’s inclusion problem the reader is recommended to refer to (Mura, 1987).
Bibliography


Research deliverables

The key deliverables of this research are listed in this section.

Journal Articles


Conference proceedings


Presentations in conferences


- Conference on Optimization Methods and Software, Cuba, 2017.


Poster contribution in conferences


Awards

Software

- OptForm v4.0 GUI was developed during this research for robust optimization and tailoring of scatter based on the methods introduced in this thesis.

*OptForm v4.0 GUI*
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Omid, It is our great pleasure to offer to you the PhD position Material property and process scattering forming of high strength steels. Congratulations, Our recruitment officer will contact you shortly.

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