Application of machine learning techniques to predict mechanical properties for polyamide 2200 (PA12) in additive manufacturing

Ivanna Baturynska

Abstract: Additive manufacturing (AM) is an attractive technology for manufacturing industry due to flexibility in design and functionality, but inconsistency in quality is one of the major limitations that does not allow utilizing this technology for production of end-use parts. Prediction of mechanical properties can be one of the possible ways to improve the repeatability of the results. The part placement, part orientation, and STL model properties (number of mesh triangles, surface, and volume) are used to predict tensile modulus, nominal stress and elongation at break for polyamide 2200 (also known as PA12). EOS P395 polymer powder bed fusion system was used to fabricate 217 specimens in two identical builds (434 specimens in total). Prediction is performed for XYZ, XZY, ZYX, and Angle orientations separately, and all orientations together. The different non-linear models based on machine learning methods have higher prediction accuracy compared with linear regression models. Linear regression models have prediction accuracy higher than 80% only for Tensile Modulus and Elongation at break in Angle orientation. Since orientation-based modeling has low prediction accuracy due to a small number of data points and lack of information about material properties, these models need to be improved in the future based on additional experimental work.

Keywords: additive manufacturing; machine learning; tensile modulus; predictive modeling; mechanical properties; polyamide 2200; PA12

1. Introduction

In polymer powder bed fusion additive manufacturing anisotropic behaviour of the material leads to the variation in dimensional and mechanical properties depending on the part orientation. Since this technology has obtained attention from automotive, aerospace and medical industries as a technology for production of end-user parts, requirements to a part quality have increased significantly including a need for consistent result. Therefore, development of new models for prediction of mechanical properties will allow meeting these requirements.

The current state-of-the-art [1–19] describes the importance of part orientation, powder morphology and machine process parameters as a means towards the control and management of variation in polymer powder bed fusion system. Among the most investigated AM machine process parameters are laser power, scan speed, hatch distance, scan strategy, beam speed, melting temperature, and powder bed temperature [2–7]. There is a number of studies [20,21], which reports that laser power, scan speed, hatch distance and layer thickness can be used to define the line energy and how their variation may influence mechanical properties of the part. In addition to energy applied to solidify polyamide, Mielicki et al. [8] have also reported on the importance of layer thickness and powder distribution in each layer. Powder distribution is dependent on the size of the particles in the powder and powder viscosity.

Besides, Drummer et al. [18] and Gümüs et al. [22] studied how size of the particles of polymer powder and its viscosity influence mechanical properties. While Drummer et al. [18] investigated...
degradation behavior of PA12 based on the analysis of phase transition temperature and melt viscosity for both virgin and aged powder, Gümüs et al. [22] have reported that size of the particles and morphology could lead to the creation of pores, gaps or/and voids in the fabricated parts. The influence of part orientation on mechanical properties has already been described in the details by [12,23,24]. Besides, there is a difference between what is reported in the literature and what is provided by EOS data sheets. While [12,23,24] have reported that Tensile modulus, Elongation at break and Maximal Stress are affected by the part orientation, EOS reports in their data sheets for PA12 - Balanced process parameters group - that Tensile Modulus is the same in all orientations. In addition, Caulfield et al. [12] report that thermal distribution in the build chamber has also an impact on mechanical properties of the fabricated parts.

However, there is a limited number of studies that have made an attempt to predict mechanical properties based on the part positioning in the build chamber. Similar research was performed for investigation of dimensional accuracy for PA12 based on the part positioning in the build chamber, part orientation and STL model properties (number of mesh triangles, volume and surface) [11]. Using similar strategy would contribute to development of the schematic approach of positioning parts in the build chamber based on their requirements, and thus, increasing area of build chamber utilization, which would lead to cheaper and more sustainable production.

Therefore, in this study the main focus is set on the development of linear and non-linear models to predict Tensile Modulus, Nominal Srtess and Elongation at break by using different machine learning techniques. Machine learning techniques have already been used for prediction of geometrical deviations, and have shown a great potential for the datasets collected from more than 100 samples [25]. Nowadays, these methods are used in different field of studies [26–28], and have also been widely used in traditional manufacturing [29–32].

Specifically, the author is aiming at addressing the following issues:

- Estimation of mechanical properties of AM-manufactured parts without prior knowledge about material (Section 3)
- Understanding of how mechanical properties are dependent on the part positioning in the build chamber (Section 3).
- Compare performance of Linear regression models and machine learning proposed models, and choose the best models for prediction of mechanical properties (Secion 3).
- Discuss which of the investigated features are the most significant and can be used to predict mechanical properties, and how mechanical properties can be control and managed based on the obtained results (Section 4).

2. Materials and Methods

Experimental work was performed on EOS P395 polymer powder bed fusion system with Polyamide 12 (PA12) used as a material. The PA12 powder was used with a 50/50 % ratio of virgin/self-aged powder respectively, and both virgin and self-aged powder were taken from the same batch. The self-aging of a powder was done based on the approach presented by Rüsenberg et al. [3]. However, part placement and orientation strategy (see Figure 1) were chosen to be different and it is described in more details in Section 2.1.

Figure 2 presents the main stages of the experiment, starting from aging powder and finishing with execution of Tensile testing. At the first aging stage, 100% of virgin PA12 (40 kg) was used in the EOS P395 machine without energy deposition. The next two aging steps have used a powder only from the build cake (from build chamber) obtained as a result of the previous aging step. Since the amount of self-aged powder from the Run 1 was not enough for execution of two experimental builds, additional run for aging powder was performed (Run 2 on Figure 2). The Run 2 consisted of three similar aging steps as in Run 1 with the same process parameters. In total 45 kg of self-aged Polyamide 12 was obtained and mixed with 45 kg of virgin powder. Then mixed powder was divided in two equal batches to be used in two experimental builds.
Since in this experiment an idea of using a self-aged powder proposed by Rüsenberg et al. [3] have been utilized to control material properties, it was of the interest to compare whether similar repeatability of the results will be obtained to the ones Rüsenberg et al. [3] had presented in their work. Therefore, build layout, process and material parameters were kept constant through the whole experiment and are shown in Table 1.

**Table 1. Material and process parameters used in the experiment**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Virgin/aged PA2200 powder ratio, %</td>
<td>50/50</td>
</tr>
<tr>
<td>EOS P395 system settings</td>
<td>Balance</td>
</tr>
<tr>
<td>AM system warm up time, min</td>
<td>120</td>
</tr>
<tr>
<td>AM system cooling down time, min</td>
<td>240</td>
</tr>
<tr>
<td>Working chamber temperature, °C</td>
<td>180.5</td>
</tr>
<tr>
<td>Removal chamber temperature, °C</td>
<td>130.0</td>
</tr>
</tbody>
</table>
2.1. Build layout

Rüsenberg et al. [3] work was taken as a reference work, but number of specimens and placement strategy were chosen to be different. It was chosen to produce in one build 217 standardized specimens of ISO 527-2 1BA type for mechanical testing. Each specimen has its own label to be able to follow part placement in terms of set of coordinates in X, Y and Z axes. Strategy for parts’ placement was set to be close to real manufacturing conditions. It means that parts are placed as close to each other as possible, but for the results verification and validation, at least 5 parts were placed close to each other to minimize variations related to part placement (coordinate). All specimens for tensile testing were placed in four different orientations (see Figure 3).

All specimens were clustered into four groups based on the ISO/ASTM 52921 standard [33]. Each orientation group name was defined based on the size of each dimensional feature, from the highest to the smallest value:

- Group 1. XYZ (XY in Fig. 3 )-oriented parts
- Group 2. XZY (XZ in Fig. 3)-oriented parts
- Group 3. ZYX (Z in Fig. 3)-oriented parts
- Group 4. Angle-oriented parts

By the Angle-oriented parts, the author mean parts oriented at 45° between X and Z axes.

Since positioning of specimens was made based on the main requirement to fit in as many of them as possible, the number of standard specimens in each orientation group differ. Thus, 65 specimens are positioned in XY orientation, 24 - in XZ orientation, 84 - in Z orientation and 22 in Angle orientation.

2.2. Conditioning of specimens and tensile testing

According to the DIN EN ISO 527-1, tensile testing was performed on universal test machine Zwick Z250 with one-week conditioning in the climate chamber at 70°C and 62% RH. This is an accelerated conditioning, which results in the same moisture content as it is mentioned in ISO 1110. In addition to one week of conditioning, specimens were kept for 1-2 days in the climate chamber at 23°C and 50% RH before testing. The Zwick Z250 machine was loaded with 2.5 kN cell. The specimens were mounted in wedge grips with grip to grip distance set to 55 mm, and an initial gauge length of the extensometer of 25 mm.
3. Results

3.1. Description of the collected data

Mechanical properties depend on the part orientation, and this phenomenon is already presented in [12]. Therefore, description of the mechanical properties should be done separately for each orientation. The four orientations were used in the current analysis, which are XYZ, XZY, ZYX and Angle (45° between X and Z axes) orientations. Tables 2 - 4 describe the data based on the Tukey range test (looking at percentiles) including standard deviation values.

Table 2. Statistical data evaluation for Tensile modulus for each orientation separately

<table>
<thead>
<tr>
<th>Statistical characteristics</th>
<th>XYZ</th>
<th>XZY</th>
<th>ZYX</th>
<th>Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>std</td>
<td>31.912</td>
<td>35.776</td>
<td>95.763</td>
<td>46.63</td>
</tr>
<tr>
<td>mean</td>
<td>1066.308</td>
<td>1051.951</td>
<td>958.25</td>
<td>1013.545</td>
</tr>
<tr>
<td>25%</td>
<td>1046.308</td>
<td>1035.374</td>
<td>908.038</td>
<td>983.455</td>
</tr>
<tr>
<td>50%</td>
<td>1067.77</td>
<td>1055.196</td>
<td>980.038</td>
<td>1010.291</td>
</tr>
<tr>
<td>75%</td>
<td>1088.461</td>
<td>1074.403</td>
<td>1032.381</td>
<td>1043.599</td>
</tr>
<tr>
<td>max</td>
<td>1148.078</td>
<td>1112.222</td>
<td>1090.35</td>
<td>1118.547</td>
</tr>
<tr>
<td>min</td>
<td>968.483</td>
<td>933.376</td>
<td>907.983</td>
<td>907.983</td>
</tr>
</tbody>
</table>

Table 3. Statistical data evaluation for Nominal Stress for each orientation separately

<table>
<thead>
<tr>
<th>Statistical characteristics</th>
<th>XYZ</th>
<th>XZY</th>
<th>ZYX</th>
<th>Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>std</td>
<td>0.665</td>
<td>0.604</td>
<td>5.101</td>
<td>3.334</td>
</tr>
<tr>
<td>mean</td>
<td>37.341</td>
<td>35.429</td>
<td>22.031</td>
<td>30.773</td>
</tr>
<tr>
<td>25%</td>
<td>36.918</td>
<td>35.019</td>
<td>18.303</td>
<td>28.478</td>
</tr>
<tr>
<td>50%</td>
<td>37.476</td>
<td>35.491</td>
<td>22.19</td>
<td>29.91</td>
</tr>
<tr>
<td>75%</td>
<td>37.832</td>
<td>35.809</td>
<td>25.826</td>
<td>31.383</td>
</tr>
<tr>
<td>max</td>
<td>39.186</td>
<td>36.576</td>
<td>32.241</td>
<td>37.744</td>
</tr>
<tr>
<td>min</td>
<td>35.519</td>
<td>34.132</td>
<td>10.09</td>
<td>26.219</td>
</tr>
</tbody>
</table>

Table 4. Statistical data evaluation for Elongation at break for each orientation separately

<table>
<thead>
<tr>
<th>Statistical characteristics</th>
<th>XYZ</th>
<th>XZY</th>
<th>ZYX</th>
<th>Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>std</td>
<td>0.727</td>
<td>0.679</td>
<td>1.096</td>
<td>2.311</td>
</tr>
<tr>
<td>25%</td>
<td>13.158</td>
<td>12.875</td>
<td>2.719</td>
<td>5.594</td>
</tr>
<tr>
<td>50%</td>
<td>13.582</td>
<td>13.497</td>
<td>3.26</td>
<td>6.343</td>
</tr>
<tr>
<td>75%</td>
<td>13.893</td>
<td>13.663</td>
<td>4.017</td>
<td>7.262</td>
</tr>
<tr>
<td>min</td>
<td>11.18</td>
<td>10.618</td>
<td>1.917</td>
<td>4.316</td>
</tr>
</tbody>
</table>

The results illustrated in Figure 4 supports anisotropic behaviour of PA 12 reported earlier [13,22]. While Tensile modulus for XYZ and XZY orientation has similar distribution, tensile modulus for ZYX orientation has the widest variance and the lowest value. Tensile modulus for Angle orientation has a narrow distribution, while the maximum value of Tensile modulus is 1065 MPa. In addition to variation between orientation, the variation between nominal value (provided by EOS for balanced machine settings for PA2200 material) and obtained results is also observed for Tensile modulus.
Similarly to the Tensile modulus, distribution of nominal stress for different orientations is presented in Figure 5. The results of XYZ and XZY orientations are similar to the Tensile modulus, although distribution for ZYX orientation is much wider and the average value of nominal stress differs from the average value of XYZ and XZY orientations. Additionally, if to compare maximal value for ZYX orientation with the value provided by EOS, one can observe that nominal stress is almost two times lower (from Table 3 it is ca. 22 MPa, while 42 MPa is expected) than provided one by EOS (dashed line in Figure 5). However, value of nominal stress for Angle orientation is better than for ZYX, it is still relatively low comparing with the results for XYZ and XZY orientations.

Elongation at break comparing with two other mechanical properties has more similar results to the ones provided by EOS, and is illustrated in Figure 6. According to EOS datasheet, elongation at break is expected to be 4 % for ZYX orientation and 18% for XYZ orientation. The average value of elongation at break for ZYX and XYZ orientations are ca.3.5% and 13.4%, respectively (are taken from Table 4). Since there is no information from the EOS for other orientations, the observed values for XZY and Angle orientations cannot be compared with nominal ones. However, it is expected the XZY orientation should have similar results to XYZ orientation due to dominating X axis, and thus slicing of the specimens is performed perpendicularly to the direction of force load in tensile test. Similarly, ZYX and Angle orientations are sliced in such way that makes easier crack generation under tensile test.
Figure 6. Distribution of elongation at break for different orientations based on kernel distribution estimation. The straight solid (18% for XYZ orientation) and dashed lines (4% for ZYX orientation) correspond to the value from EOS Balanced datasheet.

The discussion on why this wide distribution is observed for the experimental results for ZYX orientation will be provided in another article and is out of the scope of this article. In this work, different intelligent methods have been applied to discover the most important features, and obtained results are presented below.

3.2. Application of machine learning techniques to predict mechanical properties without prior knowledge about PA properties

Successful prediction of mechanical properties of fabricated parts is an important factor of future adoption of additive manufacturing to produce end-users parts. The high quality requirements and a need in the consistency are primary issues that have not been fully addressed yet. Typically, mathematical models need to be developed to make possible analysis of mechanical properties beforehand. However, the complexity of the AM process leads to the simplification of the issue in one area in order to describe another one mathematically.

Therefore, the another approach is required for obtaining robust predictions that will be less sensitive to unknown noise. Since, there are examples of successful application of machine learning techniques in traditional manufacturing [29–32], these methods could be used to predict mechanical properties with limited information about the AM process itself.

Since prediction of some output corresponds to regression task, linear regression models are compared with Gradient Boosting Regressor (GBR), Decision Tree Regressor and AdaBoost Regressor machine learning techniques. The Python programming language was used to program these algorithms with a help of Scikit-Learn libraries [34], which consist of preprogrammed methods needed for this work. One of the advantages of using such techniques is a possibility to overcome present noise and find patterns in a data that couldn’t be identify with a "human eye".

However, these methods require a large number of data points for better performance. An additional challenge is a choice of correct techniques for the assigned tasks. In this work, determination coefficient and mean square error (MSE) were considered as performance metrics for methods comparison. However, machine learning techniques often work as black boxes and models cannot be presented mathematically except for a description of model’s architecture. An additional requirement to the methods was a presence of feature importance attribute. This information is needed for better understanding of which features plays an important role in the model development to estimate Tensile Modulus, Nominal Stress and Elongation at break (or identify features that are in some way correlated to the mechanical properites).
3.2.1. Short introduction to used machine learning techniques

**Decision Tree Regressor** is a recursive algorithm that splits data into smaller subsets (separate classes) in order to form a tree, and it is important to choose correct metrics for best data split and determining when a tree node should become a terminal.

Building a decision tree for regression is similar to classification, but the main difference is in using different metrics for evaluation of the quality of the split (reduction of variance for regression task), and a leaf node is defined by numerical output. Optimization of these metrics will lead to the more stable performance of the algorithm.

However, when it comes to analysis of the big amount of data, this method has issues with scalability, stability and robustness [26,35]. Another issue that should be addressed is an increase of a complexity when large data samples are used. The total number of nodes, total number of leaves, tree depth and number of attributes are metrics that can be controlled in order to minimize the complexity of decision tree [26]. Since these issues not always can be addressed, ensemble decision trees are used instead and are more robust.

**Gradient Boost Regressor** is an ensemble of decision trees. Instead of building one tree, this method predicts the desired outcome based on the additive regression model that uses decision trees as a weak learner [36]. Sequential fitting of a parameterized function (base learner) to current "pseudo"-residuals is done at each iteration by optimizing regression loss (e.g., least squares, absolute error) [37]. Friedman [37] describes "pseudo"-residuals as minimization of the gradient of the loss function with respect to values of the regression model at each training data point for the current step.

Introduction of randomization in the process of training data set selection allows to improve accuracy and reduce the possibility of overfitting. This way of compiling a decision tree allows minimizing the errors at each next step, and therefore boosting regressor is considered as more reliable and robust method comparing to classic decision tree regressor.

**AdaBoost Regressor** (short from Adaptive Boost) is also an ensemble machine learning method. It works similarly to the Gradient Boost regressor, and the only difference is in the way weak learners are created at each iteration. Thus, AdaBoost changes the sample distribution at each iteration by changing the weights of each feature (the ones with the biggest error will have the highest weights).

Since all of the described methods needs to be trained on the data before they can be used for prediction task, the data should be divided into training and testing samples, usually with a ratio 75/25 % and 85/15 % when smaller data sets are used. For this purpose there is a library training_testing_split in Skicit-Learn [34], which was used by author in this work. Training data set is used to train the model (define the model), while testing data set is needed for evaluation of model generalization. By comparing prediction accuracy obtained for training and testing data sets separately, one can understanding whether under- or overfitting is present. Overfitting is present when model memorizes input data, while underfitting means that model cannot find any patterns in the data due to small number of data points. Both phenomena needs to be overcomed in order to obtain robust model.

3.2.2. Prediction of Tensile Modulus and comparison of models’ performance

Prediction of Tensile Modulus was performed for both different orientation groups and as a one group without separation on the orientations (called “All” in Table 5). Results show that prediction is not yet possible in XYZ, XZY and Angle orientations due to various reasons. Since large data sets is a well-known requirement for successful application of machine learning techniques, a small number of data points is one of the reasons why developed models for XYZ, XZY and Angle orientations. A limited number of investigated features could be considered as another reason of such model performance. Since many studies have earlier reported that material properties has significant impact on mechanical properties [3,13,18,22,38], and in this study they are not considered, this may have an impact on the obtained results.

However, prediction of Tensile Modulus based only on part positioning and STL model properties in ZYX orientation has promising results. Model based on the gradient boost regressor algorithm...
outperformed other models with a prediction accuracy of 0.808 out of 1 (80.8% out of 100 %) for ZYX orientation. Additionally, it can be seen that increase of number of data points (see All in Table 5, where number od data points represents number of data points used to train the model) leads to the higher prediction accuracy of 0.88 or 88 % for the developed model. This means that description of the part placement (positioning) in the build chamber in combination with part orientation and STL model properties can be used to predict Tensile Modulus especially when collected data is not divided in the groups corresponding to each orientation, but instead this information is used as an additional feature. This results show similar trend to the one Caulfield et al. [12] have reported in his study. Thermal distribution in the build chamber has an impact on the resulting mechanical properties, and presented results are in a good agreement with results reported in [12]. Besides, more details on which parameters are used in this model are described in the Section 4.

Table 5. Prediction of Tensile Modulus with a help of machine learning techniques. Linear means linear regression models, GBR stays for Gradient Boost Regressor, DTR - Decision Tree Regressor, and ABR - AdaBoost Regressor.

<table>
<thead>
<tr>
<th># data points</th>
<th>Orientation</th>
<th>Linear</th>
<th>GBR</th>
<th>DTR</th>
<th>ABR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$R^2$</td>
<td>MSE</td>
<td>$R^2$</td>
<td>MSE</td>
</tr>
<tr>
<td>110</td>
<td>XYZ</td>
<td>0.129</td>
<td>602.945</td>
<td>0.272</td>
<td>503.781</td>
</tr>
<tr>
<td>40</td>
<td>XZY</td>
<td>-0.927</td>
<td>1421.147</td>
<td>-2.297</td>
<td>2431.052</td>
</tr>
<tr>
<td>142</td>
<td>ZYX</td>
<td>0.48</td>
<td>4151.161</td>
<td>0.809</td>
<td>1524.994</td>
</tr>
<tr>
<td>74</td>
<td>Angle</td>
<td>0.03</td>
<td>1193.589</td>
<td>-0.159</td>
<td>1426.052</td>
</tr>
<tr>
<td>325</td>
<td>All</td>
<td>0.528</td>
<td>3876.678</td>
<td>0.888</td>
<td>916.721</td>
</tr>
</tbody>
</table>

3.2.3. Prediction of Nominal Stress and comparison of models’ performance

Prediction of Nominal stress (maximal nominal stress) was also done based only on the part positioning in the build chamber and STL model properties (number of mesh triangles, surface and volume). However, comparing to results obtained for Tensile Modulus, number of successful models for prediction of Nominal Stress is higher with higher prediction accuracies. While models in XYZ and XZY orientations show similar behaviour as for Tensile Modulus, the ZYX and Angle orientations have even better prediction accuracy (0.902 and 0.906 respectively).

In addition, an interesting phenomena can be observed for Angle orientation. Since number of data points for this orientation is smaller than in XYZ orientation, model performance is significantly better. This can be explained by looking at the linear regression models. In this case, prediction of Nominal Stress in Angle orientation is even possible with a use of linear model, which has prediction accuracy relatively high - 0.867 out of 1. This means that combination of part positioning and STL model properties has linear correlation with Nominal Stress in Angle orientation. Therefore, application of more advanced methods results in improved model performance with higher prediction accuracy (like AdaBoost regressor in Table 6). Prediction of Nominal Stress in ZYX orientation has similar results with Tensile Modulus, and the best model is based on GradientBoost Regressor.
Table 6. Prediction of Nominal Stress with a help of machine learning techniques. Linear means linear regression models, GBR stays for Gradient Boost Regressor, DTR - Decision Tree Regressor, and ABR - AdaBoost Regressor.

<table>
<thead>
<tr>
<th># data points</th>
<th>Orientation</th>
<th>Linear</th>
<th>GBR</th>
<th>DTR</th>
<th>ABR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>$R^2$</td>
<td>MSE</td>
<td>$R^2$</td>
<td>MSE</td>
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<tr>
<td>110</td>
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<td>2.093</td>
<td>0.197</td>
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<tr>
<td>40</td>
<td>XZY</td>
<td>-0.645</td>
<td>0.827</td>
<td>-0.013</td>
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</tr>
<tr>
<td>142</td>
<td>ZYX</td>
<td>0.252</td>
<td>15.983</td>
<td>0.902</td>
<td>2.102</td>
</tr>
<tr>
<td>74</td>
<td>Angle</td>
<td>0.867</td>
<td>0.527</td>
<td>0.855</td>
<td>0.578</td>
</tr>
<tr>
<td></td>
<td>All</td>
<td>0.763</td>
<td>10.193</td>
<td>0.964</td>
<td>1.537</td>
</tr>
</tbody>
</table>

As it can be seen in Table 6, the best model with the highest prediction accuracy and the lowest MSE corresponds to the case when gathered data is not separated into orientation-based groups. Besides, orientation is considered as an additional feature similar to the previously reported results for Tensile Modulus. The prediction accuracy of Gradient Boost regressor model is 0.964 out of 1, and this means that we can already use this model for the prediction of Nominal Stress for similar type of parts.

However, if there is a need for prediction of Nominal stress value for a specific orientation group, then prediction can be done for ZYX and Angle orientations at this moment. In order to improve models in other orientations, additional information on material as well as more data points are required. These issues will be addressed by the author in the future.

Since prediction of Nominal Stress in Angle orientation is possible by using any of the described models in Table 6. However, when higher accuracy is required, then AdaBoost model would be the best choice. Otherwise, when a mathematical model is needed, then linear regression model can be used:

$$y = -832.16 \times x_1 - 6.819 \times x_2 + 415.9 \times x_3 + 13.639 \times x_4 +$$
$$+ 416.24 \times x_5 - 6.819 \times x_6 - 7.44 \times 10^{-4} \times x_7 +$$
$$+ 0.823 \times x_8 + 0.197 \times x_9$$

(1)

where $y$ is Nominal Stress in Angle orientation, $x_1$ is central coordinate $x$, $x_2$ is central coordinate $y$, $x_3$ - min coordinate x, $x_4$ - min coordinate y, $x_5$ - max coordinate x, $x_6$ - max coordinate y, $x_7$ - max coordinate z, $x_8$ - volume, and $x_9$ - surface.

3.2.4. Prediction of Elongation at break and comparison of models’ performance

Similarly to trends observed for Nominal Stress in Angle orientation, the elongation at break in Angle orientation has also linear correlation with the investigated features. As it can be seen from the Table 7, models in XYZ, XZY and ZYX orientations has relatively low prediction accuracy and therefore cannot be used at this moment. This phenomenon can be explained by looking at the previously published results[12], which state that material properties have significant impact on mechanical properties, including elongation at break. In order to improve developed models, material properties in terms of viscosity and virgin/used powder ratio.

However, when data is not separated on orientation-based groups, prediction accuracy increases significantly. Thus, one can assume that the number of data points is an important factor. Besides, AdaBoost Regressor has outperformed all other algorithms with prediction accuracy 0.987 out of 1 with relatively low MSE comparing with other methods.
Table 7. Prediction of Elongation at break with a help of machine learning techniques. Linear means linear regression models, GBR stays for Gradient Boost Regressor, DTR - Decision Tree Regressor, and ABR - AdaBoost Regressor.

<table>
<thead>
<tr>
<th># data points</th>
<th>Orientation</th>
<th>Linear</th>
<th>GBR</th>
<th>DTR</th>
<th>ABR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$R^2$</td>
<td>MSE</td>
<td>$R^2$</td>
<td>MSE</td>
</tr>
<tr>
<td>110</td>
<td>XYZ</td>
<td>0.261</td>
<td>0.0907</td>
<td>0.0146</td>
<td>0.121</td>
</tr>
<tr>
<td>40</td>
<td>XYZ</td>
<td>0.476</td>
<td>0.667</td>
<td>0.46</td>
<td>0.681</td>
</tr>
<tr>
<td>142</td>
<td>ZYX</td>
<td>0.269</td>
<td>0.963</td>
<td>0.67</td>
<td>0.434</td>
</tr>
<tr>
<td>74</td>
<td>Angle</td>
<td>0.889</td>
<td>0.500</td>
<td>0.795</td>
<td>0.927</td>
</tr>
<tr>
<td>325</td>
<td>All</td>
<td>0.965</td>
<td>0.739</td>
<td>0.987</td>
<td>0.284</td>
</tr>
</tbody>
</table>

Since, Linear regression model in Angle orientation has relatively high prediction accuracy (0.889 out of 1), this model can be used in cases when mathematical description is required:

$$y_{eb} = 49.54 \times x_1 - 2.757 \times x_2 - 25.02 \times x_3 + 5.516 \times x_4 - 9.45e - 06 \times x_5 - 24.52 \times x_6 - 2.757 \times x_7 + 2.497e - 03 \times x_8 - 2.41e - 02 \times x_9$$

(2)

where $y_{eb}$ is Elongation at break in Angle orientation, $x_1$ is central coordinate $x$, $x_2$ is central coordinate $y$, $x_3$ -min coordinate $x$, $x_4$ - min coordinate $y$, $x_5$ - min coordinate $z$, $x_6$ - max coordinate $x$, $x_7$ - max coordinate $y$, $x_8$ - max coordinate $z$, and $x_9$ - surface.

4. Discussion

Defining importance of the features can be done with a help of different techniques. However, each of them typically provides slightly different assumptions. Therefore, in order to avoid this uncertainty, the author propose to use model performance metrics, namely the coefficient of determination and mean square errors (MSE) as key criteria for decision making process. Among investigated features are STL model properties (surface, volume and number of mesh triangles), part orientation (angle for $x/y/z$ axes), and part placement (positioning) in the build chamber in terms of maximal, minimal and central coordinates in $x$, $y$ and $z$ axes. These features were extracted from build layout prepared in Magics 22.03 software (see Figure 1). More details about build layout have been provided in Section 2.1.

In this work, feature analysis based on the developed models is performed in Python programming language with a help of already programmed methods in terms of different libraries provided by Scikit-Learn [34]. Linear AdaBoost Regressor was used to obtain the first assumption on the feature importance, and then based on this assumption linear regression model was developed and used as a reference model for comparison with other non-linear models. The choice of non-liner models were based on possibility to extract information about feature importance. Thus, Gradient Boost Regressor (GBR), Decision Tree Regressor (DTR) and AdaBoost Regressor (ABR, with updated features) were applied in this work since they have shown the best accuracy among other methods and contain the feature importance attributes.

4.1. Feature importance for prediction of Tensile Modulus

Prediction of Tensile modulus with model prediction accuracy higher than 0.8 out of 1 was considered as successful. However, when the author have made an attempt to develop model for each orientation separately, models for XYZ, XZY and Angle orientation appeared to be unsatisfactory, and therefore it is not possible to extract robust evaluation of which features are important. One of
the reasons why this is not possible at this moment is related to the number of data points (which is much lower comparing with ZYX orientation and all data together). It is well known fact, the the more data points one have, the better performance machine learning techniques have. Additionally, lack of information about material properties is crucial for mechanical properties and adding this information in the future may improve models significantly.

Since evaluation of relative importance of the features on Tensile Modulus is possible only for ZYX orientation and without data separation on orientation-groups, namely All orientations, Figure 7 illustrates differences observed for these two groups. According to the results shown in Figure 7a, one of STL model properties, which is volume, is depicted as relatively the most important feature for non-linear model based on gradient boost regressor in ZYX orientation.

![Figure 7a](image1.png)  
**Figure 7a.** Relative importance of features for Tensile Modulus in ZYX orientation.

Since, it is known from EOS that volume and surface parameters helps to define energy concentration for specific part. The larger volume value of the part (it means that part is larger), the more energy will be concentrated in the build chamber where part is placed. In addition to this feature, part placement will also play an important role. Since, it was already previously reported that in polymer powder bed fusion system temperature distribution within a build chamber is different and it influence the mechanical properties [12,20], it can be assumed that coordinates in x, y and z axes help to identify regions where specimens are placed, and in combination with volume parameter, they provide much better description of energy concentration and temperature distribution in specific regions of the build chamber. Besides, machine learning techniques have unique possibility of determining hidden patterns between feature and output, which are not visible to a “human eye”.

In order to understand better why coordinates in x and z axes are listed in top 5 the most important features for ZYX orientation, visualization of Tensile modulus as a function of x and z coordinates is needed. As Figure 8 (sum of relative importance for all features is equal to 1) shows that when central coordinates in x axis are larger than 250 mm, the tensile modulus has the lowest values. This clearly indicates the correlation between coordinates in x axis and Tensile Modulus. Since part positioning in the build chamber is always described as a combination of all three axes, then the coordinates in y and z axes provide an additional information on how Tensile Modulus changes depending on the position in the build chamber.

![Figure 7b](image2.png)  
**Figure 7b.** Relative importance of features for Tensile Modulus in All orientations.

However, when all orientations are analyzed as one data set, the list of the most important features differs from the one proposed for ZYX orientation. Another STL model property is listed as relatively the most important, which is surface, and as it has been already mentioned earlier, surface feature similarly to volume describes in more details about energy concentration for specific part, and thus contributes to the description of temperature distribution for specific are in the build chamber. The coordinates follows the surface feature but in different order. While minimal coordinate x is second
in the list, it relative importance is a bit higher than for ZYX orientation. Additionally, maximal
coordinates in z and x axes are important to the same extend.

Difference in the order of the coordinates in different axes comparing with feature importance
list proposed for ZYX orientation could be caused by the number of parts in each orientation group
and their placement in the build chamber. For example, the biggest number of specimens is in the
ZYX orientation (168 from two builds) and XYZ is the second largest group (130 specimens from two
builds). Therefore, one can assume that results for XYZ orientation group will significantly influence
on the importance of coordinates in x, y and z axes. Another assumption could be made for description
of temperature distribution in the build chamber. In other words, including parts from other areas in
the build chamber allows define patterns regarding values of Tensile Modulus, and thus leading to
better prediction accuracy of the model.

4.2. Feature importance for prediction of Nominal Stress

The Nominal Stress can be predicted for ZYX, Angle and All orientations with a higher prediction
accuracy (0.902, 0.906 and 0.964 respectively) than for Tensile Modulus. For example, list of the features
based on the relative importance in ZYX orientation for Nominal stress is different (see Figure 9a) from
the list proposed for Tensile Modulus. Gradient Boost Regressor algorithm has weighted number of
mesh triangle as the most important feature, which is followed by such features as surface, central
and minimal coordinates in x axis, number of mesh triangles and volume in the listed order. The
positioning of the sample is also highlighted by the algorithm in terms of the coordinates in x axis and
maximal coordinate in z axis. Since connection between STL model properties and part positioning has
been described for Tensile Modulus as a possible way of defining temperature distribution in the build
chamber, with special attention to the energy concentration, similar trends are observed in models
developed to predict Nominal Stress. Number of mesh triangles influence the way part is sliced on
the layer, which results in construction of parts’ contours at each layer for additive machine, and thus
contributes to the energy concentration for each specific part. This assumption is in a good agreement
with previously published studies [39,40].

However, when it comes to the analysis of features’ importance for developed model in Angle
orientation, STL model properties are still in the list of being important but their contribution is less
significant comparing to the ZYX/All orientations (see Figure 9b). One of the reasons why volume
and surface features are among the least significant for the developed model can be the distribution of
actual values for all specimens in Angle orientation. Thus surface values are in the range 1401.787 –
1432.563 mm², while values range for volume is even smaller (1029.925 – 1035.427 mm³). However,
value range for surface feature for all specimens (without separation on orientations) has significant
difference (e.g. 1381.555 − 1441.187 mm²) comparing with volume values (1029.925 − 1035.427 mm³).
However, comparison of these ranges rises another question on why such small range for volume
feature is important for prediction of both Tensile Modulus and Nominal Stress in ZYX orientation. In
order to be able to answer on this question more experimental work is needed to be done in the future,
where variation of the STL model properties should be of main concern. Another assumption could be
made by looking at prediction accuracy for linear model, which is equal to 0.867 out of 1. This could
mean that linear correlation between investigated features and Nominal Stress is present for angle
orientation, while correlation between STL model properties and Nominal Stress is absent.

Figure 9. Feature relative importance based on the specimens orientation (a) Nominal stress - ZYX
orientation. (b) Nominal Stress - Angle orientation.

Figure 10. Feature relative importance for Nominal Stress - All orientations.

Results obtained when all orientations are analyzed together are illustrated on Figure 10. As it can
be seen positioning in the x axes is listed as the most important feature, and especial attention is paid
to the minimal coordinate in x axis. In order to understand better why minimal coordinate in x axis
is chosen to be more important than, for instance central or maximal coordinates, there is a need for
visualizing how Nominal Stress is dependent on these coordinates. Since the graphical representation
for central and maximal coordinates in x axis looks alike, the minimal coordinate in x axis is compared
only with central coordinate x, and their comparison is shown in Figure 11. Even though Figure 11a
has similar dependencies comparing with Figure 11b, one can still observe better defined correlation
between minimal coordinate x and Nominal Stress. Even though at this moment it is not possible to
confirm the proposed assumptions, it is also important to highlight that feature importance in this
work is described from the perspective of developed models instead of making conclusions whether
these parameters influence the values of mechanical properties.

In other words, if another model with high accuracy is proposed, the list of the most important
features will be different and it also differs depending on the machine learning techniques used
4.3. Feature importance for prediction of Elongation at break

While developing models to predict elongation at break, especially when all orientation groups were joint, the features that described orientation angle have dominated over other parameters and have negatively influenced on the model robustness. Therefore, it was decided by author to develop models based on the specimens’ placement in the build chamber and STL models, and exclude orientation angle from the feature’s list. This has resulted in lower prediction accuracy, but has helped to overcome an issue of overfitting (memorized data instead of defined patterns and dependencies). However, it is still important to keep in mind that part orientation has the biggest impact on the elongation at break (see Figure 6, which raw values are in the range 1.917 – 33.715%).

Prediction of elongation of break has higher prediction accuracy in Angle orientation (0.903 out 1) than in ZYX orientation (0.67 out of 1) even though the number of data points for ZYX orientation is almost two times larger. While it seems that number of data points is not an important factor for machine learning techniques, there are other reasons that explains observed phenomena. Development of robust model with good generalization requires not only many datapoints but also features that influence parameter, which model is predicting. Therefore, in the future studies, there is a need for introducing material properties and additional information that will explain temperature distribution in the build chamber in more detailed way. Additionally, it is important to analyze linear model performance in Angle orientation because this model has also prediction accuracy of 0.889, which could mean that Elongation at break has linear correlation with positioning of the specimens in the build chamber similarly to the Nominal Stress.

Figure 12 illustrates that the most significant parameter is a minimal coordinate in x axis. This feature is important for the model, but it doesn’t mean that minimal coordinate x influences the value of elongation at break. However, positioning of specimens in the build chamber allows identifying changes of the temperatures in the build chamber, which influences mechanical properties similarly to other reports [12].

Additionally, it is important to mention that speed under which force was loaded on the specimens has also an impact on the values of elongation at break. Since the difference between...
values mentioned in EOS datasheets and obtained in the experimental work are similar, one can assume that this factor can be neglected.

While Elongation at break for Angle orientation could be predicted based on four features (see Figure 12a), when all orientations are joint into one dataset the number of important features for the model is different (see Figure 12b). As it can be seen from Figure 12b based only on the positioning of the specimens in the build chamber, there is a high potential in predicting elongation at break. Similarly to Tensile Modulus and Nominal Stress, coordinates in x and z axes are defined as the most important ones. These results could be different for other AM machine, and therefore, in the future work more data needs to be collected based on experimental work, which will be focused on the moving specimens within build chamber with special attention to the features listed as the most important. Since, the author could not find any similar reports in order to compare the obtained results, verification and validation of these results will be done in the future based on the additional experiments.

5. Conclusions

Additive manufacturing (AM) is an attractive technology for manufacturing industry due to flexibility in design and functionality, but inconsistency in quality is one of the major limitations that does not allow utilizing this technology for production of end-use parts. Mechanical properties are dependent on both process and material parameters of additive manufacturing process, but there is limited number of studies that set focus to the STL model properties and part positioning in the build chamber as features that can be used to describe and predict mechanical properties in addition to material and process parameters.

Since both material and process parameters were kept the same for two builds analyzed in this study, this information is neglected and the main focus is set to the analysis of build layout. From Figures 4 - 6, it can be seen that repeatability from two build is good, and this means that control of material properties can help to avoid inconsistency in the quality that usually appears from build-to-build. However, distributions in ZYX orientation for Tensile Modulus and Nominal Stress are wide and it has not been reported earlier, and therefore, this issue should be analyzed in more details in another article.

When it comes to the prediction of mechanical properties by using traditional methods like linear regression, it can be seen from the Tables 5 - 7 that prediction accuracy for linear regression (except for Nominal Stress and Elongation at break in Angle orientation) is low, and therefore more advanced techniques needs to be used. Since machine learning techniques have also been widely used in traditional manufacturing [29–32], these methods were applied in this study to develop non-linear prediction models.
Machine learning techniques require large datasets for better performance, and this trend can be observed based on the different model accuracies for orientation-based modeling and when all orientations are joint in one dataset. Models developed on the largest datasets (“All orientation” in Tables 5 - 7) have the highest prediction accuracy and, therefore, have potential to be used for prediction of mechanical properties for similar type of parts. When it comes to the prediction of mechanical properties for each orientation group individually, Tensile Modulus could be predicted only in ZYX orientation, Nominal Stress could be predicted in ZYX and Angle orientation, and Elongation at break could be predicted in Angle orientation. All other models require to include additional information about material and increase number of specimens that are analyzed.

Since two builds were identical, there is a need for introducing to the models more variations in the data such as; include material properties, change specimens’ positioning and orientations, produce specimens with other size and design, and change values of STL model properties. In addition, more attention should be paid to energy description for each part based on their placement in the build chamber.

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**Abbreviations**

The following abbreviations are used in this manuscript:

- GBR Gradient Boosting Regressor
- ABR AdaBoost Regressor
- DTR Decision Tree Regressor

**References**


