

Machine Learning for the Prediction of Bending Pa- rameters

some hyped-up tagline

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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.

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List of Abbreviations

ML Machine Learning	6
SVM Support Vector Machine	10
SVR Support Vector Regression	26
ANN Artificial Neural Network	9
FEM Finite Element Method	10
DSR Design Science Research	15
GQM Goal-Question-Metric	vii
RF Random forest	22
DT Decision tree	26
rmse root mean squared error	22
MSE mean squared error	38
LOOCV Leave one out cross validation	40
CV Cross-validation	40
ELA Equalized Loss of Accuracy	37
MLA Mean Loss of Accuracy	38

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)

Springback 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 minimum 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)

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 trial 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.

2.1.0.1 | 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)

2.1.0.2 | 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.

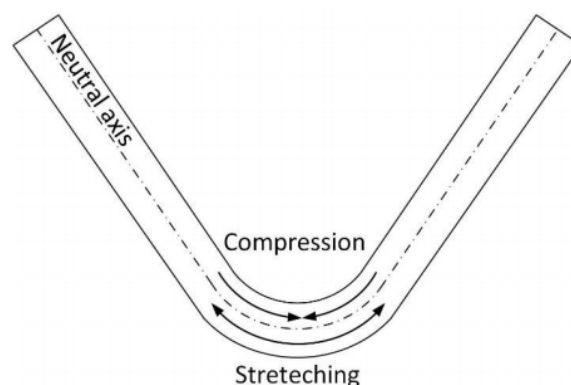


Figure 2.1: Bending plane, compression and stretching of sheet metal (Baig et al., 2021, p. 3)

2.1.0.3 | 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)

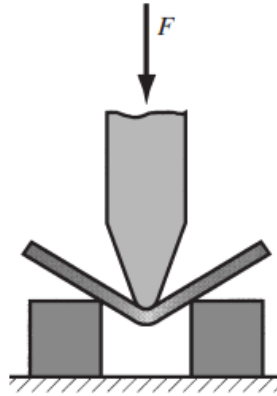


Figure 2.2: Air bending (Groover, p. 416)

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)

2.1.0.4 | 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)

$$\delta\alpha_{SB} = \alpha_i - \alpha_f \quad (2.1)$$

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.

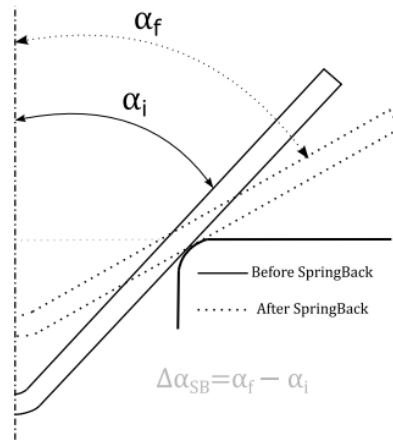


Figure 2.3: Spring back (Cruz et al., 2021, p. 5)

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 numerical value, therefore this work focuses on supervised learning for a regression problem and does not further consider classification problems. "There are two major types of supervised machine learning problems, called classification and regression."

2.2.3 | Overfitting and Underfitting

"In supervised learning, we want to build a model on the training data and then be able to make accurate predictions on new, unseen data that has the same characteristics as the training set that we used. If a model is able to make accurate predictions on unseen data, we say it is able to generalize from the training set to the test set. We want to build a model that is able to generalize as accurately as possible." (Müller and Guido, p. 35)

"Usually we build a model in such a way that it can make accurate predictions on the training set. If the training and test sets have enough in common, we expect the model to also be accurate on the test set. However, there are some cases where this can go wrong. For example, if we allow ourselves to build very complex models, we can always be as accurate as we like on the training set." (Müller and Guido, p. 35)

"The only measure of whether an algorithm will perform well on new data is the evaluation on the test set. However, intuitively³ we expect simple models to generalize better to new data. If the rule was "People older than 50 want to buy a boat," and this would explain the behavior of all the customers, we would trust it more than the rule involving children and marital status in addition to age. Therefore, we always want to find the simplest model. Building a model that is too complex for the amount of information we have, as our novice data scientist did, is called overfitting. Overfitting occurs when you fit a model too closely to the particularities of the training set and obtain a model that works well on the training set but is not able to generalize to new data. On the other hand, if your model is too simple—say, "Everybody who owns a house buys a boat"—then you might not be able to capture all the aspects of and variability in the

data, and your model will do badly even on the training set. Choosing too simple a model is called underfitting." (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 indicates a model with a complex fit to the training data and therefore overfits (Neal, p. 20)

Variance measures how much the model's prediction varies, 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 has 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)

2.2.5 | Ensemble Learning

Ensemble techniques in machine learning 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 in sheet metal forming with the goal to reduce costs and increase manufacturing quality. Bock et al. (Cao et al.) 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. (Inamdhar 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 ich "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)

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 ("artifacit"). (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 learning 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 divided into the superordinate phases "Build" and "Evaluate". This thesis follows these phases.

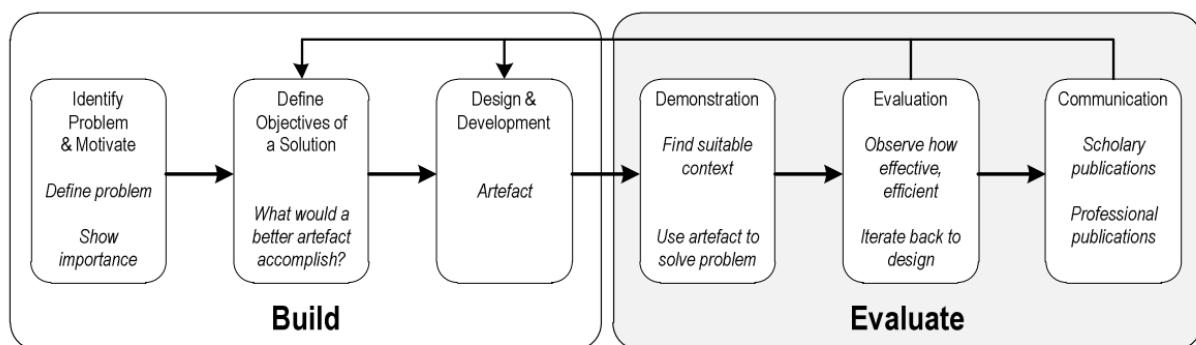


Figure 3.1: Design Science Research Approach according to Peffers et al.
Picture: (Sonnenberg and vom Brocke, 2012, p. 72)

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 artifact 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 parameters can be used to measure the performance of the artifacts (Peppers 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 artifact and its benefit are communicated externally (Peppers 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 then be DPs. (Koppenhagen et al., 2012, p. 6)

3.2 | Evaluation of Machine Learning Models

In the field of software engineering there are already standards that define the quality of software systems and its components like ISO/IEC 25010. (Siebert) noted, that such standards can not applied directly to ML and therefore need to be adapted. Therefore they re-interpreted and extended these existing quality models to the ML context. (Siebert, p. 1) In order to define the Design Principles for the artifacts in this work, the considerations of (Siebert) are used. This enables a systematic process in order to assess the quality of the developed artifacts.

3.2.1 | 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 1

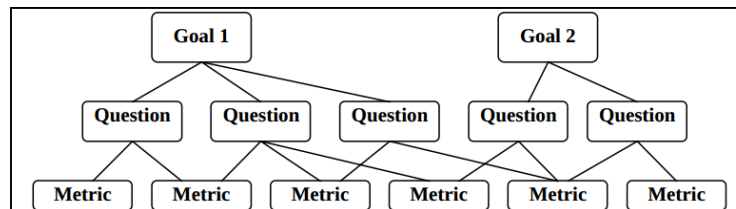


Figure 3.2: Goal-Question-Metric Ansatz (Basili et al., 2002, p. 3)

Build

4.1 | Design Principles

The following design principles is a selection of Siebert'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 minimized. (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. (Siebert, 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 learners 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 noise 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 perform

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, 1mm 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 | Preliminary Tests

A number of preliminary tests were conducted to determine the influence of the punch penetration on the spring back.

4.2.1.1 | Multiple Cycles

One approach was to test if multiple spring back can be measure using only one sheet. Therefore, the machine was programmed to perform multiple cycles in one attempt and bend the metal sheet multiple times. The benefit of this approach would have been a faster generation of the dataset because spring backs could be measured in on attempt, also less material would have been used.

Figure 4.1 shows one of these attempts. The metal sheet was bent 4 times using y_p values from 5 to 8. The results show, that 4 different spring backs can be measured, but the spring back does not vary like expected. It was observed as well, that the spring backs are different in every attempt, this is shown in Figure 4.2. Bending 4 different metal sheets each only one time returned very different results. A possible explanation

could be the cold deformation of the steel, which is not reversible. Because this approach did not work, the machine was programmed to perform one cycle at a time.

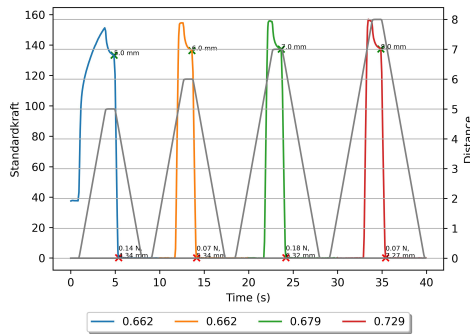


Figure 4.1: Experiment: Bending one metal sheet multiple times with different y_p values.

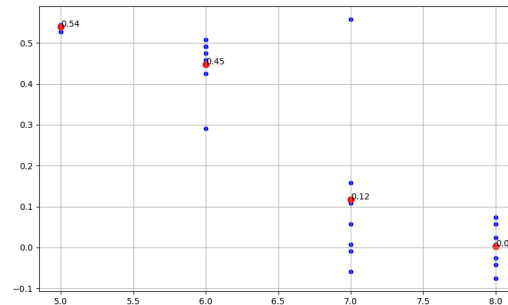


Figure 4.2: Inconsistent results bending one metal sheet multiple times. The spread of the results is very large.

4.2.1.2 | Brake Bending Machine

Before using the three point bending machine, a brake bending machine was used to test the influence of the bending on the spring back. The brake bending machine is a machine used to bend metal sheets. It is a very common machine in the industry and is used to bend metal sheets to a specific radius. The brake bending machine used is a *Bendmaster 1000* from *Bendmaster*.

After a series of bends it was observed, that the spring back values were much higher than expected. The explanation for that behavior was, that altering the position the bending beam of that specific machine was not enough to get the desired angle. Thus, the machine was excluded for the generation of the data and the three point bending machine was used instead.

Despite the inaccurate data, it was later observed, that the distribution of the spring backs was very similar to the later experiments with the three point bending machine.

4.2.2 | Experimental setup

The setup consists of a three-point-bending machine with a punch and a die with no bottom. The machine used is the *Zwick MX 25A* material testing machine. The machine is equipped with a load cell and a displacement sensor. The load cell is used to measure the force applied to the sheet and the displacement sensor is used to measure the dis-

placement of the punch. The machine is controlled by a computer and a software called *ZwickRoell TestXpert*. The software is used to control the machine and to save the output data.

The experimental setup and the process parameters are shown in Figure 4.3 where V is the die opening, y_p is the punch penetration which is the distance the punch is moved into the sheet. The parameter t is the sheet thickness, α is the sheet corresponding bending angle. Parameter r_p is the punch radius which is the radius of the tip of the punch and r_m is the die radius.

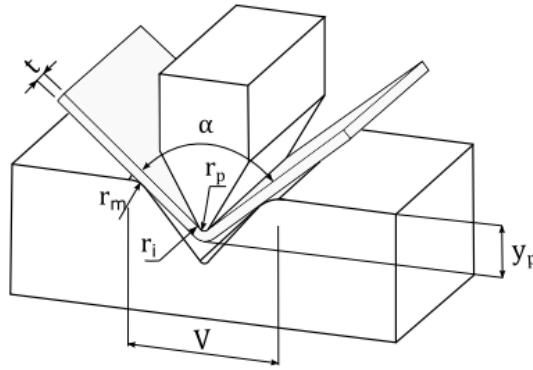


Figure 4.3: Process parameters: Sheet bending angle (α), sheet thickness (t), punch penetration (y_p), die opening (V), punch radius (r_p), die radius (r_m), inside bending radius (r_i).

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 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. The sheet thickness was varied between 0.5 and 3 mm. The constant parameters are shown in Table 4.2 and the varying parameters are shown in Table 4.1.

Parameter		Value	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 4.1: Experimental setup varying parameters

Parameter	Value	Unit
Punch radius	5	mm
Die radius	5	mm
Sheet width	20	mm
Sheet length	100	mm
Punch speed	100	mm/min
Punch speed after penetration	8	mm/min
Punch force	1	N

Table 4.2: Experimental setup constant parameters

4.2.3 | 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 4.4 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.

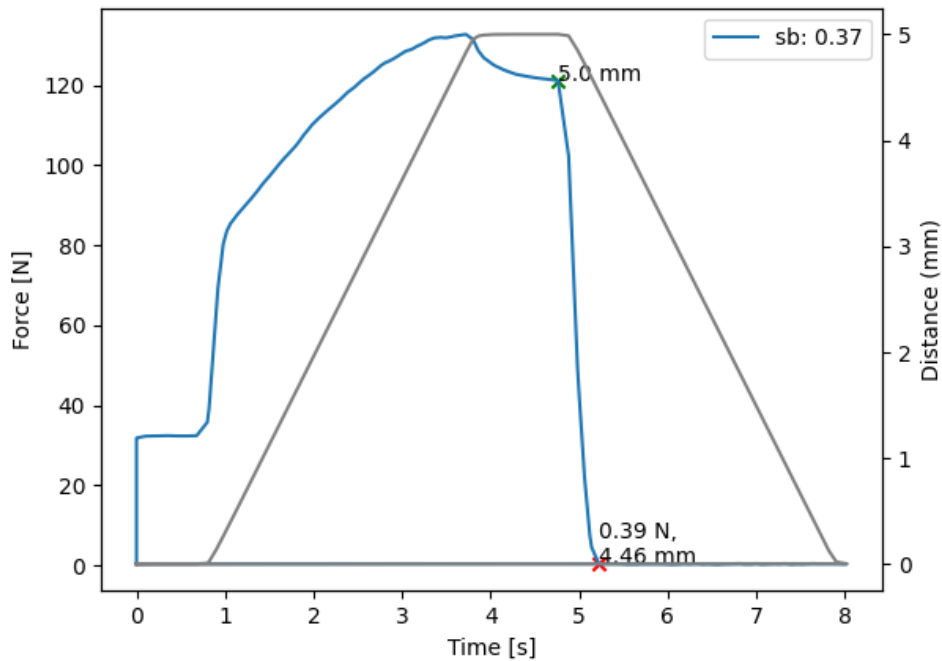


Figure 4.4: A steel metal sheet was bent with a punch penetration of 5 mm the spring back is 0.37 mm. The blue line shows the force and the blue line shows the punch penetration.

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

4.2.4 | 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

4.2.3. The final dataset therefore contained 3 features plus the added spring back. In total 396 data points were created using the described approach. An example of the dataset is shown in Table 4.3.

	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: Features used for the machine learning models

■ ~~TODO: Describe Figure 4.5~~

With 100 estimators in Random forest (RF) a **mse!** (**mse!**) of 0.15 and root mean squared error (rmse) 0.39 was achieved. Figure 4.5 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.

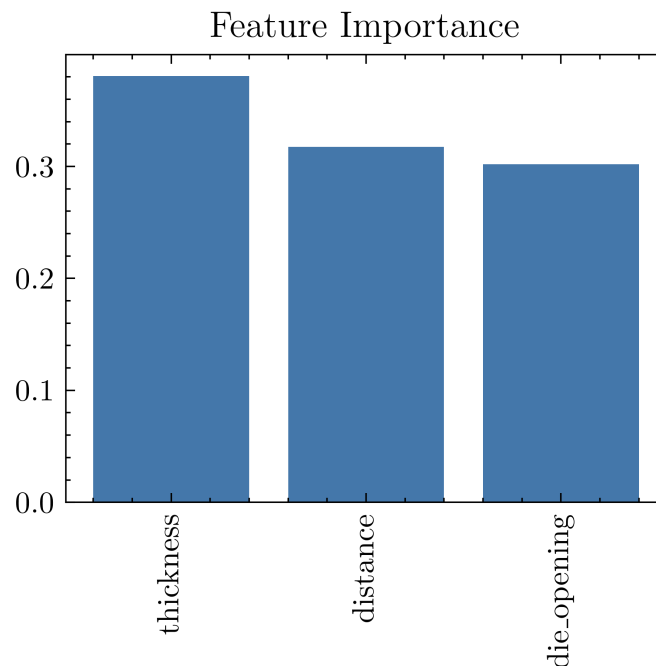


Figure 4.5: Relative feature importance

4.2.5 | Visualizing The Data

Figure 4.6 shows the spring backs for the V30 dataset. In general, it can be seen that the spring back 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.

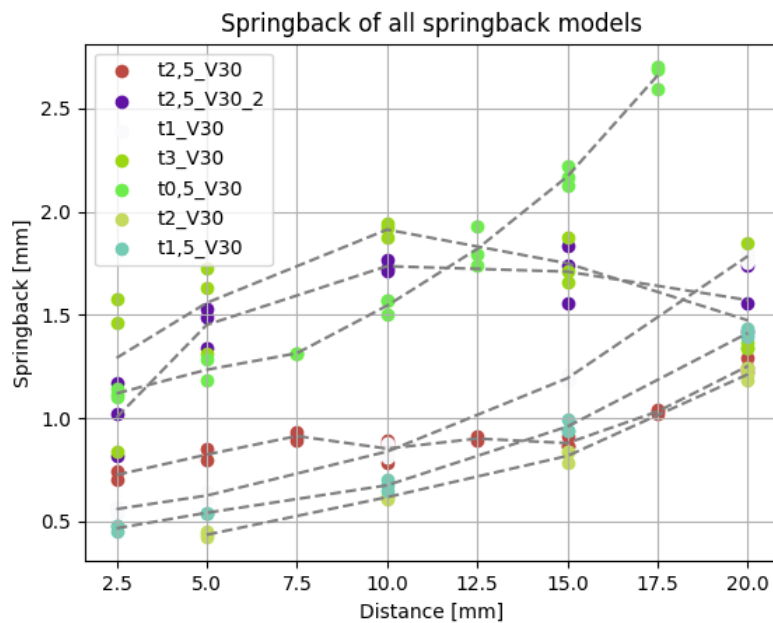


Figure 4.6: Springbacks for V30

Notes

- TODO: Add better picture. Ordered by t , better colors, scienceplot, punch penetration instead of spring back

4.2.5.1 | Data Quality

The dataset was created in an experimental environment and the samples were carefully measured. Therefore the dataset does not contain many outliers and the data quality is high. Furthermore, the dataset was continuously extended with new data points

throughout the project. During this process multiple outliers and wrong measurements were 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 considered 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 dependent 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 4.8.

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 4.8.

Notes

- *TODO: Outlier handling is not done and mentioned. Is this necessary?*

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 4.4.

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 4.7 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.

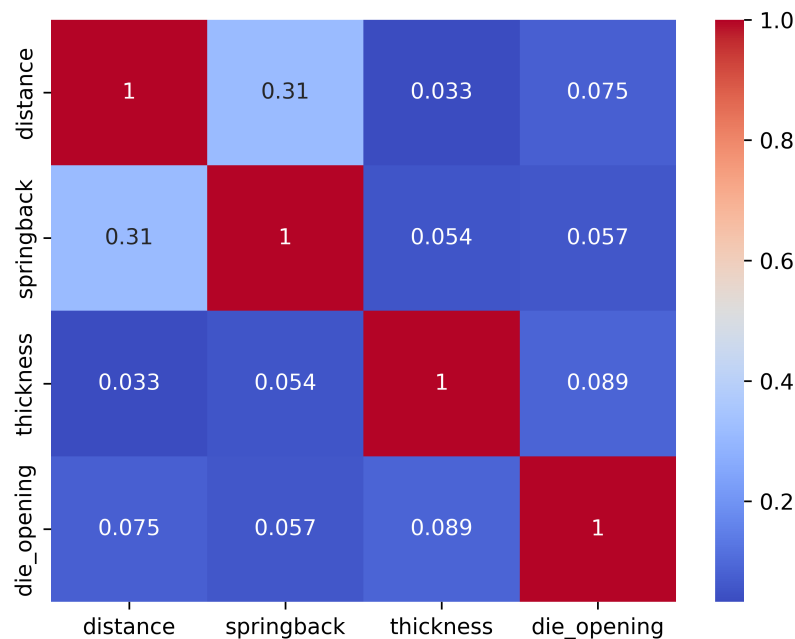


Figure 4.7: Correlation matrix

4.3 | Model Selection

4.3.1 | Support Vector Regression (SVR)

Support Vector Machines SVM are 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 is not suitable for this problem. It therefore is a generalization of classification problems, where the model returns continuous values instead of finite set of values. The Support Vector Regression Support Vector Regression (SVR) algorithm is derived from the SVM algorithm and accomplishes this generalization by introducing an ϵ -intensive region around the function ($\epsilon - tube$). (Awad and Khanna, p. 67)

4.3.2 | Multi Linear Regression

4.3.3 | Polynomial Regression

4.3.4 | Decision Tree Regression

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 Decision tree (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 drawback of DTs is the tendency to overfit and poor generalization performance, what makes them not patically for most use cases. Therefore usually 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 random-

ized 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 algorithm in which multiple decision trees are combined 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.

Results

4.4 | Model Training

4.4.1 | Training-Test Split

Figure 4.8 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 use 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. All models are trained with the same data set and the same parameters. The only difference is the used algorithm.

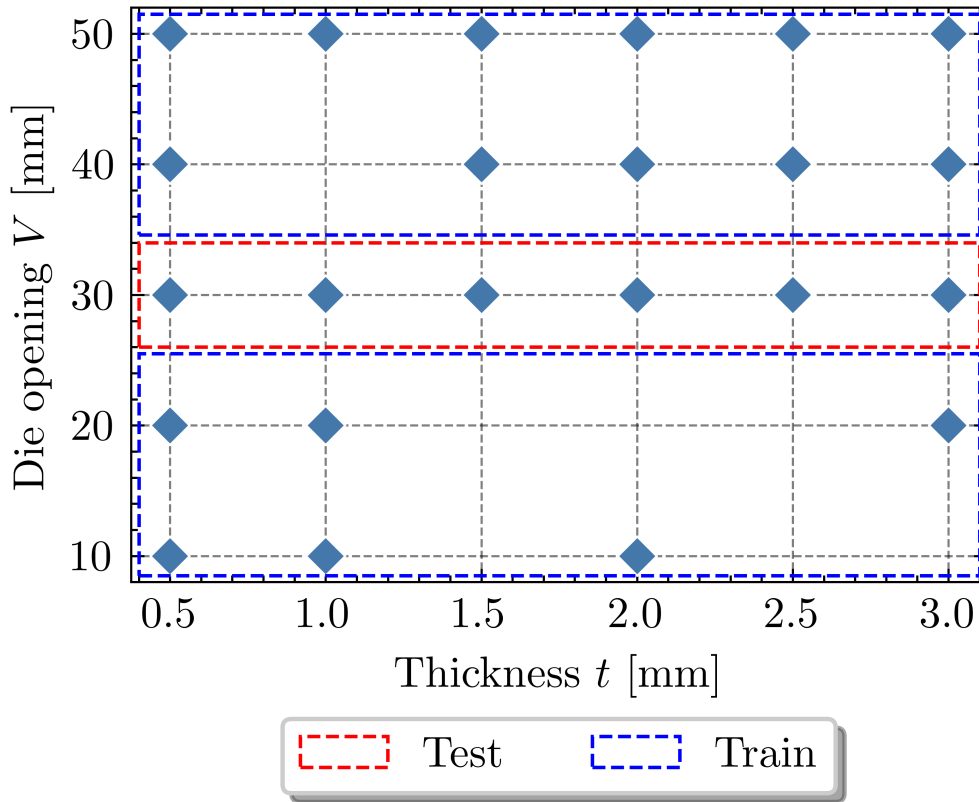


Figure 4.8: The training and test dataset. (Data especially for V_{40} is still missing)

Additional to the data split shown in Figure 4.8 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*

4.4.2 | 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 4.5. The *criterion* hyperparameter was set to *absolute_error* because the absolute error is the metric used to evaluate the model. The *n_estimators* were 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 described 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 therefore the models does use all available features. As described in Figure 4.5 only limited features are available and all of them are important for the dependent variable spring back

Table 4.5: 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.

Notes

- With a test test split (V30) the models does not achieve a good R2 score. That means that the model is not able to generalize well to new data (0.0something).
- When using a random test train split the R2 score is much better (0.9something).
- Look again at spring back calculation

4.4.3 | 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)

4.5 | Structure of The Code

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

Evaluation

This chapter critically examines the machine learning models conceived and partially implemented in the previous chapter. Table ?? shows an overview of the evaluated criteria. These are structured according to the Goal-Question-Metric approach.

The quality metrics are oriented on the quality model from (Siebert), which is based on the ISO/IEC 9126 standard for the evaluation of software quality. (?). The standard was changed to fit the requirements of machine learning models.

The metrics of the goal *Robustness* were original only defined for classification models and therefore needed to be changed. *TODO: Explain what has been changed*

Goal	Question	Metric
Appropriateness	How well does the model type fit the current task?	Prerequisites for model type
Correctness	Ability of the model to perform the current task measured on the development dataset and the runtime dataset	Precision, Recall, F-score
Relevance	Does the model achieve a good bias-variance tradeoff? Which means neither overfitting or underfitting the data.	Variance of cross-validation and fit
Robustness	Ability of the model to outliers, noise and other data quality issues	Equalized Loss of Accuracy (ELA)
Stability	Does the artifact generate repeatable results when trained on different data?	Leave-one-out-cross validation stability
Interpretability	How well can the model be explained?	Complexity measures (e.g., no. of parameters, depth)
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.

Notes

- TODO: Improve layout of table

5.1 | DP1: Appropriateness

5.2 | DP2: Correctness

The model must be able to perform well on the selected task. To 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)

$$MAE = \frac{1}{n} \sum_{i=1}^n |e_i| \quad (5.1)$$

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)

$$MSE = \frac{1}{n} \sum_{i=1}^n e^2 \quad (5.2)$$

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)

$$RMSE = \sqrt{MSE} \quad (5.3)$$

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

5.2.1 | Results

Model Name	MAE	MSE	RMSE
Random Forest (rand split)	0.14	0.05	0.22
Random Forest	0.16	0.04	0.21
Boosting	0	0	0
Linear Regression	0	0	0
Support Vector Regression	0	0	0

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

Explanation of results...

Notes

- *TODO: Compare model against baseline regression model (Cookbook)*

5.3 | Relevance

The model is relevant if it is able to achieve a good bias-variance tradeoff. This means neither overfitting or underfitting the data. The variance of cross-validation scores gives an idea on how stable the model's performance is when it is trained and evaluated on different subsets of data. If the variance is low, it means that the model's performance is relatively consistent across different folds, and you can have more confidence in the evaluation. On the other hand, if the variance is high, it means that the model's performance can vary significantly depending on which data points are used as the test set, and you should be more cautious when interpreting the results.

If the variance is low, it means that the model's performance is relatively consistent across different folds, and you can have more confidence in the evaluation. On the other hand, if the variance is high, it means that the model's performance can vary significantly depending on which data points are used as the test set, and you should be more cautious when interpreting the results.

Variance of cross-validation

R²

$$R^2 = 1 - \frac{\text{Variance}_{\text{cross}}}{\text{Variance}_{\text{fit}}} \quad (5.4)$$

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
Random Forest	0.034	0.771
Boosting	0.000	0.000
Linear Regression	0.000	0.000
Support Vector	0.000	0.000

Table 5.3: Overview of the used machine learning models and their metrics.

5.4 | Robustness

According to Sáez et al. robustness "is 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). In this context the metric Equalized Loss of Accuracy (Equalized Loss of Accuracy (ELA)) was established to measure the robustness of different machine learning models. But the ELA is only usable for classification models, therefore a different metric has to be found.

There are a number of ways to evaluate the performance of regression models, including mean squared error (MSE), mean absolute error (MAE), and root mean squared error (RMSE). You can use these measures to compare the performance of different regression models on a given task. Also the R^2 can be used to measure the robustness of the model.

As mentioned in section 4.2.3 dataset exploration the dataset has a high quality with no outliers and no missing values. Therefore, these data quality issues will be added to the dataset to measure the robustness of the model.

5.4.1 | Missing values

When applying the model to real-world data, there is a chance that some values are missing. Two possible scenarios are possible:

1. **Missing Vt -combinations:** There is no data available about a metal with a certain thickness and die opening. Reasons could be that the metal is not used in the industry or the data was never measured.
2. **Missing values:** There is data for the Vt combination but some values are missing because of general data quality issues.
3. **Outliers:** There are values that are not in the range of the dataset. Reasons could be that the data was measured incorrectly.

To measure all three of these scenarios, three different tests were created. The first test measures the robustness of the model.

1. Missing Vt -combinations

As can be seen Figure 4.8 of the test and training dataset, all possible Vt combinations in the set parameter range were measured. This is not the case in real-world data. Therefore, the robustness of the model has to be measured with missing Vt combinations.

Therefore, certain Vt combinations were removed from the training dataset. The removed Vt combinations were chosen randomly. The number of removed Vt combinations was 10% of the total number of Vt combinations in the training dataset. Subsequently the model was trained on the training dataset with the removed data and evaluated on the test dataset. The performance of the model is measured against the performance of the model trained with all data.

Calculation of the loss of accuracy

The process described above was done 100 times, to mitigate the effect of the random selection of the Vt combinations. The calculation of the loss of accuracy follows Equation 5.5, the metric is called Mean Loss Of Accuracy (Mean Loss of Accuracy (MLA)).

Mean Loss Of Accuracy

$$MLA = \frac{1}{100} \sum_{i=1}^{100} (MSE_{all} - MSE_{missing}) \quad (5.5)$$

To calculate the loss of accuracy the models trained with missing Vt combinations were compared to the model trained with all data. The difference between the mean squared error (MSE) of the models was calculated. The total loss of accuracy was calculated by averaging the difference of the MSE of the models.

2. Missing values

3. Outliers and wrong data

To measure the robustness of the model, outliers were added to the data. The outliers were added to the data in the following way:

Outliers were added to the training dataset. The model was trained on the training dataset. The model was evaluated on the test dataset. The outliers were removed from the training dataset. The process was repeated 100 times.

Noise

Not sure if I want to measure that.

Note: This process of measuring the robustness of the model differs from the approach used by Siebert and Sáez et al..

5.4.2 | Results

Model Name	Missing V_t -combinations loa	Missing Values loa	Outliers loa
Random Forest	0.034	0.000	0.771
Boosting	0.000	0.000	0.000
Linear Regression	0.000	0.000	0.000
Support Vector	0.000	0.000	0.000

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

Notes

- An alternative metric instead of ELA could be the approach of Scher and Trügler. But it would be necessary to implement the metric in Python.
- Decide if I want to evaluate noise as well or if the rest is enough.
- TODO: Visualize effect of training set size (Cookbook)

5.5 | Stability

Stability is the ability of the model to generate repeatable results when trained on different data. (Siebert, p. 16) To measure the stability of the model, leave-one-out cross-validation (Leave one out cross validation (LOOCV)) was used. LOOCV is

Leave-one-out cross-validation LOOCV

$$LOO = \frac{1}{n} \sum_{i=1}^n \frac{1}{\hat{y}_i} |y_i - \hat{y}_i| \quad (5.6)$$

LOOCV is another method that is commonly used. It can be thought of as a type of k-fold cross-validation where each fold consists of a single sample. During each split, a single data point is selected to be the test set. This method can be very time-consuming, especially for large datasets, but it may provide more accurate estimates for small datasets. (Müller and Guido, p. 257-258)

The variance of all Cross-validation (CV) scores is calculated with the formula ???. A low variance indicates that the model is stable which means that the model's performance is consistent across different training and testing sets. This is generally a desirable property for a model to have, as it suggests that the model is not overfitting to the training data and is able to generalize well to unseen data.

On the other hand, a high variance indicates an unstable model and is a sign of overfitting, as the model may be too closely tied to the training data and not generalize well to unseen data.

5.5.1 | Results

Model Name	Variance of LOOCV
RF	0.053
RFB	0.000
LR	0.000
SVM	0.000

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

Explanation of the results

Notes

- *Why exactly does the variance of LOOCV measure the robustness and the variance of CV the relevance?*

5.6 | 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, p. 16) It is the extent to which the inner workings of the model and the reasoning behind its predictions can be understood by human users. 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. To measure the interpretability of the model, the following metrics are used:

The number of parameters in the model Measured as integer, representing the total number of parameters in the model. Models with more parameters are generally more complex and more prone to overfitting

Depth of the model Measured as an integer, representing the number of layers in the model. A model with many layers, is generally more complex than a shallow network with fewer layers.

Inference time Measured in milliseconds. Time it takes to make a prediction. A model that takes longer to make predictions may be more complex than a model that is able to make predictions more quickly.

Level of interpretability Harder to measure but some ideas:

- *Partial dependence plots: These plots show the relationship between a single feature and the model's predictions, holding all other features constant. This can help to identify which features are most important for the model and how they influence the predictions.*
- *LIME (Local Interpretable Model-Agnostic Explanations): This is a method for explaining the predictions of any black-box classifier. It works by training an interpretable model locally around the prediction of interest, and using this local model to explain the prediction of the black-box model.*

- **SHAP (SHapley Additive exPlanations):** This is another method for explaining the predictions of black-box models. It works by assigning importance to each feature based on its contribution to the model's prediction.

Amount of training data required Will be the same for all models so this metric may not be used.

5.6.1 | Results

Model Name	Number Parameters	Depth	Inference	Interpretability
RF	0.000	0.000	0.000	0.000
RF Bossing	0.000	0.000	0.000	0.000
LR	0.000	0.000	0.000	0.000
SVM	0.000	0.000	0.000	0.000

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

Explanation of the results

5.7 | 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.

Runtime 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.

The runtime is measured using the `time.time` function in python. On value is picked out of the test set and the time is measured before and after the prediction is made. The difference between the two times is the runtime.

Storage space Measured in kilobytes. It refers to the amount of storage space required to store 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.

Model Name	Training time s	Runtime ms	Storage space kb
RF	0.0222	2.0275	80.2
LR	0.000	0.000	0.000
SVM	0.000	0.000	0.000

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

5.8 | Summary

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

Conclusions

6.1 | Revisiting the Aims and Objectives

6.2 | Critique and Limitations

6.3 | Future Work

6.4 | Final Remarks

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