Enhancing Manufacturing Quality Prediction Models Through the Integration of Explainability Methods

Dennis Gross¹, Helge Spieker¹, Arnaud Gotlieb¹ and Ricardo Knoblauch² ¹Simula Research Laboratory, Oslo, Norway ²Ecole Nationale Supérieure d'Arts et Métiers, Aix-en-Provence, France

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Abstract: This research presents a method that utilizes explainability techniques to amplify the performance of machine learning (ML) models in forecasting the quality of milling processes, as demonstrated in this paper through a manufacturing use case. The methodology entails the initial training of ML models, followed by a fine-tuning phase where irrelevant features identified through explainability methods are eliminated. This procedural refinement results in performance enhancements, paving the way for potential reductions in manufacturing costs and a better understanding of the trained ML models. This study highlights the usefulness of explainability techniques in both explaining and optimizing predictive models in the manufacturing realm.

1 INTRODUCTION

Milling is a subtractive manufacturing process that involves the removal of material from a workpiece to produce a desired shape and surface finish. In this process, a cutting tool known as a milling cutter rotates at high speed and moves through the workpiece, removing material. The workpiece is typically secured on a table that can move along multiple axes, allowing for various orientations and angles to be achieved (Fertig et al., 2022). The energy consumption during the milling process can vary significantly based on several factors, including the specific setup and the materials being processed. However, it is often considered to be a relatively energyintensive process. Being able to foresee and avert potential quality issues means that less energy is expended and fewer resources are wasted on creating defective parts, which would otherwise be rejected or require reworking (Pawar et al., 2021).

Machine learning (ML) models are capable of identifying patterns and structures in data to make predictions without being directly programmed to do so. These models can be a useful tool in forecasting the final quality of a workpiece at the end of the milling process, helping to improve both the efficiency and the reliability of the manufacturing process (Mundada and Narala, 2018).

Lack of Data. However, the available milling experiment data is typically small because the costs for each manufacturing experiment are very high (Postel et al., 2020). This lack of data makes it difficult to learn ML models to predict the workpiece quality.

Explainability Problem. Even if abundant data were available, utilizing complex ML models, such as deep neural network models, presents a significant challenge due to their "black box" nature. This term denotes the lack of transparency in understanding these models' internal workings, which often remain inaccessible or unclear (Kwon et al., 2023). In the realm of turning process quality prediction, an explainability problem arises when practitioners and stakeholders can not fully understand the predictions given by these models due to their complex and opaque nature.

Leveraging Explainability Techniques for Optimized Model Training. Explainability methods are, therefore, crucial in unraveling the complex prediction mechanisms embedded within ML models. Furthermore, they facilitate enhanced performance of ML models by identifying and addressing potential inefficiencies, thereby steering optimization efforts more effectively (Bento et al., 2021; Sun et al., 2022).

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Gross, D., Spieker, H., Gotlieb, A. and Knoblauch, R. Enhancing Manufacturing Quality Prediction Models Through the Integration of Explainability Methods. DOI: 10.5220/0012417800003636 Paper published under CC license (CC BY-NC-ND 4.0) In Proceedings of the 16th International Conference on Agents and Artificial Intelligence (ICAART 2024) - Volume 3, pages 898-905 ISBN: 978-989-758-680-4; ISSN: 2184-433X Proceedings Copyright © 2024 by SCITEPRESS – Science and Technology Publications, Lda. Approach. We use less computational processingintense ML models, such as decision tree regression or gradient boosting regression, and improve their performance via explainability methods. We do this by training these models on a milling dataset, identifying the important features for these models for their predictions, removing the less important features from them, and retraining a new model on stretch on the feature-pruned data set. Our results show, on a case study from the manufacturing industry in the context of milling, that we can improve the performance of ML models and reduce financial manufacturing costs by pruning the features. These findings indicate that the strategies used in recent studies for enhancing ML model performance through explainability (Bento et al., 2021; Sun et al., 2022) can be effectively adapted for manufacturing processes.

Plan of the Paper. The rest of the paper is organized as follows: Section 2 covers existing works on using AI for manufacturing/machining problems; Section 3 presents our explainability methodology and how to apply it to ML models; Section 4 explains how to deploy our explainability methodology to quality prediction model used in surface milling operations. Eventually, Section 5 and Section 6 respectively discuss the benefits and drawbacks of using explainability methods in machining and conclude the paper by drawing some perspectives to this work.

2 RELATED WORK

The usage of ML in manufacturing/machining tasks has been recognized as an interesting lead for at least a decade (Kummar, 2017). For instance, ML has been used initially to optimize turning processes (Mokhtari Homami et al., 2014), predicting stability conditions in milling (Postel et al., 2020), estimating the quality of bores (Schorr et al., 2020), or classifying defects using ML-driven surface quality control (Chouhad et al., 2021).

However, it is only recently that Explainable AI (XAI) methods have been identified as an interesting approach for manufacturing processes (Yoo and Kang, 2021; Senoner et al., 2022). The ongoing European XMANAI project (Lampathaki et al., 2021) aims to evaluate the capabilities of XAI in different sectors of manufacturing through the development of several use cases. In particular, fault diagnosis seems to be an area where XAI can be successfully applied (Brusa et al., 2023). Also, there exists work that focuses on feature selection on the dataset without taking the ML model directly into account (Bins and Draper, 2001; Oreski et al., 2017; Venkatesh and Anuradha, 2019). Our approach in this paper is to explore the potential of XAI for enhancing quality prediction models by eliminating unnecessary sensors. Even though the approach of improving ML models via explainability methods is known in the context of explainable ML (Bento et al., 2021; Sun et al., 2022; Nguyen and Sakama, 2021; Sofianidis et al., 2021), to the best of our knowledge, it is the first time that XAI is used for that application. In particular, identifying unnecessary features through XAI methods to improve quality prediction models in milling processes is novel.

3 METHODOLOGY

Our approach works as follows: First, we train an ML model on the given data set. Second, we apply an explainability method to the ML model and the data set to identify the most important features for the prediction accuracy. Third, we rank the features based on their feature importance in a descending ordered sequence and incrementally increase the number of features being used for the training (for each new setting a new ML training). Fourth, we take the features that led to the best-performing model. We now explain the different steps in more detail.

3.1 Machine Learning Models

In this study, we use decision tree regression, gradient boosting regression, and random tree regression models for the prediction process. These ML models are less data-intensive than neural networks and are considered easier to interpret.

Decision Tree Regression Models. Decision tree regression models partition the input space into distinct regions and fit a simple model (typically a constant) to the training samples in each region. For a new input x, the prediction \hat{y} is obtained from the model associated with the region R_m that x belongs to. The prediction can be expressed formally as:

$$\hat{y}(x) = \sum_{m=1}^{M} c_m I\{x \in R_m\}$$

where c_m represents the constant fitted to the samples in region R_m , M is the number of regions, and $I\{\cdot\}$ is an indicator function. This model is capable of capturing non-linear relationships through a piecewise linear approach (Myles et al., 2004).

Gradient Boosting Regression Models. Gradient boosting regression models optimize a given loss function $L(y, \hat{y}(x))$ by combining multiple weak models. The model starts with an initial approximation $F_0(x)$ and iteratively refines this through the addition of weak models $h_m(x)$. The update at each iteration *m* is described by:

$$F_m(x) = F_{m-1}(x) + \alpha \cdot h_m(x)$$

where $F_m(x)$ is the model at iteration m, α is the learning rate, and $h_m(x)$ is a weak learner aimed at correcting the errors of the previous models. This iterative process results in a robust predictive model (Otchere et al., 2022).

Random Tree Regression Models. Random Tree Regression models also employ an ensemble learning strategy, building multiple decision trees during the training phase and aggregating them for predictions. The final prediction \hat{y} for an input *x* is the average prediction across all trees in the ensemble:

$$\hat{y}(x) = \frac{1}{T} \sum_{t=1}^{T} y_t(x)$$

where T is the total number of trees and $y_t(x)$ is the prediction of the *t*-th tree. This aggregation helps enhance the model's generalization capabilities and mitigates the risk of overfitting (Prasad et al., 2006).

3.2 Explainability Methods

Feature Permutation Importance. A critical aspect of our approach is employing feature permutation importance as a significant explainability method. This technique operates by evaluating the importance of different features in the model. The general procedure involves the random permutation of a single feature, keeping others constant, and monitoring the change in the model's performance, often measured through metrics like accuracy or mean squared error (Huang et al., 2016).

Mathematically, the feature importance I_i of a feature *i* can be defined as the difference in the model's performance before and after the permutation of the feature and can be formulated as:

$I_i = P_{original} - P_{permuted(i)}$

where $P_{original}$ is the model's performance with the original data and $P_{permuted(i)}$ is the performance with the *i*-th feature permuted.

By iterating this process across all features and comparing the changes in performance, we can rank the features by their importance, offering deeper insights into the model's decision-making process and enabling the identification of areas for optimization and refinement.

Shapley Values. The Shapley value, originating from cooperative game theory, allocates a fair contribution value to each participant based on their marginal contributions to the collective outcome. In the context of machine learning models, Shapley values are used to quantify the contribution of each feature to the prediction made by the model (Sundararajan and Najmi, 2020).

Given a predictive model $f : \mathbb{R}^n \to \mathbb{R}$, where *n* is the number of features, the Shapley value of the *i*-th feature is calculated as follows:

$$\phi_i(f) = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|! \cdot (n - |S| - 1)!}{n!} \left[f(S \cup \{i\}) - f(S) \right]$$

where:

- *N* is the set of all features.
- *S* is a subset of *N* not containing feature *i*.
- |S| denotes the number of features in subset S.
- f(S) is the prediction of the model when only the features in *S* are used.
- The term $f(S \cup \{i\}) f(S)$ represents the marginal contribution of feature *i* when added to the subset *S*.

The Shapley value $\phi_i(f)$ captures the average contribution of feature *i* to the model's prediction, averaged over all possible subsets of features. This comprehensive averaging process ensures a fair distribution of contributions, considering all possible interactions between features.

It is important to note that the computation of Shapley values can be particularly intensive, especially in scenarios where the number of features is large. This is due to the necessity to evaluate the model's prediction for every possible combination of features, resulting in a total of 2^n model evaluations for *n* features. Therefore, practical implementations often employ approximation methods or sampling strategies to mitigate the computational demands.

4 CASE STUDY

In this case study, we apply our method to a dataset generated at MSMP - ENSAM. A series of surface milling operations were performed on aluminum 2017A using a 20 mm diameter milling cutter R217.69-1020.RE-12-2AN with two carbide inserts XOEX120408FR-E06 H15 from SECO, and a

synthetic emulsion of water and 5% of Ecocool CS+ cutting fluid.

In total, 100 experiments have been carried out varying the following process parameters: depth of cut, cutting speed, and feed rate. For each one of these experiments with different control parameters, cutting forces F_z (normal force) and F_a (active force), and surface profiles are measured on-machine using a Kistler 3-axis dynamometer 9257A and a STIL CL1-MG210 chromatic confocal sensor (non-contact) respectively. In the feature engineering step, the following surface roughness amplitude parameters are calculated using MountainsMap software. Ra is the most commonly used in the industry.

- Ra (Average Roughness): Average value of the absolute distances from the mean line to the roughness profile within the evaluation length.
- Rz (Average Maximum Height): Average value of the five highest peaks and the five deepest valleys within the evaluation length.
- Rt (Total Roughness): Vertical distance between the highest peak and the deepest valley within the evaluation length.
- Rq (Root Mean Square Roughness): Square root of the average of the squared distances from the mean line to the roughness profile within the evaluation length.
- RSm (Mean Summit Height): Average height of the five highest peaks within the evaluation length.
- RSk (Skewness): Measure of the asymmetry of the roughness profile around the mean line.
- Rku (Kurtosis): Measure of the peakedness or flatness of the roughness profile.
- Rmr (Material Ratio): Ratio of the actual roughness profile area to the area within the evaluation length.
- Rpk (Peak Height): Height of the highest peak within the evaluation length.
- Rvk (Valley Depth): Depth of the deepest valley within the evaluation length.
- Rdq: It is a hybrid parameter (height and length). It is the root mean square slope of the assessed profile, defined on the sampling length. Rdq is the first approach to surface complexity. A low value is found on smooth surfaces, while higher values are found on rough surfaces with microroughness.

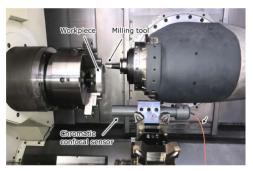


Figure 1: Milling machine that produces workpieces.

4.1 Objective

The aim is to develop a predictive model for each quality metric associated with roughness amplitude parameters. This necessitates not only the training of accurate models but also an elucidation of the predictive rationales behind their outputs. Concurrently, there is a need to identify and eliminate superfluous features from the models. This is a strategic step to minimize both installation and maintenance expenses related to redundant sensors, thereby optimizing resource allocation and reducing overall costs.

4.2 Data Preprocessing

Since we are dealing with variable time series lengths, we calculate the box plot values for each time series in the time and frequency domain. Additionally, metadata within the dataset comprises experiment parameters with various focuses.

4.3 ML Model Training

We trained a decision tree regression, gradient boosting regression, and random forest models for each quality measure. See the overall input-output of the models in Figure 2. We employ a 5-fold crossvalidation approach for each model training. In this method, the data is divided into five equal parts. In each iteration, four parts (80%) are used for training the model, and the remaining one part (20%) is utilized for testing. This process is repeated five times, with each of the five parts serving as the test set exactly once. The performance of the model is then averaged over the five iterations to obtain a more robust estimate of its effectiveness.

4.4 Analysis

In this section, we analyze our approach. First, we evaluate the ML model performance. Second, we an-



Figure 2: The ML prediction model receives the box plots (for time and frequency domains) and machine configuration parameters to output the quality measures.

alyze the predictive mechanisms of the ML models. Third, we evaluate the effect on the ML model performances by removing features.

4.4.1 Evaluating the Predictive Quality of the Models

The objective of this study is to evaluate the predictive accuracy of three distinct ML models: gradient boosting regression, decision tree, and random forest. In assessing the quality of the predictions, the key metric employed is the *Mean Absolute Percentage Error (MAPE)*. A prediction is considered to be of high quality if its MAPE is below 5%.

Setup. Preprocessed dataset with 100 samples.

Execution. We trained three different machine learning models: gradient boosting regression, decision tree, and random forest on the preprocessed dataset and used k-fold cross-validation to measure their MAPE.

Findings. By employing these ML techniques on an exhaustive set of quality features, we achieved predictions for Rdq with an error rate of less than 5%. Specifically, the Gradient Boosting Regression model yielded an error rate of 4.58%, while the Random Forest model yielded an error rate of 4.88%.

4.4.2 Understanding the Predictive Mechanisms of the ML Models

This study assessed the importance of various attributes in forecasting quality metrics.

Setup. Given the trained models, we focus here on the gradient-boosting regression model, which achieved the highest performance.

Execution. We applied feature permutation importance and Shapley value to the prediction model.

Findings. We observed that the different explanation methods yield different reasons. For instance, permutation feature importance highlights fa_ts_max more important than the Shapley method (see rank one vs. rank two Figure 3). In the justification of our experiment, it is crucial to acknowledge that employing various explanation methods to interpret ML models is expected to yield divergent explanations. This disparity stems from the intrinsic differences in methodological approaches, the complexity of the models, the data dependence of explanations, and the approximations and assumptions inherent in each explanation method. These factors collectively contribute to variations in identifying important features (Lozano-Murcia et al., 2023).

4.4.3 Performance Improvements

In this experiment, we aimed to explore the potential benefits of integrating explainability methods into the ML model development process, focusing on enhancing model performance.

Setup. To initiate this, we categorized the variables in our ML model based on their respective feature importance, arranging them in descending order. This categorization enabled us to identify and quantify the significance of each feature in the context of model training. We did this for feature permutation importance, Shap values, and a baseline feature selection method. The baseline method is *SelectKBest method*, a component of the Scikit-learn library (Pedregosa et al., 2011), for the purpose of univariate feature selection. This technique operates on the principle of evaluating individual features based on statistical tests, ultimately selecting the k features that demonstrate the highest relevance or significance.

Execution. Following the setup phase, we conducted a series of trials where we systematically varied the top percentage (p) of important features incorporated into the training dataset. In each trial, a new model was trained exclusively on the top p% of the most significant features, excluding potentially less impactful features from the model training process.

Findings. We enhanced the ML models' performance by integrating only the most critical features into the training dataset (see Figure 4). This approach effectively streamlined the model by removing unnecessary features, improving performance, and potentially allowing for more transparent and explainable model operations. For example, by choosing only the

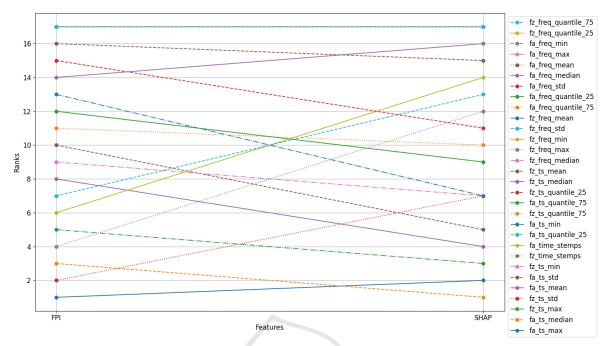


Figure 3: Visualization demonstrating the feature importance rank of Rdqmaxmean predictions, as elucidated by the feature permutation importance permutation (FPI) and Shapley value (SHAP) method.

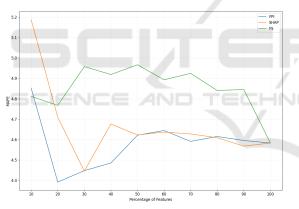


Figure 4: Using a different percentage of the most important features based on the different methods for the Rdq prediction. *FS* refers to feature selection.

top 20% of features deemed most critical (as determined by permutation importance), we enhanced the MAPE from approximately 4.58 to 4.4.

5 DISCUSSION

Our case study shows the benefit of explainable ML techniques for quality prediction models in manufacturing. Explainability scores, as provided by the feature importance studied in our case study, allow to interpret the results and determine the relevance of individual features for the predictive power of a model. This interpretation can be utilized by human domain experts for the analysis of the trained model and a plausibility check, whether those features with high importance are meaningful for the predictive task. While it is known that ML models might reveal previously unknown relationships between input features and the prediction target, this is a rather unlikely case in our quality prediction setting. Instead, an overreliance on a specific feature can be an indicator for learning a spurious correlation between an input and the target, potentially caused by a lack of relevant data in the small data regime. Explainability can, therefore, serve as an instrument for model validation and human inspection.

Furthermore, the feature importance scores support the improvement of models, as demonstrated in Section 4.4.3 by removing low-ranked features. Besides improving the prediction accuracy of the actual models, feature removal has additional benefits for deploying ML models for manufacturing quality prediction. If the removed features relate to sensor data, their removal also removes the necessity of frequently reading and preprocessing that sensor, which reduces the computational cost of making predictions. When doing real-time quality prediction to detect potential faults or deviations from the process plan during production, minimizing the time needed to make a prediction and increasing the frequency in which predictions can be made is crucial.

In cases where the model development for quality

prediction is considered during the prototyping phase and construction of the manufacturing machine, the relevance of features can inform the selection of physical sensors to be deployed on the machine. The prototype machine is equipped with a larger set of sensors, and only after evaluating the prediction models is the final set of relevant sensors determined.

Finally, besides the direct relation to the manufacturing case study, we see the benefit of deploying smaller, less complex, and ideally interpretable models (Breiman, 2001; Rudin et al., 2022). At the same time, there is a trade-off between simplicity and accuracy, referred to as the Occam dilemma (Breiman, 2001). The simpler a model is made, the less accurate it gets. We see this in the case study from the error difference between the simpler decision tree vs. the more complex gradient-boosting trees or random forest. By applying explainability methods to reduce the feature space, we again reduce the model complexity, making the final model more interpretable.

6 CONCLUSION

This study showcases the potential of combining ML and explainability techniques to enhance the performance of predictive models of surface quality in the manufacturing sector, specifically in the context of the milling process. Despite the limitations imposed by data availability, our approach successfully leverages less data-rich ML models, enhancing their efficacy through feature selection based on explainability methods.

For future work, we are interested in extending the application of explainability methods in ML models to other manufacturing processes of our partners beyond milling to create a more comprehensive predictive system. Additionally, utilizing these ML models as digital twins for the corresponding physical machinery opens new avenues for employing parameter optimization methods. This integration not only enhances the accuracy of the models but also provides an opportunity for real-time fine-tuning of machine operations, thereby potentially improving efficiency and reducing costs.

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