Data-driven approach to optimize the relative density in additive manufacturing processes

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ABSTRACT

Additive manufacturing (AM) is a modern production technology to manufacture complex designs which are otherwise impossible to produce with conventional production technologies. However, the inherently large number of influential parameters, such as layer height and extrusion rate, lead to difficulties during the ramp-up phase for new products until the optimal parameter combination is found. Unfortunately, conventional techniques for optimization (e.g. finite element analysis) are resource-intensive and mostly design specific. Additionally, even though sophisticated methods from the domain of machine learning can be utilized as well, to the best of our knowledge, existing research largely focuses on in-situ process monitoring or ex post quality inspection. However, these methods do not support the selection of suitable process parameters in advance. Thus, a combined methodology consisting of traditional aspects and machine learning is proposed. First, supposedly influential factors are selected, a repeated factorial design of experiments is conducted to generate high-quality data samples, and the target value is measured. Second, the random forest algorithm is utilized to determine the feature importance of each influential factor. Third, the most relevant features are used to train several machine learning models to predict the target quality characteristic. Fourth, a repeated k-fold cross validation is employed to evaluate the models, so that the best model can be selected in spite of the small data set. This methodology was validated for the relative density of extrusion-based AM parts. As it was shown, the best model can reliably (R-squared of 0.92) predict the relative density purely based on process parameters. Consequently, the resulting model can be utilized to support an efficient ramp-up phase and future work can focus on extending the methodology for other AM technologies and quality characteristics.

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CCS CONCEPTS

• **Computing methodologies** → **Cross-validation**; **Classification and regression trees**; **Ensemble methods**; • **Applied computing** → **Industry and manufacturing**.

KEYWORDS

additive manufacturing, machine learning, process optimization

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1 INTRODUCTION

Additive manufacturing (AM) represents a modern production technology from the group of prototyping [2], with which physical components are generated through layer-by-layer material application. In contrast to conventional, mostly subtractive manufacturing technologies, such as turning, milling or drilling, no material is removed from existing solid parts, but is usually applied without a geometrically defined tool shape. The volume of a component is created by iteratively joining horizontal material layers in X- and Y-direction to form volume elements in the Z-direction. The hypernym additive manufacturing combines different processes which are based on the same manufacturing principle of layer-by-layer material application, but which differ from one another in terms of the specific procedure. Depending on the process type, the raw material is either in a solid (e.g. wire, powder, films, sheets), liquid (e.g. viscous pastes, low-viscosity liquids) or gaseous (e.g. gasified material) aggregate state [3].

Due to selective material application, one major advantage of AM is that components can be deliberately underfilled (relative density < 100 %), resulting not only in weight and cost advantages, but also in accelerated production times. However, this approach becomes problematic in the case of mechanically stressed structural components. Compared with their fully filled counterparts, the resistance against external forces is much lower with a relative density below 100 % [18]. This is particularly critical in extrusion-based AM processes such as fused filament fabrication (FFF), since the deposition of material is based on tool paths in the X/Y and Z directions. Thus, as shown in Figure 1, due to the characteristics of the FFF technology, components are either unwillingly underfilled (deadzones) or the geometrical accuracy is negatively influenced by deliberately overlapping the paths (over-extrusion). In case of

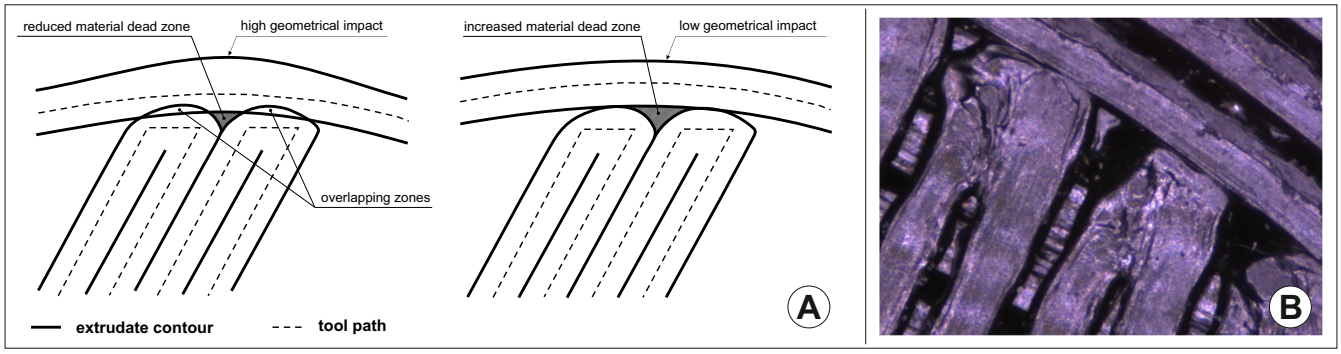

Figure 1: A: Deliberate over-extrusion (left) increases the relative density, but also influences the geometrical accuracy. Maximizing dimensional accuracy is inevitably accompanied by increased dead zones (right) [4].
B: Image taken with measuring microscope shows the material dead zones on the real printing part.

the latter, the AM part is physically strengthened, whereas the geometric properties deteriorate.

Furthermore, due to its low level of technological maturity [9], the industrial form of AM is a challenging field of activity that requires an extended level of know how. Nevertheless, in the area of end-use parts, customers generally place the same requirements on AM parts as on classically subtractively manufactured components. Therefore, companies focused on extrusion-based AM processes face particular challenges, since in addition to basic quality factors, such as geometrical accuracy and surface finish, the relative density of the component is an important quality characteristic, as it has a significant influence on the structural integrity of a part [19].

To ensure consistent quality characteristics (e.g. relative density), traditional methods (e.g. finite element analysis or design of experiments) are often applied. However, associated costs and design-specific results lead to additional challenges. Apart from these traditional methods, machine learning approaches are successfully applied in additive manufacturing processes during or after the process to determine the product quality [5, 16]. Nevertheless, instead of focusing on an in-situ quality prediction, the following work utilizes machine learning to predict quality characteristics during the design stage, to reduce the number of faulty processes in advance.

Thus, the following paper proposes a method for data-driven modeling of the relative density and is structured as follows. Section 2 elaborates on related work, in particular on traditional methods and machine learning approaches. In section 3 the methodology is discussed in detail, whereas section 4 describes the experimental setup. Afterwards, the results are shown and discussed in section 5 and the paper is concluded in section 6.

2 RELATED WORK

2.1 Conventional methods

The complex customer requirements for additively manufactured components usually lead to extended ramp-up phases and increased time-to-market, especially in the course of new product developments. To increase efficiency, it is typically attempted to transfer experience from already produced components to new designs. However, this is usually only possible to a limited extent, especially in the case of complex parts or different materials.

In the *manual trial and error* approach, attempts are made to optimize the target variables (e.g. the relative density) by manually adjusting printing parameters. This approach requires the operator to have a high degree of expertise in the key production factors of the manufacturing process, the material and the 3D printer itself. In the course of the manual trial and error approach, an extensive pilot series is usually produced, which are accompanied by corresponding time and cost expenditures [19]. To systematize the attempts of manual trial and error, the *Design of Experiments* (DoE) comes into focus. It is an effective approach for maximizing the learning effect while consciously limiting required resources. The combination of mathematics and statistics applied to the AM process makes it possible to determine which controllable and uncontrollable manufacturing parameters are influencing the process output [14]. In addition to an experimental approach, *numerical methods* can be applied. In particular, finite element analysis (FEA) is used for complex components. FEA represents a numerical method for determining approximate solutions of partial differential equations. In the course of FEA, a complex solid body, is divided into a finite number of trivial partial bodies (= finite elements). The behavior of these simple geometries can be calculated, which finally leads to insights about the behavior of the entire component. FEA is used in additive manufacturing especially for strength and deformation analyses, which are implicitly also related to the density, and even for coupled thermomechanical and thermal analyses. The application of numerical simulation methods makes it possible to reduce repetitive, material-intensive experiments to a minimum. However, numerical methods usually entail significant computational efforts in addition to high complexity, which means that simulations can sometimes take days or even weeks. This fact often limits the applicability of FEA in the context of AM [17].

2.2 Data-driven methods

Apart from conventional methods, such as FEA or DoE, which require extensive resources, machine learning approaches are increasingly used for applications along the entire AM process, from the design stage to post-production quality inspection [12, 19]. In

this regard, machine learning can be generally categorized in supervised, unsupervised and reinforcement learning, whereas the latter is hardly used in the context AM. Supervised learning requires training data consisting of input variables and associated output values (labels) to train a model which can be used to predict the target, such as the tensile strength. On the other hand, unsupervised learning does not require labeled data, but identifies patterns within the data without a given target variable. Consequently, the effort for labeling the data set is reduced (or avoided) at the cost of explicit information about the target variable [19].

Therefore, a combined approach utilizes the advantages of both, supervised and unsupervised learning. In this regard, Gobert et al. combined OTSU thresholding (unsupervised) with convolutional neural networks (CNN, supervised) to detect porous areas in X-ray computed tomography (XCT) images of metallic products produced with metal powder bed fusion technology. Even though, this accelerates and improves the quality inspection of produced pieces, the ex post approach cannot mitigate faulty products [5]. Hence, as noted by Li et al., an ex post quality inspection leads to unnecessary waste in terms of time and material in case of detected quality issues. Thus, they introduced an in-situ detection for surface issues, whereas several machine learning algorithms were evaluated. Additionally, to reduce the number of features for the model, the importance of each feature was quantified with the random forest algorithm. In order to reduce the costs associated with each manufactured product, the authors relied on synthetic data for training purposes and only validated the models with 3D-scans of actual parts [10].

On the other hand, Shevchik et al. focused on in-situ prediction of porosity based on acoustic emissions and a CNN. The data was collected for one manufactured cuboid during a selective laser melting process, whereas the energy density was modified during the process. Thus, a sufficient variation of acoustic signals paired with porosity values were generated for training and testing purposes [15]. Similarly, Khanzadeh et al. also proposed a method for in-situ prediction of porous areas. However, in contrast to Shevchik et al., melt pool images in combination with XCT were used as input for supervised learning techniques to predict porosity [8]. These research articles demonstrate the wide range of suitable approaches for predicting the same properties. Moreover, the same data source, for instance XCT images, are used for predicting different properties as well. As shown by Snow et al., layer-wise XCT images as input for a CNN model can also be used for in-situ detection of internal flaws and prediction of the resulting fatigue performance [16]. However, even though these in-situ applications of machine learning models can be used to employ repair measures during the process [16], they are unfit to optimize process parameters in advance. This is particularly relevant during the ramp-up phase of new AM products, in which the optimal parameters are usually unknown. Importantly, the input variable for the actual machine learning model are usually limited to sensor signals during the process and neglect the overall process parameters [11, 15, 16]. Thus, these approaches do not make use of a priori data and cannot be used for selecting suitable process parameters in advance.

To address these issues, Jiang et al. trained and employed a machine learning model solely based on process parameters (extrusion rate, print speed, layer height, line distance) to predict inner-line connections. These connections were classified into 5 categories, ranging from gaps between neighboring lines (paths) to overlapping lines. The resulting model is used for selecting process parameters before the production. However, no quantitative details were presented regarding the labeling process and the prediction was purely used as an indicator for dimensional accuracy. Moreover, only one repetition of the experiments was performed leading to potentially biased results [7]. Thus, even though similar factors are relevant for the relative density investigated in this paper, additional work is required for a comprehensive methodology.

In particular, even though, porosity was investigated in several studies, to the best of our knowledge, the relative density of extrusion-based AM parts was not subject to any related research. Moreover, the majority of literature sources is focused on in-situ or ex post quality inspection, which cannot be used to optimize the process parameters in advance. Hence, the methodology, elaborated in the following section, addresses these research gaps.

3 METHODOLOGY

To address the shortcomings of related work, we propose to use DoE as a conventional method, which is usually used for individual process optimization, to generate the data base for training a machine learning model to predict quality characteristics of AM parts before they are produced. In contrast to individual process optimizations based on a DoE, a ML model with generic input parameters, for instance, layer height and extrusion width, can be applied for different designs. Thus, the remaining part of this section elaborates on the methodological steps.

3.1 Design of Experiments

Similar to related research [7, 11], a DoE is employed to generate the data for training and validating the machine learning models. In this regard, four process parameters were selected for investigating their influence on the relative density of the final part. First, the *infill pattern*, such as rectilinear or conical infill paths, is investigated due to its impact on the calculated tool paths. Second, the *layer height* (or thickness) describes the height of each single layer in the production process. Third, the *extrusion width* represents the line (or path) width, which is used to calculate the number and position of individual paths in the slicer software. This value corresponds to line distance [7]. The layer height, extrusion width and print speed (statically defined in this work) are used by the slicer software to calculate the extrusion rate (material flow). However, as fourth investigated parameter, the *extrusion multiplier* is used to manually adjust this extrusion rate, so that the calculated material flow is either decreased (multiplier < 1.0) or increased (multiplier > 1.0) depending on the extrusion multiplier. Consequently, in the case of a multiplier larger than 1.0, potential dead zones between the lines are (partially) filled while leaving the number and position of individual paths as originally calculated by the slicer software. In addition to these process parameters, the influence of the *slicer* (methodology) used to generate machine code, itself is assessed as fifth parameter, since it is the main component which calculates the paths and extrusion rates. Moreover, due to its layer- and path-based build up process, the influence of the *geometrical features* of the product is investigated as sixth parameter. Particularly, since the path of individual lines is affected by the geometry (sharp corners

or large radius) which could lead to larger or smaller gaps between paths.

3.2 Density Measurement

These six factors including their specific boundaries and instances (see below) are used to conduct experiments as basis for the measurements. In this regard, the density of each printed part can be measured with the Archimedes principle, whereas the part weight is measured in air and a defined liquid, so that the density of the product can be calculated based on the known density of the liquid at a known temperature and the difference in weight between air and liquid measurements.

The calculated value represents the absolute density of the corresponding part, which is mainly influenced by the properties of the filament. Thus, the relative density is of greater importance to quantitatively determine what proportion of the ideal volume of the product is filled with material. For that purpose, the absolute density of the input raw material (filament) must be known or measured in advance. Consequently, the relative density in this work is calculated as follows:

$$RD = \frac{M_{air}/V_{ideal}}{\rho_{fil}} = \frac{\rho_{part}}{\rho_{fil}} \tag{1}$$

As shown by the equation, the relative density of the part *RD* is calculated in relation to the measured density of the filament ρ_{fil}. The density of the part ρ_{part} is calculated with the actual weight of the product in air M_{air} and the ideal volume of the design V_{ideal}. As a result, *RD* can be interpreted as the degree to which the ideal volume is filled with the filament. Thus, if an overlap, as defined by Jiang et al. [7], occurs, the *RD* could exceed 100 %, meaning that the dimensional accuracy is not guaranteed.

As an alternative, the *RD* of the product could be calculated on the basis of the actually measured volume (through the Archimedes principle), which yields the degree of filled volume in relation to the overall volume including overflows. Consequently, the *RD* based on the actual volume cannot exceed 100 % and therefore, cannot be used to infer issues regarding overflows in the production process. Thus, the remainder of this work is focused on *RD* calculated based on the ideal volume of the part.

3.3 Data Preparation and Feature Selection

Preparing the data for later usage consists of two main steps. First, concerning categorical features, such as the slicer software, part geometry and infill pattern, are one-hot encoded, so that the information can be properly accessed by subsequent processes. Consequently, each category within the respective categorical feature is transformed into a boolean feature indicating if this particular category is present. Thus, a three-level categorical feature is represented with three individual boolean columns. Second, to ensure each numerical features are equally considered in subsequent processes, z-normalization is applied to transform each feature on the same scale.

To determine the actual relevance for each considered parameter (see above), the random forest feature importance is used. As described by Li et al., this approach is based on the characteristic of the random forest algorithm, which creates several uncorrelated decision trees to train the overall ensemble model. Thus, the non-linear importance of each feature can be calculated based on all individual decision trees [11]. As a consequence, selecting a subset of features simplifies the model complexity and also leads to new insights regarding the influential factors.

3.4 Machine Learning Algorithms and Validation

To create an adequate model for predicting the relative density based on process parameters, several machine learning algorithms are evaluated. First, the *random forest* algorithm as an ensemble method consisting of a number of individual decision trees is used for feature selection on the one hand and on the other hand also for training a predictive model. Second, a *decision tree* model is trained on the data to have a direct comparison of one individual tree model and the random forest ensemble. In this regard, a decision tree is iteratively build, so that each fork within the tree maximizes the information gain. Interestingly, each prediction within the decision tree can be directly explained by the model, so that a user can interpret the result in greater detail [13]. Third, a regularized ridge regression as representative for linear models is considered. This specific algorithm imposes a penalty on the sum of squared coefficients, which leads to smaller coefficients and a more robust regression [6].

The evaluation of the machine learning models is conducted with k-fold cross validation, to reduce the bias originating from the train-test split. Consequently, several (k) train-predict-evaluate cycles are executed, whereas the train and test data are different for each run ensuring that each data sample was at least once used as a training and test sample. The final evaluation score is calculated as the average of all individual cycles [20]. In this regard, as suggested by Chicco et al., the R-squared error metric is used to evaluate the machine learning models, whereas the following formula is used for calculating the score [1]:

$$R2 = 1 - \frac{\sum_{i=1}^{N}(y_i^{obs} - y_i^{pred})^2}{\sum_{i=1}^{N}(y_i^{obs} - \bar{y}_i)^2} \tag{2}$$

The observed (true) target values are represented by y^{obs} and the predicted values of the model by y^{pred}. Additionally, $\bar{y}$ denotes the mean of observed values, whereas N indicates the number of values for both y^{obs} and y^{pred}. As the formula shows, possible values for the R-squared score range from minus infinity to 1.0, meaning a perfect model fit.

4 EXPERIMENTAL SETUP

To train and evaluate the machine learning models an adequate data set is required. For this purpose, a DoE is set up based on 6 influential factors described above. Thus, each factor is associated with either a list of options or min/max boundaries. To investigate the influence of geometrical features, three conceptionally different products, a cuboid (l=40 mm, w=20 mm, h=30 mm), a cylinder (h=30 mm, r=20 mm) and a cone (h=30 mm, r=20 mm), are produced. Moreover, two slicer software solutions – Cura and Simplify – are considered for these experiments. Since the infill pattern mainly determines the paths of the infill, two different patterns are evaluated. On the one

Table 1: Parameters including values and boundaries for the DoE

No.	Parameter	Min. value	Max. value	Options
1	Part geometry	-	-	Cuboid, Cylinder, Cone
2	Slicer software	-	-	Ultimaker Cura, Simplify3D
3	Infill pattern	-	-	rectilinear, conical paths
4	Layer height	0.05 mm	0.3 mm	-
5	Extrusion width	0.6 mm	1.0 mm	-
6	Extrusion multiplier	1.0	1.15	-

Table 2: One-fourth fraction experimental design for factors 2-6.

No.	Slicer	Infill pattern	Layer height	Extrusion width	Extrusion multiplier
1	Simplify	rectilinear	0.6	0.3	1.15
2	Simplify	rectilinear	1.0	0.3	1.0
3	Simplify	conical	0.6	0.05	1.15
4	Simplify	conical	1.0	0.05	1.0
5	Cura	rectilinear	0.6	0.05	1.0
6	Cura	rectilinear	1.0	0.05	1.15
7	Cura	conical	0.6	0.3	1.0
8	Cura	conical	1.0	0.3	1.15

hand, a rectilinear pattern leads to layer-wise alternating diagonal lines. On the other hand, a conical pattern fills each layer from the outside to the inside in conical paths. These categorical factors, in addition to the min/max values for the numerical factors are summarized in Table 1.

Due to the high costs, in particular regarding required production time, the number of experiments is significantly reduced with a one-fourth fraction factorial experimental design. However, this configuration is only used for the factors 2-6, whereas each experiment is conducted for all geometries. These specifications, as shown in Table 2, are produced three times to reduce the bias of individual runs. As a result, the total number of experiments is reduced from 288 to 72.

The experiments are conducted on an industrial 3D-printer (HAGE140L) with an ABS-filament from Form Futura (TitanX, diameter of 1.75 mm). Since the density of the filament is not known in detail, but is required for the calculation of the relative density, the filament density ρ_{fil} is measured, whereas 15 samples of 5 cm each were collected from three independent filament spools. The resulting mean density of 1.1347 g/cm^3(std=0.00812) is used for further calculations. The measurements of both, the filament and the produced parts, are conducted with a precision balance of Mettler Toledo. In this regard, two measurements were performed for each product to reduce the bias of individual results.

The software implementation for preparing the data, selecting the features, and training as well as evaluating the machine learning models is based on Python 3.9.5 and scikit-learn 0.24.2. Additionally, the following specification for the machine learning algorithms were used:

- Random Forest: number of estimators=100, no limit regarding the depth of individual trees
- Decision Tree: no limit regarding the tree depth
- Ridge Regression: regularization strength alpha=1.0

5 RESULTS & DISCUSSION

After the printing experiments are conducted, the weight of every individual part is measured and the relative density is calculated. The resulting values are used as targets in the features selection phase. Accordingly, the six considered factors (described above) are prepared (one-hot encoding, z-normalization) and included as input features for the random forest training process. As a result, the relative importance (sum of individual importance is 1.0) for each feature is shown in Figure 2, whereas the categorical values are included as one-hot encoded boolean features, leading to a total of 10 explanatory variables.

As depicted by Figure 2, the extrusion multiplier is the most influential factor for predicting the relative density. Additionally, the extrusion width and the slicer software (Simplify, Cura) have a notable impact on the prediction. Importantly, the significant influence of the slicer software implies that both investigated solutions employ different slicing methodologies to generate the commands for the printer (g-codes). However, the three remaining factors (layer height, geometry, infill pattern) are neglectable for the relative density. As a consequence, the three most relevant factors are considered for training the machine learning models and evaluation process. Only one ("Slicer - Cura") of the one-hot encoded slicer features is included, since the boolean characteristic leads to mutually exclusive features, meaning that only one of them can be true for a given data entry. Thus, no information is added when both, instead of one, one-hot encoded features are considered.

Based on a repeated 10-fold cross validation all three machine learning models are trained on a sub-set of the experimental data and evaluated on the remaining samples (90 % training, 10 % test). Hence, the R-squared score is calculated for each test set, resulting

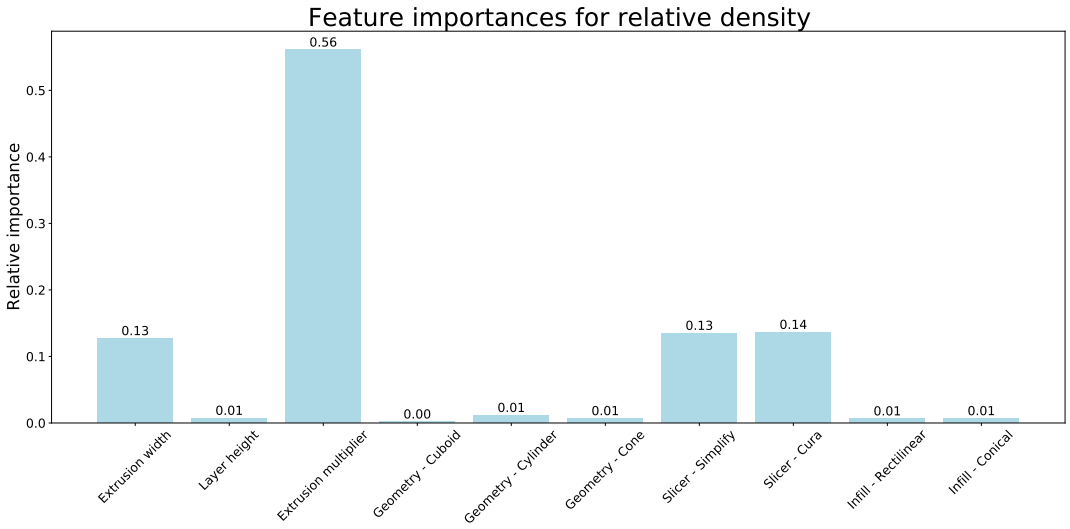

Figure 2: Relative importance for each feature for predicting the relative density.

Table 3: Results of 10-fold cross-validation randomly repeated 10 times based on the R-squared error metric.

Algorithm	Count	Mean	Std.	Min.	25 %	50 %	75 %	Max.
Random Forest	100	0.918	0.068	0.613	0.900	0.933	0.962	0.987
Decision Tree	100	0.918	0.068	0.609	0.900	0.931	0.963	0.988
Ridge Regression	100	0.442	0.316	-1.134	0.418	0.533	0.628	0.723

in 100 individual scores (10 repetitions). As shown in Table 3, the overall mean R-squared score of 0.918 is equal for both, the random forest and the decision tree model. Therefore, the additional computational costs and complexity due to the ensemble approach of the random forest algorithm does not lead to quantifiable improvements.

The ridge model performs significantly worse with an average score of 0.442, whereas even the maximum R-squared score of 0.72 remains below the 0.25 % quantiles of its non-linear counterparts (0.9), thus, implying that certain non-linear dependencies are present within the experimental data, which cannot be represented with a linear model. Even though the mean R-squared score for both, the random forest and the decision tree model, indicate a good model fit, the detailed statistical values, in particular the gap between the minimum score (0.61) and the 25 % quantile (0.9), reveal that some dependencies within the data are not accounted for.

6 CONCLUSION

Due to a large number of influential parameters, it is inherently difficult to determine the optimal production parameters for additive manufacturing processes. This leads to complex dependencies and difficulties during the ramp-up phase for new products until the optimal parameter combination is found to ensure consistent quality.

In particular for extrusion-based technologies, such as FFF, the relative density is often one of the main quality characteristics. Even though, conventional techniques, such as FEA and DoE, are used for optimizing AM processes, theses approaches are resource-intense and typically design-specific, so that the results are only suitable for individual designs. In contrast to that, data-driven methods based on generic input features, such as vibration data or layer height, offer interesting results for large-scale applications.

Consequently, a methodology, consisting of a DoE for data generation, measuring and calculating relevant target values, feature selection, machine learning models and cross-validation, was proposed for predicting the relative density. For the DoE, six supposedly influencing factors, such as geometrical features and extrusion width, were considered and a one fourth fraction factorial test design was performed to decrease the number of experiments. Afterwards, the input factors and the target values (relative density), were utilized during the feature selection process to determine the relative importance of each feature with the random forest algorithm. It was found, that layer height, geometrical features and infill patterns are of minor relevance for predicting the relative density. Thus, only the extrusion width and multiplier as well as the used slicer software were included in the training and validation procedure for the machine learning models. In this regard, three algorithms – random forest, decision tree and ridge regression – were evaluated on the mean R-squared score, achieved in a 10-fold cross-validation, which was randomly repeated 10 times.

As a result, both, the random forest and the decision tree model, learned the non-linear dependencies within the data and proved to be applicable with an average R-squared score of 0.92. Thus,

the proposed methodology for predicting the relative density of extrusion-based parts was validated and is suitable to be applied during the ramp-up phase for new designs to increase the efficiency. However, some dependencies are not accounted for, since the minimum R-squared score is 0.61 for both models, indicating that additional work is required for training a robust model. Moreover, several future research directions are determined based on the results of this work. On the one hand, an extension and validation of the methodology for other quality characteristics, such as surface roughness or warping degree, as well as other AM technologies is necessary to create a holistic methodology for optimizing AM processes. On the other hand, an active learning procedure, which recommends the next best experiment for the current model status, can reduce the number of required experiments, while retaining the effectiveness. Additionally, the methodology for predicting the relative density can be adapted and used as an indicator for dimensional accuracy, similar to Jiang et al. [7]. Furthermore, combining ex ante and in-situ approaches to create an overall AM quality framework, could increase the applicability of AM process in general.

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