Hochschule
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Stuttgart

Utilizing Supervised Learning for the Prediction of Bending Parameters

some hyped-up tagline

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February, 2023

A dissertation submitted in partial fulfilment of the requirements for the degree of M.Sc. in Software Technology.

Abstract

This is the abstract. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

Contents

List of Figures

List of Tables

List of Abbreviations

1

Introduction

Sheet metal forming has been used for centuries in different manufacturing industries to create a wide range of products for different applications. Sheet metal bending and stamping can be considered as the most important variants in the forming industry. (Cruz et al., 2021, p. 1) Therefore these have been continuously improved in recent decades to meet the growing demand especially in automotive and aircraft industries with the goal to reduce energy efficiency and emissions. (Zheng et al., p. 4)

Sprinback is a common phenomenon in sheet metal forming processes. It is a deformation of the sheet metal that occurs when the sheet metal is bent. Therefore, predicting the spring back is important to reduce the number of trial and error cycles in the manufacturing process. (Cruz et al., 2021, p. 1) Sheet metal forming is a complex process that involves a large number of variables and parameters Therefore, it is difficult to predict the spring back accurately, which makes it an interesting case for machine learning.

In order to predict springback with minimium errors, this thesis build and evaluates different machine learning models to predict the springback of a sheet metal. The models are evaluated based on the mean absolute error (MAE) and the root mean squared error (RMSE). The best model is then used to predict the springback of a sheet metal with different parameters.

1.1 | Problem Statement

"There are two major types of supervised machine learning problems, called classification and regression." (**?**, p. 34)

"For regression tasks, the goal is to predict a continuous number, or a floating-point number in programming terms (or real number in mathematical terms). Predicting a person's annual income from their education, their age, and where they live is an example of a regression task. When predicting income, the predicted value is an amount, and can be any number in a given range. Another example of a regression task is predicting the yield of a corn farm given attributes such as previous yields, weather, and number of employees working on the farm. The yield again can be an arbitrary number." (Müller and Guido, p. 34)

2

Theoretical Foundations

2.1 | Sheet Metal Bending

The process of sheet metal bending involves using force to shape sheet metal into a desired form. It is usually used to produce large quantities of components at a low cost in various industries. (Dib et al., p. 1) One aspect which makes the the process of sheet metal forming complex is that it is characterized by highly non-linear behavior due to large deformations of the metal sheet and is therefore hard to predict. As a result, traditional methods often rely on trail and error approaches, (Dib et al., p. 1), such as creating 'technology tables' which contain bending parameters and resulting spring back data. These tables are created by performing a lot of different experiments with different bending angles and metal sheets. This process is time and cost intensive and therefore often not suitable for the production of high-volume and low-cost components.

2.1.1 | Sheet Metal

Sheet metal is any form of metal that has a relatively large length to thickness ratio , their thicknesses are typically from 0.4 mm to 6 mm. Above is considered to be plate and below is considered to be foil. Sheet metal is usually manufactured by flat rolling. Low-carbon steel is the most commonly used type of sheet metal. Its low cost and has a good formability as well as its sufficient strength for most applications. (Groover, p. 405) Therefore it is used in this work as well. Sheet metals play a vital role in many industries. A significant number of consumer and industrial products such as automobiles contain sheet metal parts. Most sheet metal forming operations are performed on machines called presses and these operations are known as pressworking. These presses usually use tooling called punch and die or stamping die . Three main processes are categorize the sheet metal forming processes: cutting, bending and drawing, where bending is the the most common and only relevant process for this thesis . Bending and drawing are used to shape sheet metal parts into their required forms. (Groover, p. 405)

2.1.1.1 | Bending

Bending is a forming operation that is used to change the shape of a sheet metal by apply a load to it. The load is applied in way that exceeds the yield strength of the metal, but is below its ultimate tensile strength, which allows the metal to bet permanently deformed into a new shape. (Baig et al., 2021, p. 1)

During the bending process, the metal on the outside of the neural plane (the plane that is perpendicular to the bending axis) is stretched, while the metal, while the metal on the inside is compressed. This results in a curvature of the sheet metal in the direction of the applied load. (Baig et al., 2021, p. 3) The amount of curvature that is achieved in the bending process is determined by the amount of load applied, the thickness and properties of the metal, and the location and length of the neutral plane. By controlling these factors, it is possible to achieve precise and consistent results in the bending of sheet metal.

Figure 2.1 shows the neutral plane after the bending operation, it is visible, that is is closer to the inside of the bend than to the outside of the bend. The arrows show where the metal was stretched and where it was compressed.

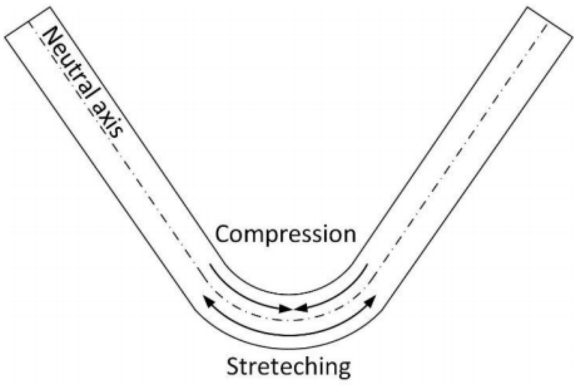


Figure 2.1: Bending plane, compression and stretching of sheet metal (Baig et al., 2021, p. 3)

2.1.1.2 | Air Bending

Air bending is a variant in the V-Bending process which is performed using puch-and-die tooling. (Groover, p. 416) As illustrated in Figure 2.2 the punch pushed the sheet metal which is placed in the die down. In other bending forms the die is also used to shape or form the metal in a specific way. This is where the term "die" comes from in this context. (Source missing) In other bending methods the die is fully closed and provides a form where the sheet metal is pressed into. In air bending this is not the case, but the term stays the same. (Source missing)

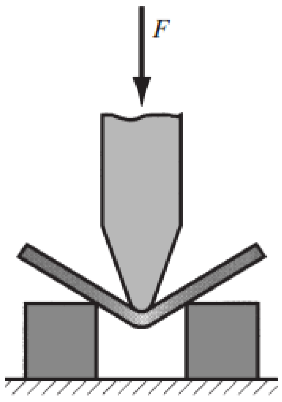


Figure 2.2: Air bending (Groover, p. 416)

Air bending is commonly used in automotive industry to manufacture sheet metal parts. (Kim et al., p. 342) In this process the punch sheet metal comes in contact of the outside edges of the die , as well as the punch tip, but it does not come in contact with the die surface. It is typically the preferred bending method because, its high flexibility because it is possible to achieve different bending angles using the same punch-and-die tooling. (Miranda et al., p. 3)(Cruz et al., 2021, p. 1)

Today sheet metal bending machines like air bending machines are usually equipped with "copmputer numeral control" (CNC) systems that can automatically control the bending process and produce the desired shape." (Miranda et al., p. 3) The air bending process is shows strong nonlinear behavior, considering its parameters and their interrelationships. (Miranda et al., p. 3)

2.1.1.3 | Spring Back

When the punch and therefore the bending pressure is removed at the end of the deformation operation, elastic energy remains in the bent part. This elastic energy is released, and the metal sheet partially returns to its original shape. (Groover, p. 113-114) In metal forming this process is called spring back and is illustrated in Figure 2.3. The solid line shows the metal plate in its original for when the punch was still applied. The dashed line shows the metal plate after the punch was removed. The metal plate is partially returned to its original shape. The angle before the spring back is usually denoted as α_f and the angle after spring back as α_i. The spring back ($\Delta\alpha_{SB}$) is therefore the difference between α_f and α_i as show in equation 2.1. (Cruz et al., 2021, p. 6)

$$\delta\alpha_{SB} = \alpha_i - \alpha_f \tag{2.1}$$

To address this issue there are several methods to compensate the spring back. For example one common method is over bending, which means that the punch angle and radius are fabricated smaller than the specified angle. (Groover, p. 114) Prerequisite for all compensation methods is that the spring back is known therefore the accurate prediction of the spring back play an important role in the manufacturing process.

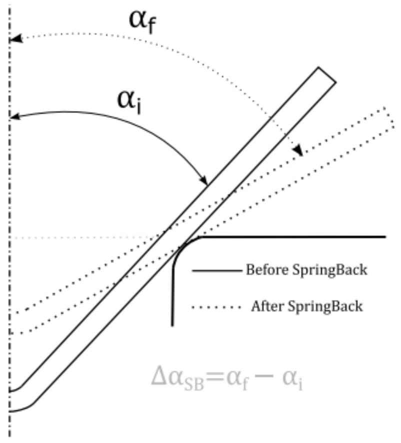


Figure 2.3: Spring back (Cruz et al., 2021, p. 5)

2.2 | Machine Learning

Machine learning also called Machine Learning (ML) is a field of study that involves using statistical and computational techniques to analyze and learn from data. (Müller and Guido, p. 1)

2.2.1 | Supervised Learning

Supervised learning is a type of machine learning where we have a set of input/output pairs that we use to train a model to predict an outcome for a given input. We use this model to make predictions on new, unseen data, the training set. It consists of the input/output pairs, needs to be created manually, but once the model is trained, it can automate and potentially improve upon tasks that would be time-consuming or difficult for humans to perform. (Müller and Guido, p. 25)

2.2.2 | Regression

There are two main types of supervised machine learning problems: classification and regression. For regression problems it is the goal to predict a continuous numerical value. This can be a real number in mathematical terms or a floating-point number in programming terms. (Müller and Guido, p. 226) Classification problems involve predicting a class label, which is a choice from a predefined list of possible options. (Müller and Guido, p. 25)

Predicting the spring back is a regression problem because the spring back is a continuous-valued output. Therefore, this work focuses on supervised learning for a regression problem and does not further consider classification problems.

2.2.3 | Overfitting and Underfitting

In supervised learning, the goal is to construct a model using training data that can accurately predict outcomes for new, unseen data that shares similar characteristics as the training data. The ability of a model to make accurate predictions on unseen data is referred to as generalization. The objective is to develop a model that generalizes as effectively as possible. (Müller and Guido, p. 35)

The effectiveness of an algorithm on new data is determined by its performance on a test set. Simple models tend to generalize better to new data. Overfitting occurs when a model is too complex for the amount of information available and does not generalize well, while underfitting occurs when a model is too simple and does not perform well on the training set. The goal is to find the simplest model that captures the variability in the data. (Müller and Guido, p. 35)

2.2.4 | Bias-Variance Tradeoff

Bias measures how well the central tendency of a learner's model approximates the actual function it is trying to learn. If the model consistently learns the true function accurately, it is unbiased. Otherwise, it is biased. (Neal, p. 7-8) In essence the bias is the differences between the predicted values by the model and the actual values. A high bias indiactes a model with a complex fit to the training data and therefore overfits (Neal, p. 20)

Variance measure how much the model's prediction vary, when trained on different subsets of the data. That means that a model with low variance generalizes one new data. A high variance indicates that the model as a complex fit to the data and therefore is overfitting the training data. This means it will not perform well on new data. (Neal, p. 7-8)

Both, high variance and high bias are undesirable properties for a model. The goal is, to find a model with low bias and low variance. This is called the bias-variance trade off. (Neal, p. 9)

Regularization

Regularization refers to a group of techniques that force a model to be simpler. this usually results in a slight increase in bias but a substantial decrease in variance (**?**, p. 12).

The regularization method used in this thesis and in general the most popular are L1 and L2 regularization. In order to construct a regularized model, the objective function is altered by including a penalizing term that increases the value as the model becomes more complex (**?**, p. 12)

2.2.5 | Ensemble Learning

Ensemble techniques in machine learning to involve the construction of multiple models , called "learners," for a given task. The primary goal of these methods is to improve the accuracy and performance of the model by combining the predictions of multiple learners. Ensemble techniques differ from single classifier methods by constructing multiple models and combining them using a voting strategy in order to highlight different aspects of the data. This can potentially lead to improved overall performance. (Shaik and Srinivasan, p. 253)

2.2.6 | Evaluations and Improvements of Models

2.2.6.1 | Cross Validation

Cross-validation is a method of evaluating the performance of a model by training multiple models on different subsets of the data and evaluating their performance. The most common version of cross-validation is k-fold cross-validation, in which the data is divided into k folds , and k models are trained, each using a different fold as the test set and the remaining folds as the training set. The accuracy of each model is then evaluated, and the average accuracy across all k models is used as an estimate of the generalization performance of the model. This process helps to reduce the variability in model performance due to the specific choice of training and test sets, and is therefore considered to be a more stable and reliable way to evaluate the performance of a model. (Müller and Guido, p. 252-260)

2.2.6.2 | Grid Search

Each machine learning method has a number of parameters that can be tuned to improve the performance of the model. Parameters are often not known in advance and must be tuned to the data. This is a common task in machine learning and therefore there are standard methods like grid search to find the best parameters. Grid search is a method of systematically working through multiple combinations of parameters (called grid), cross-validating as it goes to determine which tune gives the best performance. (Müller and Guido, p. 260-275)

2.3 | State of research

With the availability of data there has been an increased use of Machine Learning **ML!** (**ML!**) in sheet metal forming with the goal to reduce costs and increase manufacturing quality. Bock et al. (Cao et al.) lesen The ML algorithms can be divided into the main categories supervised learning, unsupervised learning and reinforcement learning. (Liu et al., a) Supervised learning is generally used in classification problems and regression problems while unsupervised learning is used to find patterns in data (Cruz et al., 2021, p. 2).

Spring Back Prediction Using Unsupervised Learning

Artificial Neural Networks Artificial Neural Network (ANN)s are widely used in sheet metal forming because of their high accuracy and generalization performance. (Cruz et al., 2021, p. 2) (Narayanasamy and Padmanabhan) which compared regression and neural network modeling for predicting spring back of steel sheet metal during the air bending process. They observed that ANN was able to predict the spring back with higher accuracy. But they had a sample size of 25 and suggested further research. (Inamdar et al.) developed an ANN for the air bending process to predict spring back as well as the punch travel to achieve the desired angle in a single stroke. (Kazan et al.) developed an ANN trained with FEM simulation data to predict the spring back for the wipe-bending process.

Because ANNs need a large amount of data to train the model generating the data with real machines is a time-consuming process. Therefore, it is common to use ANNs trained with Finite Element Method Finite Element Method (FEM) simulation data. *Was sind die Nachteile von FEM? Warum nutze eich "echte" Experimente?*

Spring Back Prediction Using Supervised Learning

Liu et al. (2019) used a Support Vector Machine Support Vector Machine (SVM) to predict the spring back of micro W-Bending operations. Liu et al. (b) Dib et al. (2019) compared different ML techniques (logistic regression, SVM, KNN , ANN, random forest, decision tree, naive Bayes, MSP) to predict the spring back and the occurrence of defects in sheet metal. (Dib et al., p. 1) The authors conclude that the MLP and the SVM are the best performing algorithms and suggest further studies of ML regressions models and kriging regression models. (Dib et al., p. 13)

3

Research methodology

The research method used in this thesis follows the design science research (DSR) approach (von Rennenkampff et al., 2015, p. 17). DSR is a research paradigm in which the designer tries to create artifacts to answer questions for problems.

DSR is a research paradigm in which the designer creates artifacts and uses them to answer questions for problems and generate new scientific knowledge. The designed artifacts are both useful and fundamental to understanding the problem (Hevner and Chatterjee, 2010, p. 10)

Design, according to Peffers et al. (2007), is the creation of an applicable solution to a problem (Peffers et al., 2007, p.47)

According to Hevner et al. (2010) design" is both a process ("a set of activities") and a product ("artifactt"). (Hevner and Chatterjee, 2010, p .78) The design-oriented research approach as a methodological framework seems well suited to answer the research questions. Predicting spring back and bend deduction is a relevant problem in business practice. Also, the conception and implementation of machine learning models is a design activity.

The term artifacts is intentionally broad and can take on different forms. In this work, the artifact is different machine leaning models which are applied on the generated data. DSR can be implemented in various ways, a prominent example is provided by Peffers et al. and shown in Figure 3.1 The approach comprises six steps, which are dived into the superordinate phases "Build" and "Evaluate". This thesis follows these phases.

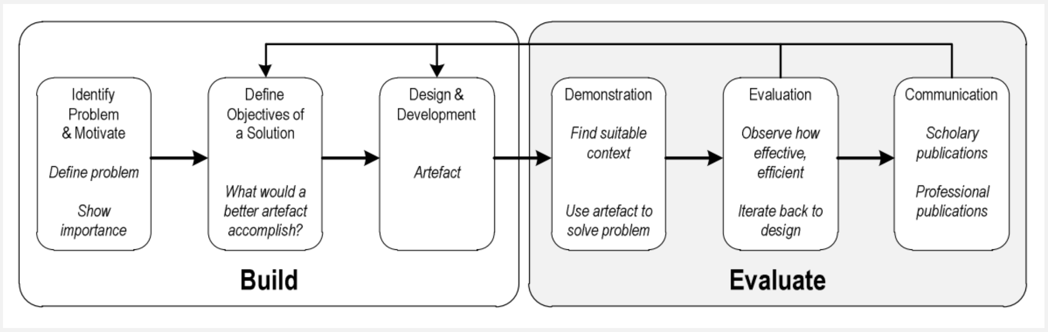

Identify Problem & Motivate
Define problem
Show importance
Define Objectives of a Solution
What would a better artefact accomplish?
Design & Development
Artefact
Demonstration
Find suitable context
Use artefact to solve problem
Evaluation
Observe how effective, efficient
Iterate back to design
Communication
Scholary publications
Professional publications
Build
Evaluate

Figure 3.1: Design Science Research Approach according to Peffers et al. Picture: (Sonnenberg and vom Brocke, 2012, p. 72)

Also, I'm not quite clear on the distinction between Demonstration and Evaluation in your context, since Demonstration would most likely be showing that your model predicts springback reliably, which refers back to evaluation?

Activity 1 - Problem identification and motivation This activity includes defining a specific research problem and the value of a potential solution. The problem is used for the development of the artifact. To reduce complexity, the problem should be divided into sub-problems. For problem-solving, explicit methods such as system requirements gathering or an implicit method such as programming and/or data analysis. (Peffers et al., 2007, p. 52)

Activity 2: Define the objectives for a solution The goals of a solution are derived from the problem definition. These are derived in the context of what is possible and feasible. Objectives can be quantitative or qualitative. Objectives should be derived from the problem specification and are thus based on the previous step. For knowledge about previous solutions and their effectiveness are required (Peffers et al., 2007, p. 55)

Activity 3: Design and development This step involves the creation of the artifact. An artifact can potentially contain models, methods or constructs, it can be anything that contributes to the solution of the research question. This step includes the definition of the functionality and architecture of the artifacts, followed by the creation of them. (Peffers et al., 2007, p. 55)

Activity 4: Demonstration The use of the previously created artifactt is demonstrated for one or more problems. This requires effective knowledge of the artifact. (Peffers et al., 2007, p. 55)

Activity 5 - Evaluation It is observed and evaluated how well the developed artifact provides a solution to the defined problems in activity 1. Knowledge of relevant metrics and methods of analysis is assumed. Depending on the nature of the problem, the evaluation can take different forms. A comparison of the functionality of the artifact and other solutions can be considered. Furthermore, quantified quantified parameters can be used to measure the performance of the artifacts (Peffers et al., 2007, p. 56) Hevner et al. suggest five different evaluation methods: Observational methods, analytical methods, experiments, testing of the artifact and descriptive methods (Hevner et al., 2004, p. 87)

Activity 6 - Communication The problem and the artifactt and its benefit are communicated externally (Peffers et al., 2007, p. 56) Hevner et al. describe in a conceptual framework guidelines for the

3.1 | Design Principles

Design Principles (DP) are seen as a central part of design-oriented research. (Gregor et al., 2013, p. 348) Design principles are characterized as "principles of form and function" as well as "principles of implementation" of an artifact. (Gregor and Jones, 2017, p.8) They are used to close the gap between researchers and user and allow prescriptive research on systems. They are used to capture knowledge about the artifact. (Sein et al., 2011, pp. 37-56). Koppenhagen et al. suggest generating design principles by grouping requirements for the solution and then creating core requirements, which can which can then be DPs. (Koppenhagen et al., 2012, p. 6)

3.2 | Evaluation of Machine Learning Models

Evaluating ML models is different from evaluating other software artifacts for several reasons. One of them is that data-driven software components, like ML models, have functionality that is not completely defined by the developer but is instead learned from data. Therefore, using machine learning presents new challenges compared to traditional software engineering (Siebert et al., 2022, p. 2).

In the field of software engineering, there are already standards that define the quality of software systems and its components. Most notable the ISO/IEC 9126 standards, which provide a quality model which is widely adapted in software engineering (Source). For above-mentioned reasons these standards are not suitable to evaluate machine learning models, therefore Siebert et al. (2022) note that they need to be adapted. They reinterpreted and extended these existing quality models to the ML context (Siebert et al., 2022, p. 1).

In order to define the Design Principles for the ML models this work, the considerations of (Siebert et al., 2022) are used. This enables a systematic process in order to assess the quality of the developed models.

In the work of Siebert et al. (2022), several quality attributes are considered, including Correctness, Relevance, Robustness, Stability, Interpretability and Resource Utilization. Alongside these attributes, the authors also provide a set of quality measures to evaluate the models, but these are nor complete and are only used as a starting point for the evaluation of the models in this work, further evaluation is described in Chapter 5.

It is important to note, that the mentioned quality attributes and measures should not be seen as a complete set of quality attributes and measures for ML models. Other studies, such as **?** have proposed additional sets of quality attributes. These additional perspectives will also be considered in the evaluation of the models, but only as a supplementary means of evaluating model performance.

Attributes like Security, Fairness and Privacy (**?**, p. 3) are not considered in this work, as they are difficult to measure and my not be relevant for the use case of this work.

3.3 | Goal Question Metric Approach

To make the defined quality attributes measurable, the “Goal-Question-Metric”-approach GQM was chosen in this work. It is one of the most common approaches in DSR and is divided into three levels. (Basili et al., 2002, p. 3)

1. Conceptual level (goal): "A goal is defined for an object, for a variety of reasons, with respect to various models of quality, from various points of view, relative to a particular environment." (Basili et al., 2002, p. 3)

2. operational level (question): "A set of questions is used to characterize the way the assessment/achievement of a specific goal is going to be performed based on some characterizing model. Questions try to characterize the object of measurement (product, process, resource) with respect to a selected quality issue and to determine its quality from the selected viewpoint." (Basili et al., 2002, p. 3)

3. quantitative level (metric): "A set of data is associated with every question in order to answer it in a quantitative way." (Basili et al., 2002, p. 3)

Objectives, questions and metrics can be presented in a hierarchical structure.

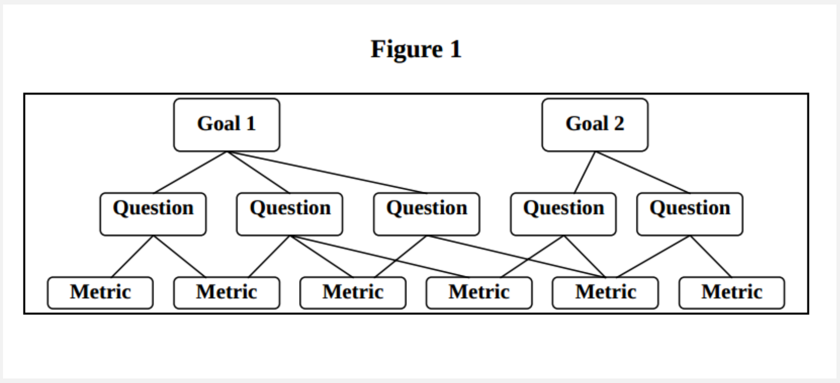


Figure 3.2: Goal-Question-Metric Ansatz (Basili et al., 2002, p. 3)

4

Build

4.1 | Design Principles

The following design principles is a selection of **?**'s quality parameters for ML models. In this Design Science Research (DSR) work the artifacts are ML models therefore these design principles are used to evaluate them.

Design Principle 1: Correctness

Does the artifact predict the spring back of a sheet metal with a high accuracy and correctness? With progression in manufacturing there is a growing demand for high-quality products, that means that the meta parts needs to be produced with high precision and accuracy. Here the sprin back is an undesired side effect which need to be mimimized. (Baig et al., 2021, p. 1) Sheet metal forming in manufacturing need a high level of quality and precision. Therefore, the spring back of a sheet metal is an important parameter to consider. (Cruz et al., 2021, p. 1) Predicting spring back is important to reduce the number of trial and error cycles in the manufacturing process. Also predicting spring back is complex because of many variables and parameters and often not all of them are known. Therefore, a machine learning model should predict the spring back of a sheet metal with a high accuracy and correctness. When using the ML model small errors in the prediction can cause fitting problems in the manufacturing process.

Design Principle 2: Appropriateness

Is the artifact appropriate for the given problem? While selecting a model it is important that it fits the problem/task and can deal with the given data. (**?**, p. 16)

Design Principle 3: Relevance

Does the artifact achieve a good bias-variance trade-off?

In addition to measure the correctness it is important to understand "why" the learner has this performance. This is important to understand the limitations of the model and to improve it. Therefore, it is important to understand the bias-variance trade-off. (Zhou, p. 50) Bias measures the differences between the learnesrs expected prediction and the ground-truth label. This results in the fitting ability of the learner. Variances measures the change of learning performance of the learner because of changes in the training set. This results in the impact of data disturbance on the results. (Zhou, p. 51)

Design Principle 4: Robustness

How well does the artifact handle outliers, noise and missing data? Using real-world data noice is a common problem and can have a negative impact on the performance of the learner. Therefore, it is important to measure how good the artifact performs when dealing with impact data. Sáez et al. proposed a new measure to establish the expected behavior of a learner with noisy data trying to minimize the problems: the Equalized Loss of Accuracy (ELA). (Sáez et al., p. 3)

Design Principle 5: Stability

Does the artifact generate repeatable results when trained on different datasets?

Design Principle 6: Interpretability

Is the artifact easy to understand and explain?

It should be noticed, that there are many parameters and variables involved in the sheet metal forming process. That makes the process design quite complex, particularly in the production of components which require several stages, and thus more than one set of tools. (Dib et al., p. 1) A model which allows conclusions how the results where generated is better.

Design Principle 7: Resource utilization

How many resources does the artifact need to train and predict?

Conventional processes are often based on empirical trial and error approaches. (Dib et al., p. 1) A common approach is to experimentally create so named 'technology tables' which contain the bending parameters and the resulting spring back. (Quelle: Hochstrate?) This process is time and cost intensive and therefore often not suitable for the production of high-volume and low-cost components. Therefore, one of the benefits of using machine learning should be the reduction of the number of trial and error cycles in the manufacturing process. Furthermore, training the model should take not too much time and resources. As mentioned before often FEM-simulation are used to virtually try out metal forming processes. However, fully exploring the design space is computationally expensive and often not possible. (Dib et al., p. 3) The number of experiments can be reduced using a meta-model like ANN. (Dib et al., p. 3) A approach fully based on ML should perfor

4.2 | Dataset generation

For the dataset generation, bending experiments were performed on metal sheets with different thicknesses. The material used is cold rolled steel sheets of the norm DIN EN 10130. The thicknesses used were 0.5mm, 1mmm and 2mm. The material was used because it is commonly used in bending processes and its high availability. In previous tests, it was observed, that the spring back are well observable with this material. Using this material, 200 single bending pieces of the dimension 20×100 mm have been cut. Each piece was bend one time using a *Zwick* three-point-bending machine.

Python script where developed to covert the output data format from the machine to CSV files. The following describes the experimental setup used for the experiments performed.

4.2.1 | Experimental setup

The experimental setup comprises of a three-point bending machine, consisting of a punch and die, with the latter lacking a bottom, which allows only air bending metal-sheet. The material testing machine utilized is the *Zwick MX 25A*, which is equipped with a load cell and a displacement sensor. The load cell measures the force applied to the sheet (in N), while the displacement sensor measures the displacement of the punch (y_p). The punch is mounted on the top of the machine and is stationary, while the die is mounted on the bottom and is the part which can be moved. The machine is operated via a computer and the *ZwickRöll TestXpert* software, which is used for both machine control and data collection.

The experimental setup and the process parameters are shown in Figure 4.1 where V is the die opening which is the opening between the the two points between the sheet metal is placed. The parameters y_p is the punch penetration, which is the distance the punch is moved into the sheet. The parameter t is the thickness of the metal sheet while α is the corresponding angle after the bending process.. Parameter r_p is the punch radius which is the radius of the tip of the punch, which was never replaced in all experiments and therefore remains constant.

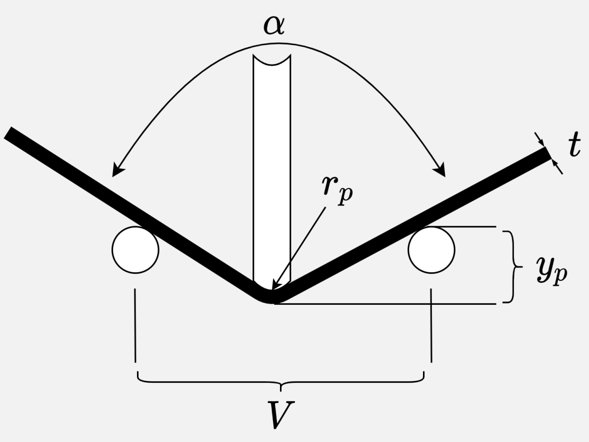


Figure 4.1: Process parameters: Sheet bending angle (α), sheet thickness (t), punch penetration (y_p), die opening (V) and punch radius (r_p)

In order to get consistent results, a number of constant and variable parameters were chosen. The parameters include the punch-and-die tooling made of steel where die punch had a radius (r_p) of 5 mm and and die radius (r_m) of 10 mm. The die opening V was varied between 10 and 50 mm and the punch penetration y_p was varied between 0 and 20 mm.

The machine was configured to move the punch with a constant speed of 100 mm/min until it measured a resistance of 1 N. That meant, that the punch reached the metal plate and the actual bending process can start. After a hold time of 1 second the punch was moved with a slower speed of 8 mm/min until the specified punch penetration was reached. The length and width of the metal sheet was 100 mm and 20 mm respectively.

Using the *ZwickRöll TestXpert* software, the following parameter where set for the experiment, which are summarized in Table **??**. The punch of the machine was never replaced and therefore the radius of the punch remained 5 mm. The width and length of metal sheets where 100 mm and 20 mm respectively. The punch speed was set too 80 mm/min and the hold time was set to 1 second, latter is the time the punch stays at the end of the metal sheet and has to be a least 1 second which is a limitation of the machine. After the bending process, the punch was moved back to the starting position with a speed of 8 mm/min. This speed was chosen significantly lower than the speed used for the bending process in order to accuratly measure the spring back to avoid any damage to the metal sheet. The punch force threshold was set to 1 N, which means, that the punch starts bending the metal a soon as it touches the sheet metal.

Parameter	**Values**	**Unit**
Punch radius	5	mm
Sheet width	20	mm
Sheet length	100	mm
Punch speed	80	mm/min
Punch speed up (after bend)	8	mm/min
Hold time	1	s
Punch force threshold	1	N

Table 4.1: Constant parameters in th eperimental setup

The following parameters where varied in the experiments, which are summarized in Table **??**. The die opening V was varied between 10 and 50 mm and the punch penetration y_p was varied between 0 and 20 mm. The thickness of the metal sheet t was varied between 0.5 and 2 mm. Also the punch penetration y_p was varied between 0 and 20 mm.

Parameter	**Values**	**Unit**
Punch penetration y_p	2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20	mm
Die opening V	10, 20, 30, 40, 50	mm
Thickness t	0,5, 1, 1.5, 2, 2.5, 3	mm

Table 4.2: Varying parameters in the experimental setup

4.2.2 | Measuring The Spring Back

The output data contained different data points, which were used to calculate the spring back. Important parameters for the calculation are the force, punch penetration and testing time. As shown in Figure 4.2 at the y_p maximum the punch penetration and the force are maximized as well. The punch stays at that position for 1 second and then moves back with a slower speed. This hold time a limitation of the machine and can not be changed. After the punch is moved back, the force is reduced and the punch penetration is reduced as well, until the punch is at the initial position. For a short time after the lift, the load cell still measures a force. That is because the metal sheet springs back and the punch is still in contact with the sheet. This was measured using a python script, the green and the yellow point represent the resulting spring back distance.

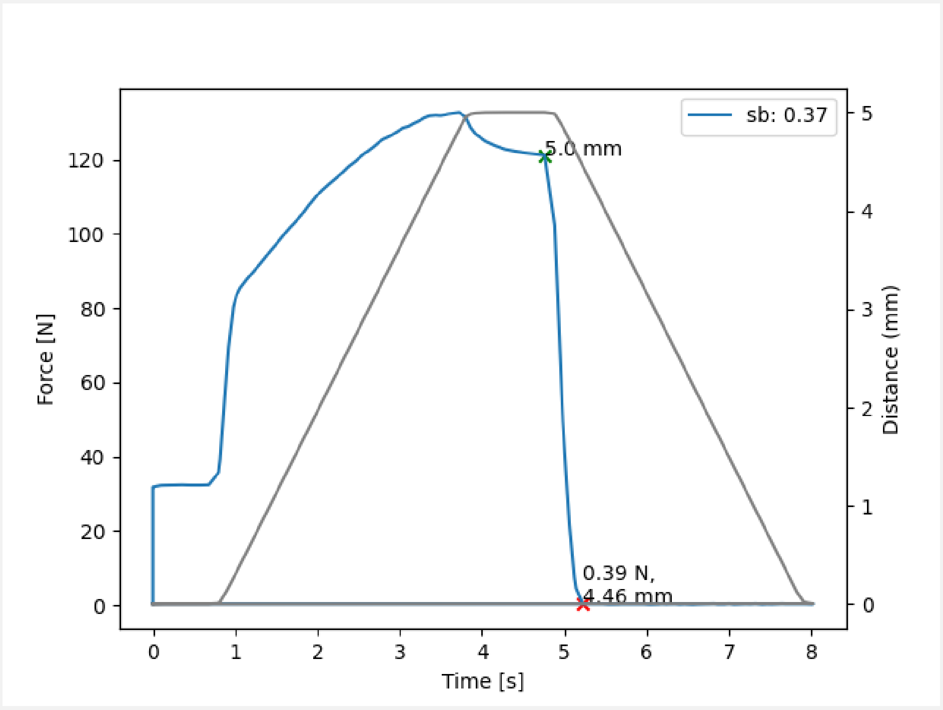


Figure 4.2: A steel metal sheet was bent with a punch penetration of 5 mm the spring back is 0 .37 mm. The blue line shows the force and the blue line shows the punch penetration.

Notes

- *Why is an initial force measured before the punch is moved?*
- *TODO: Add legend for grey line (punch penetration) and blue line (force))*
- *TODO: More dpi for the image*

4.2.3 | Adding Features to the Dataset

The current dataset includes three independent and one dependent feature. These features will be discussed in more detail in the following section. On goal was it to enhance the dataset with more features, this would improve the performance of models and provide greater insight into the bending process.

On potential candidate for a new feature is the tension. A drawing test was carried out for this which is described more in detail in the next section...

Notes

- *TODO: Add drawing test*

4.2.4 | Dataset Exploration

4.2.4.1 | Features

The output data of the bending machine contained 26 features which can be found in the appendix. Out of these features only the standard power and the distance y_p and the force are relevant for calculating the spring back which was described in the last section 4.2.2. The final dataset therefore contained 3 features plus the added spring back. In total 396 data points where crated using the described approach. An example of the dataset is shown in Table **??**.

With 100 estimators in Random forest (RF) a mean squared error (MSE) of 0.15 and Root Mean Squared Error (RMSE) 0.39 was achieved. Figure 4.3 compares and visualizes the relative importance of the features used for training the model. As shown, the thickness is the most important feature followed by distance and die open. The results show, that all three featured are relevant for the outcome and so no feature can be removed from the dataset to get a better performance of the model.

index	Distance	Spring Back	Thickness	Die Opening
1	5	0.6667	2.0	50
2	15	0.9164	2.0	50
3	10	0.6829	2.0	50
...	...	...	...	...
396	5	0.6667	3.0	10

Table 4.3: Varying parameters in the experimental setup

.6.6

Figure 4.3: Relative feature importance

4.2.5 | Visualizing The Data

Figure 4.4 shows the spring backs for the $V30$ dataset. In general, it can be seen that the spring backs is less for lower thicknesses and higher for higher thicknesses. Also, the spring backs for lower thickness tend to go up with increasing punch penetration, while the spring backs for higher thicknesses tend to go down with increasing punch penetration.

The factors for the behavior of the spring back can't be fully understood with the available data, which makes it a good case for machine learning.

Notes

- *TODO: Add better picture. Ordered by t, better colors, scienceplot, punch penetration instead of spring back*
- *Experimental setup methodology like Jonas.*

4.2.5.1 | Data Quality

The dataset was created in an experimental environment and the samples where carefully measured. Therefor the dataset does not contain many outliers and the data quality is high.

As shown Figure 4.6 data for all possible V and t combinations where collected. Also there the y_p values are evenly distributed and always range from 2.5 to 20 mm. Fur-

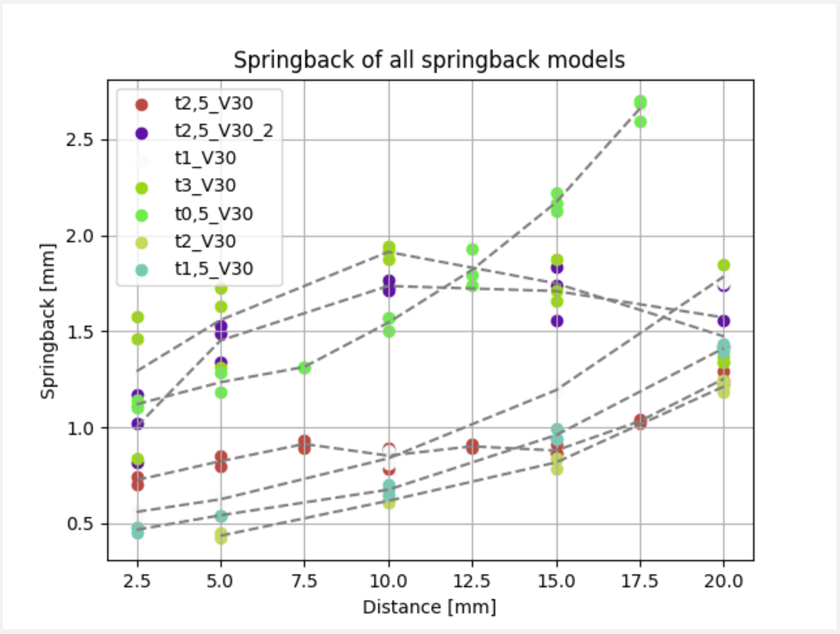


Figure 4.4: Springbacks for $V30$

thermore, the dataset was continuously extended with new data points throughout the project. During this process multiple outliers and wrong measurements where detected and removed.

It has to be noted that therefore the dataset does not model a real-world scenario, where the data quality is not as high as in the experimental environment. This has been considers in section 5.3 Robustness, where artificial noise is added to the dataset to test the robustness of the models.

Notes

- *The Figure feature importance was created using a random forest so it does not belong here. Find a*
- *different method to visualize the feature importance.*
- *Add example picture of spring back plots*
- *It is not yet decided if artificial noise will be added to the dataset.*
- *Add some data quality measure?*

4.2.6 | Data Preprocessing

The three independent features y_p, V and t as well as the dependend feature $spring\_back$ were normalized using the `MinMaxScaler`from the scikit-learn library. The `MinMaxScaler` scales the data between 0 and 1. The scaler was fitted on the training data and then used to transform the test data. The scaler was saved to be used for the prediction of the spring back of the real world data.

Scaling is only done on the training data, because cross-validation is later used to tune and evaluate the models. Scaling the whole data set before the split would lead to data leakage because the min and max values of the test data would be used to scale the training data. How the data was split can be seen in Figure 4.6.

Because cross-validation is later used to tune and evaluate the models the data was split before the scaling. How the data was split can be seen in Figure 4.6.

Notes

- *TODO: Outlier handling is not done and mentioned. Is this necessary?*
- *TODO: Use more sophisticated scaling methods, not only min-max scaling. For example for V classfication*

4.2.7 | Computational Setup

For training the machine learning models a ThinkPad X1 Carbon 2019 with an Intel Core i7-10610U CPU @ 1.80GHz and 16 GB RAM was used. The operating system used is Ubuntu 20.04.2 LTS. The code for the model is written in Python 3.8.5 using the IDE PyCharm. The libraries used are mentioned in Table **??**.

Library	Version
numpy	1.23.2
pandas	1.5.1
matplotlib	3.6.2

Table 4.4: Libraries used for the machine learning models.

Looking at the correlation matrix shown in Figure 4.5 it can be seen, that the distance and the spring back are more correlated than the other features. This is expected, because the punch penetration y_p is the main factor which influences the spring back. The other features are not correlated with each other, no multicollinearity is present which is good for the machine learning models.

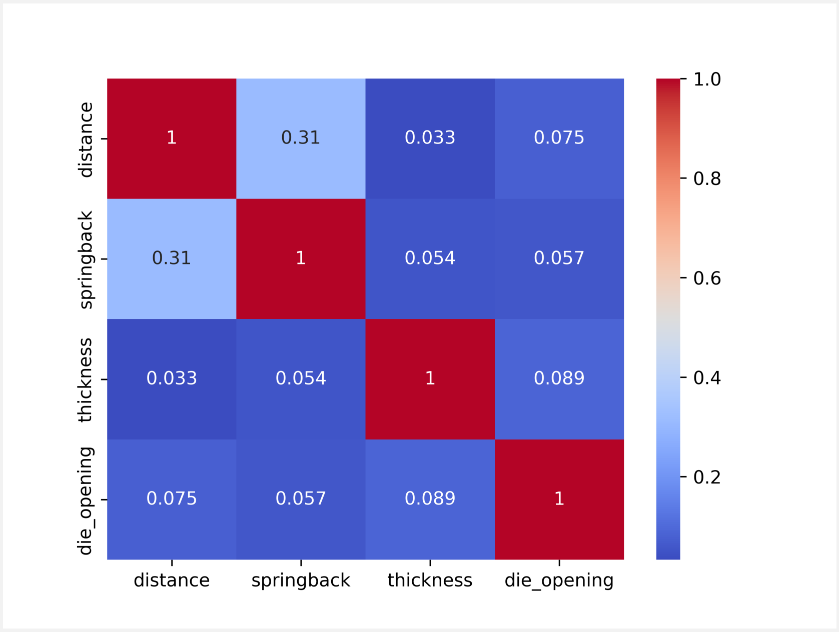


Figure 4.5: Correlation matrix

4.3 | Model Selection

4.3.1 | Support Vector Regression (SVR)

Support Vector Machines SVM are usually used for classification problems . The SVM algorithm is used to find a hyperplane in an N-dimensional space (N - the number of features) that distinctly classifies the data points. (Awad and Khanna, p. 42) Predicting the spring back is a regression problem, so the SVM algorithm need to be generalized of classification problems, where the model returns continuous values instead of finite set of values. This is done by using the Support Vector Regression (SVR) algorithm, which is inspired by SVM and uses the same principles. It fits a model to data using only residuals smaller in absolute value than a certain constant called ϵ-sensitivity

This is done by creating a "tube" of ϵ width around the data, with points inside the tube not being penalized and points outside the tube being penalized based on their distance from the predicted function. This is done similar to how SVMs penalize points in classification. Like SVM, SVR fins a well-fitting hyperplane to a kernel-induced feature space to achieve good generalization performance using the original features. (Montesinos López et al., p. 369)

Kernel Trick

The kernel trick is a method to transform the data into a higher dimensional space, where the data is linearly separable. This is done by using a kernel function, which is a function that maps the data into a higher dimensional space. Two methods are usually used for SVMs, the polynomial kernel and the radial basis function, also known as gaussian kernel. (Müller and Guido, p. 97-98) In practise the mathematical details behind these kernels are not important, but it is important to know that they are used to transform the data into a higher dimensional space, where the data is linearly separable.

4.3.2 | Multi Linear Regression

4.3.3 | Polynomial Regression

4.3.4 | Decision Trees

Decision Tree (DT)s are a commonly utilized type of model for categorizing and predicting outcomes. They construct hierarchy if rules to solve classification or regression problems (Müller and Guido, p. 70).

In DT models, the data is divided into multiple segments based on specific feature values. This division creates various subsets of the dataset, with each sample being a part of one subset. The last subsets are referred to as terminal or leave nodes while the intermediary subsets are known as internal nodes or split nodes. To predict the outcome in a particular leaf node, the mean outcome of the training data present in that nodes is taken into account (Molnar, 2020, p. 76).

4.3.5 | Random Forest Regression

A commonly used method in machine learning. The goal is to solve classification or regression problems by predicting the value of a output variable by one or multiple input variables. (Shaik and Srinivasan, p. 253) To build a DT the source dataset represents the root node of the tree this data set is split into leafs (children) by using a set of spitting rules until each leaf in the DT is "pure" and only contains one target value. Depending on the use cases this is a single class or a single regression value. (Müller and Guido, p. 70-72) The main drawbback of DTs is the tendency to overfit and poor generalization performance, what makes them not paticaly for most use cases. Therefore usualy ensemble methods are used instead of a single DT. (Müller and Guido, p. 78) (Liu et al., c, p. 251) Random forest (Breiman) is a type of ensemble learning algorithm in which multiple decision trees, which are "weak learners," are trained and combined to produce a more accurate and stable prediction, known as a "strong learner." (Awad and Khanna, p. 24) The risk of overfitting is mitigated by subset and feature randomization. Each root node uses a unique subset of the data and each leaf is split using a random features. This ensures that no single tree sees all of the data, allowing the model to focus on general patterns rather than being sensitive to noise. (Liu et al., c, p. 251) In this supervised learning method, a "divide and conquer" approach is used. This involves dividing the data into smaller samples, incrementally building a randomized tree predictor for each sample, and then combining (aggregating) these predictors together. This approach has proven to be effective. Because not only one but multiple classifiers are used the random forest learning is known as ensemble model. (Shaik and Srinivasan, p. 254)

This mechanism is flexible enough to handle classifications and regression problems, this is one of the reasons that random forests count to the most successful ML methods. (Biau and Scornet, p. 3-4) (Breiman, p. 25)

Random forests are a type of machine learning algorithm that uses bagging and the random selection of features to produce accurate results. They are effective at handling noise and can work with both continuous and categorical variables. This combination of techniques helps improve the performance of the algorithm. (Liu et al., c, p. 259) Decision trees have a limitation in their ability to overfit, which is a disadvantage. This is mitigated by the use of subset and feature randomization. Specifically, each base model uses a unique subset of the data, and each node in the decision tree is split using a random set of features. This ensures that no single tree sees all of the data, allowing the model to focus on general patterns rather than being sensitive to noise. (Liu et al., c, p. 259)

4.3.5.1 | Gradient Boosting Regression Tree

A gradient boosting regression is a type of ensemble learning 2algorithm in which multiple decision trees are combines to produce a more accurate and stable prediction. Similar to the random forest algorithm gradient boosting combines multiple weak learners to create a strong learner. The difference to a random forest is, that the trees are trained in a serial manner and each tree corrects the errors of the previous tree. (Müller and Guido, p. 88-89) Gradient boosted tree use strong pre-pruning and therefore produce shallow trees with a depth of one to five. This brings the advantage of a smaller model which uses less memory and also results in a faster prediction. Usually generating more trees improves the overall performance of the model. (Müller and Guido, p. 88-89) Also the algorithm performs well without scaling the dataset and can handle a mixture of binary and continuous features. (Müller and Guido, p. 88-89) Like other tree-based models it does not perform well on high-dimensional data.

4.3.5.2 | Multi-layer Perceptron

Should I a MLP or will it be out of scope?

Results

4.4 | Model Training

4.4.1 | Training-Test Split

Figure 4.6 shows the data set and which parts of it is used for training and testing the used models. Samples with a die opening of 30 are used to test the performance and the remaining part is used for training. A different approach would be to us a random test and train split, this would lead to a better performance of the models but would not evaluate their ability to predict new data of a different die opening. The die opening 30 was chosen because it is in the middle of the selected data set and therefore the models should be able to predict the data of this die opening. It is expected that this approach will lead to improved model performance as the data removed lies in the middle of the parameter space. This should result in the model generalizing better on that specific range of data as it has not been over-exposed to it during the training process.

All models are trained with the same data set and the same parameters. The only difference is the used algorithm.

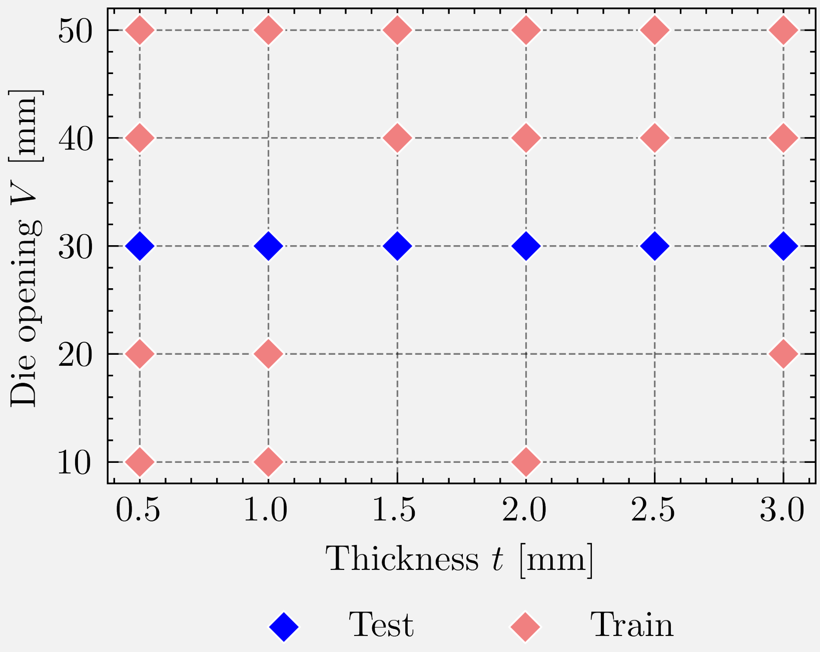


Figure 4.6: The training and test dataset. (Data especially for V40 is still missing)

Additional to the data split shown in Figure 4.6 a random test split was used to train the models. The random 80/20 split was also used to evaluate the performance of the models and to compare them to each other.

The reason for choosing to different methods for the data split is that the first one is used to evaluate the models' ability to generalize on new data. The second one is used to evaluate the models' performance on the data set. Also in real-world applications is possible that there is already data for all needed $V - t$-combinations and models could be trained on that data.

It is expected that the models perform better on the random data but the information gain about the models' ability to generalize on new data is less because the random split will most certainly contain data of all $V - t$-combinations.

Notes

- ***Dataset not yet complete***, *data for all missing Vt combinations will be added*

- *V10 does differ very much and it might be not good to include in the data set. Maybe add V60 instead*

4.4.2 | Linear Regression

A liner regression model uses the feature inputs to make prediction about the target by creating a linear relationship which is easy to understand and interpret (Molnar, 2020, p. 37).

Linear models can be used to understand the relationship between a target variable y and one or more input features x. The general formula for predicting in a linear model in regression is shown in 4.4.2 (Müller and Guido, p. 45). In this context, $x[0]$ to $x[p]$ represent the attributes (with p being the number of attributes) of a specific data point. The parameters w and b, which are learned by the model, and the predicted output $\hat{y}$, are also included (Müller and Guido, p. 45).

$$\hat{y} = w[0] * x[0] + w[1] * x[1] + ... + w[p] * x[p] + b \tag{4.1}$$

Linear Regression (LR) models estimate the target value as linear combinations of the feature inputs. The linearity of the relationship between the inputs and the target makes the interpretation of the model straightforward (Molnar, 2020, p. 37).

Linear regression has no hyperparameters to tune and therefore no hyperparameter tuning was performed.

4.4.3 | Decision Trees

Linear and logistic regression models are not effective when the relationship between input features and output is not linear or when features have interactions with one another.

Decision trees are models are useful when the relationship between features and outcome is or when features interact with one another. These models split the data multiple times based on certrain cutoff values, resulting in different subset of the dataset. The final subsets, called leaf nodes are used to predict the outocme by taking the average of the training data in that subset (Molnar, 2020, p. 76).

4.4.4 | Decision Tree

Grid search cross validation was used to find the best hyperparameters for the decision tree. All hyperparameters are summarized in Table **??**.

Table 4.5: Hyperparameters of the random forest model.

Hyperparameter	Value	Description
criterion	absolute_error	The function to measure the quality of a split.
max_depth	30	The maximum depth of the tree .
min_samples_split	4	The minimum number of samples required to split an internal node.
min_weight_fraction_leaf	0.0	The minimum weighted fraction of the sum total of weights (of all the input samples) required to be at a leaf node.
splitter	random	The strategy used to choose the split at each node.
ccp$_alpha$	0.0	Complexity parameter used for Minimal Cost

4.4.5 | Random Forest

Hyperparameter Tuning

Grid search cross validation was used to find the best hyperparameters for the random forest model using Scikit-Learn's default `GridSearchCV` function. All hyperparameters are summarized in Table 4.6.

The *criterion* hyperparameter was set to *absolute_error* because the absolute error is the metric used to evaluate the model.

The *n_estimators* where set to 10 using grid search cross validation, because the model should not be too complex and the number of trees should not be too high.

The *max_depth* was set to 10 using grid search cross validation. The default unpruned model did overfit the training data and was not able to generalize on the new data well. This is expected behavior of decision trees which is descriped by (Müller and Guido, p. 133-136) amongst others.

The *min_samples_split* was set to 2 using grid search cross validation. The default value of 2 was chosen because it is the default value of the random forest model in Scikit-Learn.

The *min_samples_leaf* was set to 1 using grid search cross validation. The default value of 1 was chosen because it is the default value of the random forest model in Scikit-Learn.

The *max_features* was set to *auto* and therefor the models does use all avialble featues. As described in Figure 4.3 only limited featues are avaialbe and all of them are important for the depenend variable spring back

Table 4.6: Hyperparameters of the random forest model.

Hyperparameter	**Value**	**Description**
n_estimators	10	The number of trees in the forest.
criterion	absolute_error	The function to measure the quality of a split.
max_depth	30	The maximum depth of the tree.
min_samples_split	4	The minimum number of samples required to split an internal node.
min_samples_leaf	2	The minimum number of samples required to be at a leaf node.
max_features	auto	The number of features to consider when looking for the best split.
max_leaf_nodes	X	Grow trees with max_leaf_nodes in best-first fashion.
max_leaf_nodes	X	Grow trees with max_leaf_nodes in best-first fashion.

4.4.6 | Gradient Boosted Regression Trees

Hyperparameter Tuning

"Gradient boosted trees are frequently the winning entries in machine learning competitions, and are widely used in industry. They are generally a bit more sensitive to parameter settings than random forests, but can provide better accuracy if the parameters are set correctly." (Müller and Guido, p. 88-89)

"Apart from the pre-pruning and the number of trees in the ensemble, another important parameter of gradient boosting is the learning rate, which controls how strongly each tree tries to correct the mistakes of the previous trees. A higher learning rate means each tree can make stronger corrections, allowing for more complex models. Adding more trees to the ensemble, which can be accomplished by increasing n estimators, also increases the model complexity, as the model has more chances to correct mistakes on the training set." (Müller and Guido, p. 88-89)

"The main parameters of gradient boosted tree models are the number of trees, n estimators, and the learning rate, which controls the degree to which each tree is allowed to correct the mistakes of the previous trees. These two parameters are highly interconnected, as a lower learning rate means that more trees are needed to build a model of similar complexity. In contrast to random forests, where a higher n estimators value is always better, increasing n estimators in gradient boosting leads to a more complex model, which may lead to overfitting. A common practice is to fit n estimators depending on the time and memory budget, and then search over different learning rates." (Müller and Guido, p. 88-89)

4.4.7 | Support Vector Machine

Hyperparameter Tuning

The *kernel*, *degree*, gamma and *epsilon* where set using grid search cross validation. Gamma controls the width of the gaussian kernel, it determines when points are close or far away. The C parameter controls the importance of each point.

The features of the dataset have different order of magnitude, this is already a problem for other models, but big effects on the kernel SVM. To resolve this problem the data was scaled using the *MinMaxScaler* between 0 and 1. The model trained on the scaled data performed better than the model trained on the unscaled data.

Notes

- *Paraphrase parameters better*

Hyperparameter	**Value**	**Description**
kernel	rbf	Kernel type used in the algorithm.
degree	1	Degree of polynomial kernel function.
gamma	0.1	Kernel coefficient for rbf, poly and sigmoid kernels.
C	4000	"Regularization parameter. The strength of the regularization is inversely proportional to C"
epsilon	0.001	"Epsilon in the epsilon-SVR model."

Table 4.7: Hyperparameters of the Suport Vector Regressor.

4.5 | Structure of The Code

- *The code is available on GitHub:* `www.github.com/...`
- *TODO: Short explanation what to do to reproduce the results.*

5 Evaluation

This chapter conducts a comprehensive analysis of the ML models implemented in the preceding chapter. An overview of the quality metrics used for the evaluation is presented in Table 5.1. The quality metrics have been structures based on the GQM approach mentioned in subsection 3.3.

The quality metrics are aligned with the quality model from Siebert et al. (2022), which is based on the ISO/IEC 9126 standard for software quality evaluation. The standard has been adapted to meet the specific requirements of machine learning models, as described in section 3.2.

As Siebert et al. (2022) mostly focuses on the evaluation of classification models, the quality metrics have been adapted to fit the requirements of the regression models implemented in this thesis. This is elaborated in each individual quality metric section.

Todo: Mention further changes

Goal	Question	Metric
Correctness	Ability of the model to perform the current task measured on the development dataset and the runtime dataset	MAE, MSE, RMSE
Relevance	Does the model achieve a good bias-variance tradeoff? Which means neither overfitting or unterfitting the data.	Variance Cross-validation (CV), R^2
Robustness	Ability of the model to outliers, noise and other data quality issues	Loss of Accuracy, Average Loss
Stability	Does the artifact generate repeatable results when trained on different data?	LOOCV stability
Interpret-ability	How well can the model be explained?	Linearity, monotonicity, interaction
Resource utilization	How much resources are required to train and run the model?	Training time, runtime, storage space

Table 5.1: Overview of the goals, questions and metrics for the evaluation of artifacts following the GQM approach.

5.1 | DP1: Correctness

The model must be able to perform well on the selected task. Siebert et al. (2022) used the metrics precision, recall and F-score to evaluate the correctness of the classification models. As the regression models implemented in this thesis are not able to predict the class of a sample, these metrics are not applicable.

Therefore measure the correctness of the model, the metrics MAE, MSE and RMSE are used. In the formulas 5.1, 5.2 and 5.3 the variable e_i is the prediction error which is the difference between the predicted value by the model the actual value. y_i is the actual value and n is the number of samples in the testing data set.

The mean absolute error (MAE) and mean squared error (MSE) are the most commonly used metrics for evaluating the performance of regression models.

Mean Absolute Error (MAE)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|e_i| \tag{5.1}$$

The MSE is the average of the squared differences between the predicted and the actual values. The MSE is more sensitive to outliers than the MAE.

Mean Squared Error (MSE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}e^2 \tag{5.2}$$

The RMSE is the square root of the MSE. The RMSE is the most popular metric for evaluating the performance of regression models. The RMSE is interpretable in the same units as the response variable. The RMSE is more sensitive to outliers than the MAE. The MAE is the average of the absolute difference between the predicted and actual values. Additionally the R^2 was added to the overview. The R^2 is a statistical measure of how close the data are to the fitted regression line. It is also known as the coefficient of determination, or the coefficient of multiple determination for multiple regression. The value of the R^2 is the percentage of the response variable variation that is explained by a linear model.

Root Mean Squared Error (RMSE)

$$RMSE = \sqrt{MSE} \tag{5.3}$$

For a full overview about the performance all three metrics are sued for the evaluation.

5.1.1 | Results

Model Name	MAE	MSE	RMSE
Linear Regression	0.199	0.092	0.303
Linear Regression (rand.split)	0.261	0.127	0.356
Decision Tree	0.193	0.076	0.266
Decision Tree (rand. split)	0.212	0.119	0.346
Random Forest	0.183	0.060	0.244
Random Forest (rand.split)	0.134	0.041	0.202
Extra Trees	0.126	0.040	0.201
Extra Trees (rand. split)	0.134	0.041	0.202
Support Vector Machine	0.09	0.04	0.20
SVM (rand. split)	0.09	0.04	0.20
MLP	0.13	0.06	0.236
MLP (rand. split)	0.161	0.051	0.225

Table 5.2: Overview of the used machine learning models and their metrics.

"The RF, **ET!** (**ET!**), and SVM models are the top performers, showing relatively equal performance. Among them, the **ET!** model boasts the best results, with an **RMSE!** (**RMSE!**) of 0.201. It's worth mentioning that the SVM model has a slightly better MSE, while still maintaining a comparable MSE compared to the other models. This could be due to the fact that the errors made by the SVM are evenly distributed across instances, or that the errors made by the other models are large for a few instances but smaller for the rest."

The algorithms LR and DC do perform worse than the other models. A likely reason for the LR not perfoming good is that the relationship between the independent and dependent variables is not linear. This cna result in an inadequate fit and reduced predictive power (Source).

DR! (**DR!**) on the other hand, can perform poorly when tey overfit the training data. Also they are pron to instability, both problems are mitigates by usng ensemble method like RF and gradient boosting which can overcome the limiations of indiviual decision trees.

5.2 | DP2: Relevance

A model is considered relevant when it achieves a balance between bias and variance, avoiding both overfitting and underfitting of the training data. The relevance of the model can be quantified through the *variance of cross-validation*, which proves insight into how the model perfoms when trained and evaluated on different subsets of data and how generalizes.

A low variance indicates that the model's performance is consistent across different folds, suggesting that the model is not overfitting the training data. Conversely, a high variance implies that the performance can vary significantly depending on the specific data points used the test set, indicating a potential overfitting problem.

Figure 5.1 shows how the variance of cross-validation was calculated. The parameter E denotes to the estimator which is used to calculate the CV score. The parameter k denotes to the number of folds, which was set to 5 in this context. As estimator for the trained models R^2 was used because this is usually the metric used to evaluate the regression models.

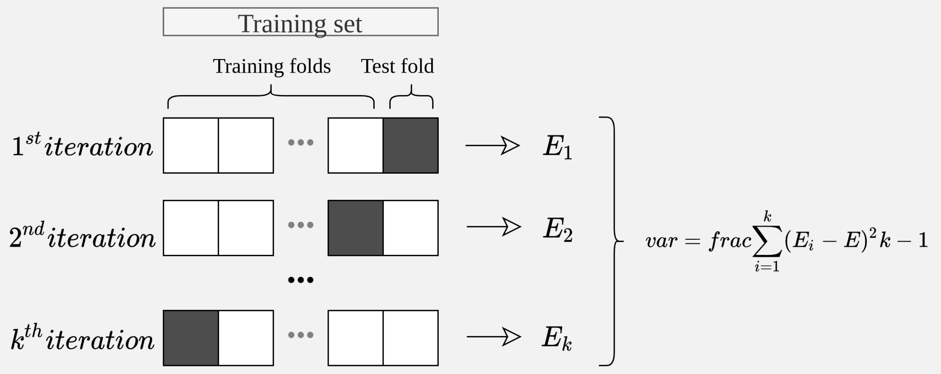


Figure 5.1: Variance of cross-validation

For completeness the R^2 score is also shown int the table. The R^2 is a statistical measure of how close the data are to the fitted regression line. It returns a score between 0 and 1, where 0 means that the model does not explain any of the variance in the response variable around its mean, and 1 means that the model explains all the variance in the response variable around its mean. Therefore, a high R^2 indicated a good model fir and good bias-variance tradeoff. (Müller and Guido, p. 43)

R^2

$$R^2 = \frac{Explained\_variance}{Total\_variance\_targert\_variable} \tag{5.4}$$

Table 5.3 shows the variance of cross-validation and the R^2 for all used machine learning models. To calculate the variance of cross-validation the variance of Scikit-Learn's `cross_val_score` was calculated. Five-fold cross-validation was used to calculate the variance of cross-validation. The R^2 was calculated with the formula 5.4.

Model Name	Variance of CV	R^2
Linear Regression	0.051	0.644
Linear Regression (rand. split)	0.034	0.771
Decision Tree	0.042	0.806
Decision Tree (rand. split)	0.068	0.784
Random Forest	0.034	0.771
Random Forest (rand. split)	0.034	0.771
Support Vector Machine	0.008	0.851
SVM (rand. split)	0.008	0.851

Table 5.3: Performance of the used machine learning models according relevance.

5.3 | DP3: Robustness

The IEEE standard glossary of software engineering terminology describe robustness as "The degree to which a system or component can function correctly in the presence of invalid inputs or stressful environmental conditions" (**?**, p. 64). **?** extend this definition to fit machine learning models and describe it as the "capability of an algorithm to build models that are insensitive to data corruptions and suffer less from the impact of noise" (Sáez et al., p. 2). Siebert et al. (2022) specifically mention data quality issued like outliers or noise (Siebert et al., 2022, p. 16).

Unlike DP1 Correctness(5.1), robustness is a non-functional characteristic of a ML model. A way to evaluate the robustness is to check the correctness of the model wit added noise to the data (Zhou, p. 18), if the model is still able to predict the correct values, it is considered robust.

As mentioned in section 4.2.2 the data set was generated in a controlled environment does not contain many data quality issues and noise. This offers the opportunity to test the robustness of the models by manipulating the data set to introduce the data quality issues missing values and noise.

5.3.1 | Missing Data

When applying the model to real-world data, it is possible that some values are missing. Looking at the available dataset two scenarios or missing data can occur: Missing Vt-pairings and missing values.

In the first scenario, there may be no data available for a specific die opening, which can be due to the die opening was never being used before or a lack of recorded information. In the second scenario, while data may exist for the desired Vt combination, certain values may be missing or the dataset may not be complete.

To address these scenarios, the following tests were conducted:

2. Missing values

To study the model's ability to handle missing data, a controlled manipulation of the dataset was performed by removing a random subset of the data. This approach allows for an evaluation of the model's performance when only a portion of the data is missing rather than all of it. This simulates scenarios where data may be missing due to various reasons such as measurement errors or missing data points.

The most accurate method would be Leave-P-Out-Cross-Validation (LPOCV), which generates all possible training and test sets by removing p samples from the complete dataset. This approach creates overlapping test sets, resulting in a large number of iterations, which is computationally expensive. Due to limitations in computing power, this method could not be used in this thesis and therefore is only mentioned for completeness.

The alternative approach chosen is to a regular CV approach, with an increasing number of folds. The minimum number of folds used in this approach was 2, while the maximum number of folds was the total number of samples in the dataset. This means that each sample was used as a test sample once. This approach allows for a gradual increase in the amount of missing data, simulating secnarios where data may be missing due to various reasons such as measurement errors or missing data points. It is expected that the model's performance will improve with fewer folds, as the model will be trained to more data.

This approach provides a more computationally efficient evaluation of the model's robustness under conditions of missing data.

For each iteration of the cross-validation, the RMSE of the model was calculated. The mean RMSE for each cross-validation was then calculated and the difference between all mean RMSEs was defined as the loss of accuracy. The total loss of accuracy was calculated by averaging the difference of the RMSE of the models for each fold of the cross-validation. An average loss function was introduced to measure the performance of the model under different levels of missing data.

To measure the performance an average loss function is introduced as follows:

$$\text{Loss of Accuracy} = \frac{1}{N}\sum_{i=1}^{N} |\text{RMSE}i - \text{RMSE}avg| \tag{5.5}$$

Where N is the toal number of folds, i is the index of the current folds.

It is worth noting that imputations of missing values can be used to mitigate the loss caused by missing data. However, this approach was not used in this thesis as the goal was to measure the robustness of the model to missing values specifically, rather than to artificially improve its performance through imputation techniques.

5.3.2 | Noise

A common practise in ML is to add noise to the training data to improve the model's generalization abilities. In this sturdy adding Gaussian Noise will be added to evaluate the robustness of the model.

There is no standard approach to adding noise to the data. The approach chosen in this thesis is to add noise to the training data, while the test data remains unchanged. To add the noise, *numpy.random.normal* function was used, which generated random numbers with a Gaussian distribution. The mean and standard deviation of each feature were calculated based on the original data, and the function was used to generate noisey values for each feature.

To study the model's reaction to increasing amounts of noise, the noise added to the training data was gradually increased starting from 1% to 50%, which means that the last iteration contains as many noisy as"clean" samples.

The difference between all RMSE's between iterations was defined as loss. The total loss was cacluclated by averaging the difference of these values as shown in Equation 5.6.

$$\text{Average Loss} = \frac{1}{N}\sum_{i=1}^{N}|\text{RMSE}i - \text{RMSE}avg| \tag{5.6}$$

Notes

- *Does the calculation of the loss make sense?*

5.3.3 | Results

Model Name	Missing Values loa	Noise loa
Linear Regression	0.070	0.251
Linear Regression (rand. split)	0 .071	0.224
Random Forest	0.071	0.224
Random Forest (rand. split)	0.067	0.233
SVM	0.070	0.251
SVM (rand. split)	0.071	0.224

Table 5.4: Results of used machine learning models regarding the design principle robustness.

5.4 | DP4: Stability

Stability is defined as the ability of the model to generate repeatable results when trained on different data (Siebert et al., 2022, p. 16).

One appropriate way to measure the stability of a model is to use Leave-one-out Cross Validation (LOOCV), which is a a form of CV where one sample is used for validation and the remaining data is used for training (Gareth et al., 2013, p. 200–201).

In order to evaluate the model the LOOCV was repeated for all samples in the dataset resulting in a total of n iterations. The stability of the model was determined by calculating the average prediction error across all iterations, using the equation provided in Equation 5.7 which is taken from (Gareth et al., 2013, p. 201).

$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n} \text{MSE}_i \tag{5.7}$$

The approach provides an unbiased estimate of the model's generalization error but this estimate is poor because only one samples is used for validation (Gareth et al., 2013, p. 201). Therefore, it can not be used to make a statement about the generalization error of the model. Since the goal is to measure repeatable results, the LOOCV is a suitable metric to measure the stability of the model.

A low $CV_{(n)}$ value indicates a high stability of the model, because the model is able to generate repeatable results when trained on different data. Note: The method can be very time-consuming, especially for large datasets, but it may provide more accurate estimates for small datasets.

5.4.1 | Results

Model Name	$CV_{(n)}$
Random Forest	0.053
Random Forest (rand. split)	0.053
Decision Tree	0.086
Decision Tree (rand. split)	0.062
Support Vector Machine	0.051
SVM (rand. split)	0.000

Table 5.5: Overview of the used machine learning models and their metrics.

Explanation of the results

5.5 | DP4: Interpretability

Interpretability refers to the ease with which humans can understand and make sense of the decisions made by a trained machine learning model (Siebert et al., 2022, p. 16). Miller (2019) define interpretability as the "degree to which a human can understand the cause of a decision" (Miller, 2019, p. 1). Good interpretability is important because it allows users to trust and rely on the model, and it can also help with debugging and improving the model (*Source*).

Interpretable models will also deliver more insights for this project, as the goal is to understand the relationship between the features and the target outcome.

When following the above definitions of interpretability, it is clear that it is not possible to measure interpretability in a quantitative way. No mathematical formula can be used to measure interpretability, but other methods can be used to measure the interpretability of a model. Interpretable models allow the usage of global model-agnostic evaluation methods which will be used later in the evaluation of the models (see Section **??**).

In a first steps it has to be defined what makes a model interpretable.

Interpretable Models

According to Molnar (2020) one way to make a model interpretable is to limit the choice of algorithms to those that produce interpretable results. Example of such algorithms include linear regression, logistic regression and decision trees (Molnar, 2020, p. 35).

Molnar (2020) defines three properties of interpretable models:

Linearity A linear model is one in which the relationship between features and the target outcome is represented as a linear equation (Molnar, 2020).

Monotonicity A model with monotonicity constraints ensures that there is a consistent relationship between a feature and the target out come across the entire range of the feature. This can make it easier to understand the relationship.

Interactions Some models can automatically include interactions between features to improve prediction, while other require manual creation of interaction features. However, too many or complex interactions can make the model more difficult to interpret.

In the model selection for this thesis the focus is on interpretable models, as they are easier to understand and explain, therefore mostly models are chosen which fulfill all three properties.

Later in the thesis, the interpretability of the models is used to explain the results.

Number of Parameters

More complex models tend to have more parameters and are therefore more difficult to interpret. The number of parameters is calculated using the the `model .get_params` function in scikit-learn.

Note: The Depth of the model could be used as well for the evaluation, but not all models have a depth therefore this metric is not suitable. The depths is representing the number of layers in the model. A model with many layers, is generally more complex than a shallow network with fewer layers.

Notes

- *Space complecity -> How much memeory is needed?*

Linear Regression

Linear regression is a linear model as it models the relationship between the features and the target as a linear equation.

This linearity usually does mean that the relationship between the feature and the target goes in the same direction over the entire range of the feature. Therefore LR is monotonic.

LR models do not include interaction features by default. To capture interaction effects in LR, interaction features need to be created and added to the model manually. This was not done in this work.

5.5.1 | Results

Model Name	Linear	Monotone	Interaction	Param.
Linear Regression	Yes	Yes	No	4
Decision Tree	No	Some	Yes	11
Random Forest	No	Some	Yes	17
Logistic Regression	No	Yes	No	XX
SVM	X	X	XX	11

Table 5.6: Overview of the used machine learning models and their metrics.

Notes

- *Reasoning for results in table.*

Explanation of the results

5.6 | DP5: Resource utilization

To measure the resource utilization of the model, the following metrics are used:

Training time Measured in seconds. Refers to the time it takes to train the model. Training a model requires resources such as memory, CPU, and GPU, therefore the longer it takes to train a model, the more resources are required. According to resources utilization a shorter training time is desirable.

The training time is measured using the `time.time` function in python . The function returns the time in seconds since the epoch. The time is measured before and after the model is fitted. The difference between the two times is the training time.

Inference time Measured in milliseconds. It refers to the time it takes to make a prediction on data once it has been trained. It is an important measure not only for real-world application but also a faster runtime uses less resources and is therefore more efficient.

Inference time Measured in milliseconds. Time it takes to make 100 predictions. A model that takes longer to make predictions may be more complex than a model that is able to make predictions more quickly. Measured using the `time.time` function in python. 100 valuees are picked out of the teset set and the time is measured before and after the prediciton is made.

Memory space Measured in Mb. It refers to the amount of memeory required to run the model. The more storage space required to store the model, the more resources are required to store it. Therefore, a smaller storage space is desirable. To measure the memory usage the `memory_usage` function from the `memory_profiler` package is used.

Model Name	**Training time** ms	**Inference time** ms	**Memory Usage** kb
Linear Regression	2.609	0.975	157.41
Decision Tree	2.600	1.055	155.734
Random Forest	0.0222	2.0275	80.2
Support Vector Machine	289.874	2.376	156.891

Table 5.7: Overview of the used machine learning models and their metrics.

5.7 | Results

Using the evaluation metrics described in the previous sections, the following results were achieved...

What are cruz et al. doing?

- They have two different data devision methods, DD1 and DD2.
- Also they use a validation set and a test set.
-

The results in Figure **??** show that the random forest

5.7.1 | Overall Results

This section will showcase the outcomes generated by the trained models in more detail and will also discuss the results in relation to the research questions.

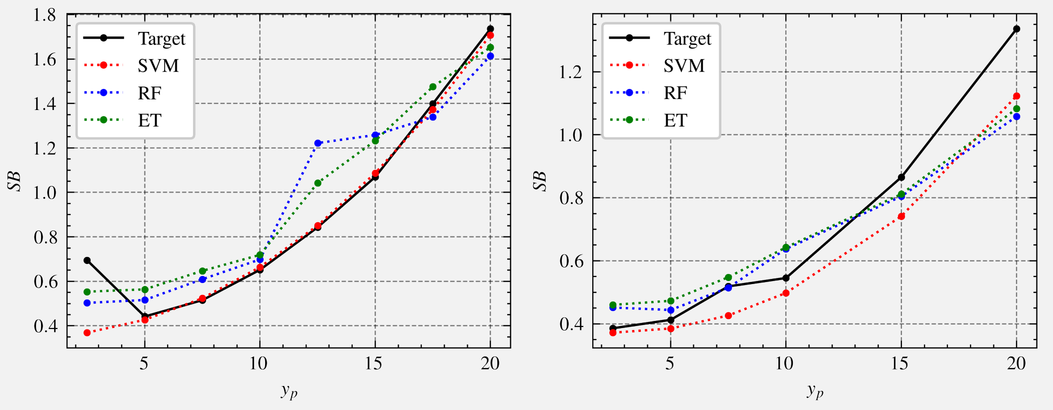
In Section 5.1 the overall correctness of the model was evaluated using different metrics. In order to evaluate the results of this problem in more detail, three test cases are used in this analysis. The V/t ratio is used to determine the bending conditions of the test cases. In the dataset used in ranged from 3.3 (V 50 and t 3)to 100 (V50 t 0.5)and the test cases are chosen to represent the different bending conditions.

Recommended V/t ratios in industrial practices are between 6 and 10 (Cruz et al., 2021, p.7). Bending operations performed outside of this range of recommended ratios may result in high spring back.

Case A is chosen, so that is is below the recommended ration, case B is chosen to be within the recommended ratios and case C is chosen to be above the recommended ratios. As can be seen, case A features a significant spring back while the other cases do not.

In order to evalute the model's performance without bias, each test case where removed from the training data set so that the model has not seen the test case before. This results in a small but notable performance decrease in the test cases.

Case 5.2a with a V/t-ratio of 20 demonstrates the models' ability to predict the spring with high accuracy. However, the performance decreases in case b)5.2b with a V/t-ratio of 6.6, particularly when predicting the spring backs. It is likely that there is a measurement error at $V = 7.5$ in case b) 5.2b, causing some models to potentially predict the correct spring back.



(a) V: 20, t: 1 (b) V: 20, t: 3

Figure 5.2: Performance plots for case A

As seen in Figure 5.3, the performance in case B is similar. The models exhibit high accuracy in predicting the spring back in case a) **??** with a V/t-ratio of 15. Additionally, the spring backs at the higher end are also predicted with high accuracy.

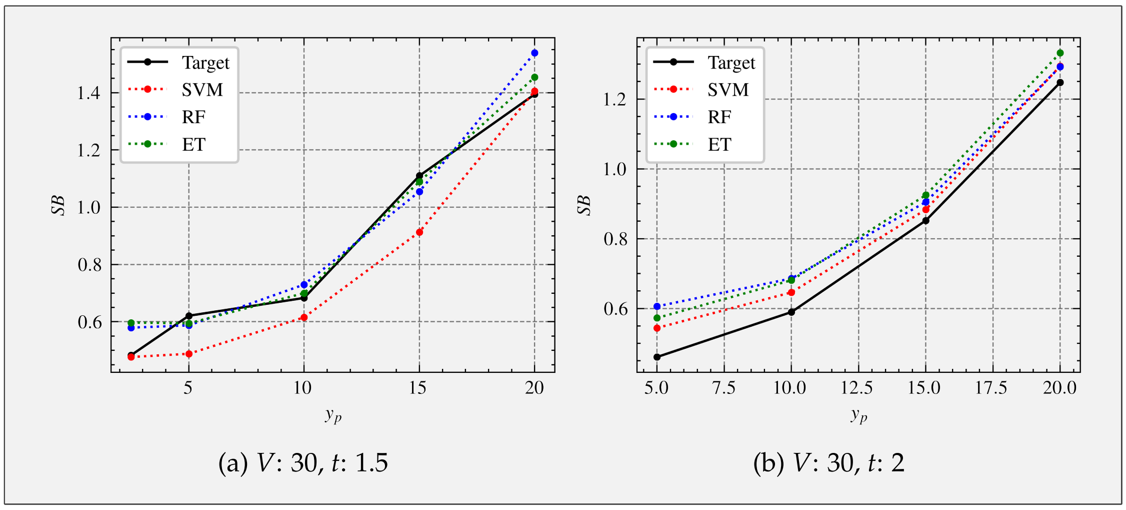


Figure 5.3: Performance plots for case B

In case C as seen in Figure 5.4 the models performance is getting worse.

Reasons for that? ...

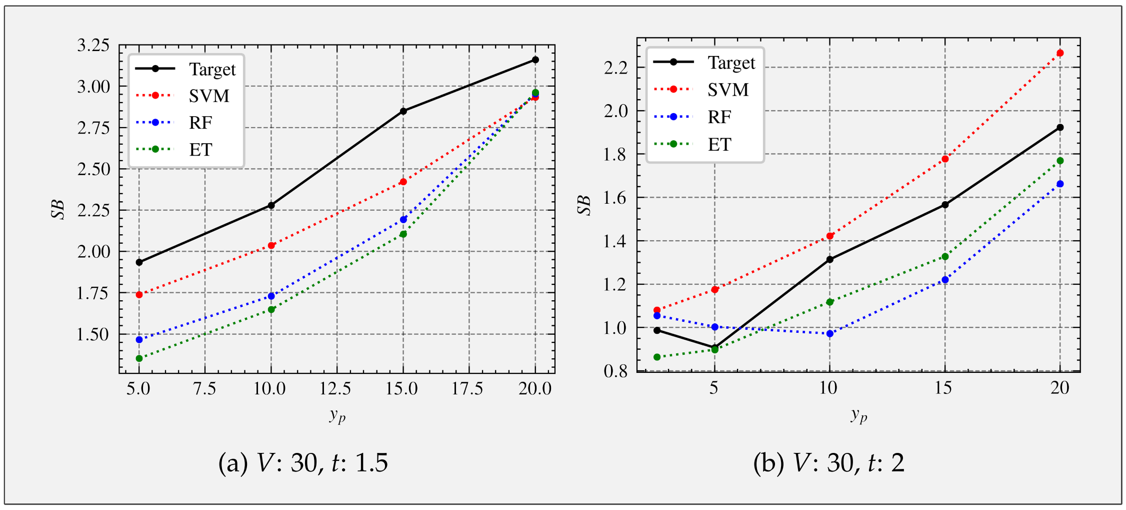


Figure 5.4: Performance plots for case C

The best performing model is the SVM model with an RMSE of 0.2. Therefore the cases A, B and C are predicted using the SVM model.

As seen in Figure **??**, the model performs consistent across all thee scenarios, indicating that it can effectively handle a broad range of V/t ratios also outside the recommended industry guidelines range.

5.8 | Intepretation

5.8.1 | Model Specific Interpretability Methods

To attain interpretability, the simplest approach is to select algorithms that generate interpretable models. Some of these models like linear regression and decision trees where used in this work.

The following section looks at the generated and uses model specific interpretability methods to interpret the results.

5.8.1.1 | Feature Importance

5.8.1.2 | Linear Regression

The linearity of the relationship between the inputs make the mode interpretable as elaborated in section 4.4.2.

In a LR model, the significance of a feature can be quantified using the absolut value of its t-statistic. The t-statistic represents the scaling of the estimated weight with its standard error (Molnar, 2020, p. 40).

Feature importance table here

Also it is possible to create visual interpretations of the model using a weight plot or effect plot.

Weight and effect plot here

And also Lasso

Lasso plot here

5.8.1.3 | Decision Trees

Feature Importance Plot possible as well

OneR algorithm

Baysan Rule List

Global Model-Agnostic Methods

As already described in section 5.5, only algorithms that are interpretable where used for the evaluation.

Molnar (2020) differentiates between model-specific and model-agnostic interpretability methods. Model-specific methods are methods that are specific to a certain model type, for example, decision trees. Model-agnostic methods are methods that can be used with any model type, for example, permutation importance.

Also Molnar (2020) differentiates between global and local interpretability. Global interpretability refers to the ability to understand the overall behavior of the model, while local interpretability refers to the ability to understand the behavior of the model for a specific instance.

For the purpose of this thesis, the focus is on global model-agnostic methods, as they can be used with any model type and provide an overview of the model's behavior.

Partial Dependence Plots

5.8.2 | Local Model-Specific Methods

5.9 | Discussion

- *Data set had only limited features, but there are many more factors influencing the spring back*

6 Conclusions

6.1 | Revisiting the Aims and Objectives

6.2 | Critique and Limitations

6.3 | Future Work

6.4 | Final Remarks

6.5 | TODO

- Stability section refinement
- Read Siebert paper and add important points to the thesis
- —
- Robustness refinement

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