

Article

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

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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

36 degradation behavior of PA12 based on the analysis of phase transition temperature and melt viscosity
37 for both virgin and aged powder, Gümüs *et al.* [22] have reported that size of the particles and
38 morphology could lead to the creation of pores, gaps or/and voids in the fabricated parts. The
39 influence of part orientation on mechanical properties has already been described in the details by
40 [12,23,24]. Besides, there is a difference between what is reported in the literature and what is provided
41 by EOS data sheets. While [12,23,24] have reported that Tensile modulus, Elongation at break and
42 Maximal Stress are affected by the part orientation, EOS reports in their data sheets for PA12 - Balanced
43 process parameters group - that Tensile Modulus is the same in all orientations. In addition, Caulfield
44 *et al.* [12] report that thermal distribution in the build chamber has also an impact on mechanical
45 properties of the fabricated parts.

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

53 Therefore, in this study the main focus is set on the development of linear and non-linear models
54 to predict Tensile Modulus, Nominal Stress and Elongation at break by using different machine
55 learning techniques. Machine learning techniques have already been used for prediction of geometrical
56 deviations, and have shown a great potential for the datasets collected from more than 100 samples
57 [25]. Nowadays, these methods are used in different field of studies [26–28], and have also been widely
58 used in traditional manufacturing [29–32].

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

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

69 2. Materials and Methods

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

76 Figure 2 presents the main stages of the experiment, starting from aging powder and finishing
77 with execution of Tensile testing. At the first aging stage, 100% of virgin PA12 (40 kg) was used in
78 the EOS P395 machine without energy deposition. The next two stages have used a powder only
79 from the build cake (from build chamber) obtained as a result of the previous aging step. Since the
80 amount of self-aged powder from the Run 1 was not enough for execution of two experimental builds,
81 additional run for aging powder was performed (Run 2 on Figure 2). The Run 2 consisted of three
82 similar aging steps as in Run 1 with the same process parameters. In total 45 kg of self-aged Polyamide
83 12 was obtained and mixed with 45 kg of virgin powder. Then mixed powder was divided in two
84 equal batches to be used in two experimental builds.

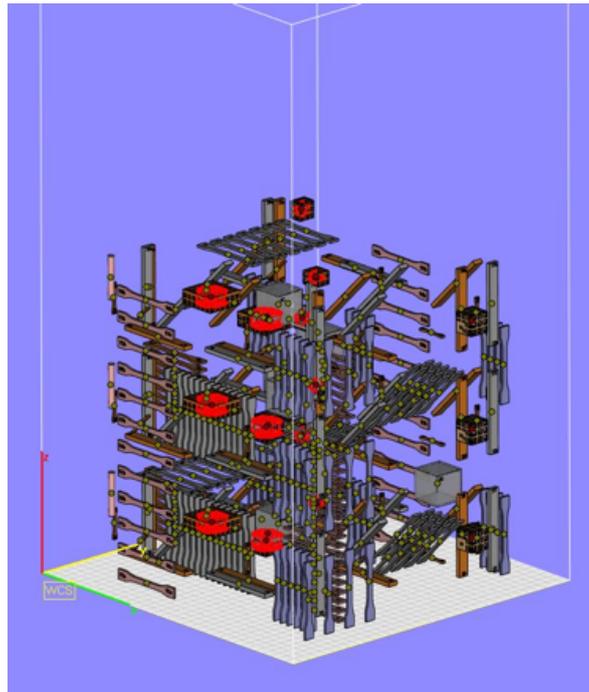


Figure 1. Build layout in Magics 20.0

Table 1. Material and process parameters used in the experiment

Parameters	Value
Virgin/aged PA2200 powder ratio, %	50/50
EOS P395 system settings	Balance
AM system warm up time, min	120
AM system cooling down time, min	240
Working chamber temperature, °C	180.5
Removal chamber temperature, °C	130.0

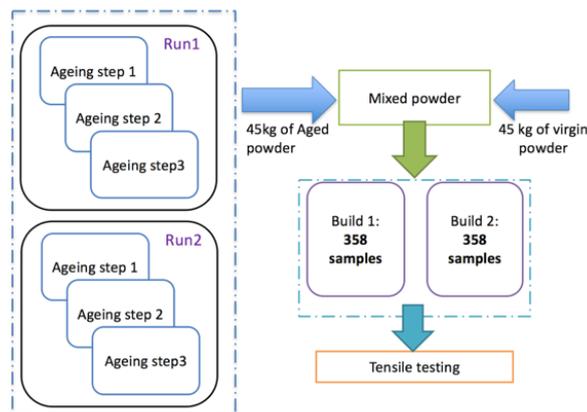


Figure 2. Schematic representation of main stages of the experiment

85 Since in this experiment an idea of using a self-aged powder proposed by Rösenberg *et al.* [3]
 86 have been utilized to control material properties, it was of the interest to compare whether similar
 87 repeatability of the results will be obtained to the ones Rösenberg *et al.* [3] had presented in their
 88 work. Therefore, build layout, process and material parameters were kept constant through the whole
 89 experiment and are shown in Table 1.

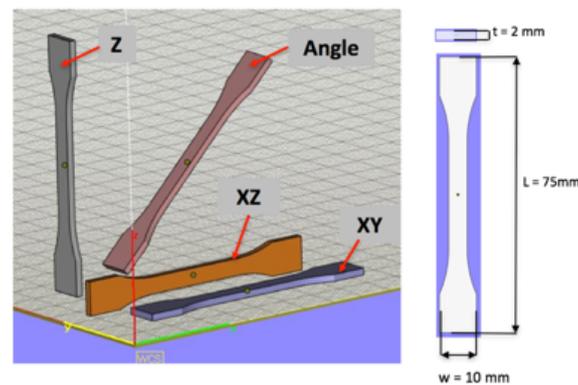


Figure 3. Schematic visualization of parts' orientation and dimensional features (where t – thickness, w – width and L – length)

90 2.1. Build layout

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

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

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

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

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

110 2.2. Conditioning of specimens and tensile testing

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

118 3. Results

119 3.1. Description of the collected data

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

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

Statistical characteristics	XYZ	XZY	ZYX	Angle
std	31.912	35.776	95.763	46.63
mean	1066.308	1051.951	958.25	1013.545
25%	1046.308	1035.374	908.038	983.455
50%	1067.77	1055.196	980.038	1010.291
75%	1088.461	1074.403	1032.381	1043.599
max	1148.078	1112.222	1090.35	1118.547
min	968.483	933.376	648.079	907.983

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

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

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

Statistical characteristics	XYZ	XZY	ZYX	Angle
std	0.727	0.679	1.096	2.311
mean	13.383	13.265	3.499	7.079
25%	13.158	12.875	2.719	5.594
50%	13.582	13.497	3.26	6.343
75%	13.893	13.663	4.017	7.262
max	14.353	14.287	7.451	12.537
min	11.18	10.618	1.917	4.316

125 The results illustrated in Figure 4 supports anisotropic behaviour of PA 12 reported earlier [13,22].
 126 While Tensile modulus for XYZ and XZY orientation has similar distribution, tensile modulus for
 127 ZYX orientation has the widest variance and the lowest value. Tensile modulus for Angle orientation
 128 has a narrow distribution, while the maximum value of Tensile modulus is 1065 MPa. In addition to
 129 variation between orientation, the variation between nominal value (provided by EOS for balanced
 130 machine settings for PA2200 material) and obtained results is also observed for Tensile modulus.

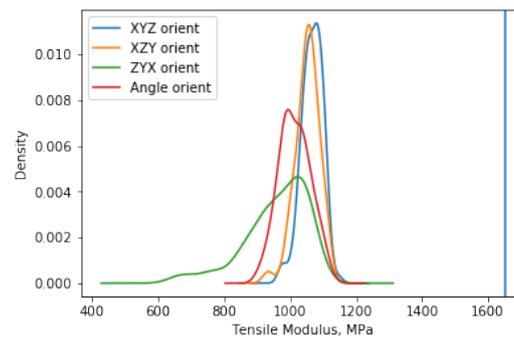


Figure 4. Distribution of tensile modulus for different orientations based on kernel distribution estimation (The straight line (1650 MPa) corresponds to the value from EOS Balanced datasheet)

131 Similarly to the Tensile modulus, distribution of nominal stress for different orientations is
 132 presented in Figure 5. The results of XYZ and XZY orientations are similar to the Tensile modulus,
 133 although distribution for ZYX orientation is much wider and the average value of nominal stress
 134 differs from the average value of XYZ and XZY orientations. Additionally, if to compare maximal
 135 value for ZYX orientation with the value provided by EOS, one can observe that nominal stress is
 136 almost two times lower (from Table 3 it is ca. 22 MPa, while 42 MPa is expected) than provided one by
 137 EOS (dashed line in Figure 5). However, value of nominal stress for Angle orientation is better than for
 138 ZYX, it is still relatively low comparing with the results for XYZ and XZY orientations.

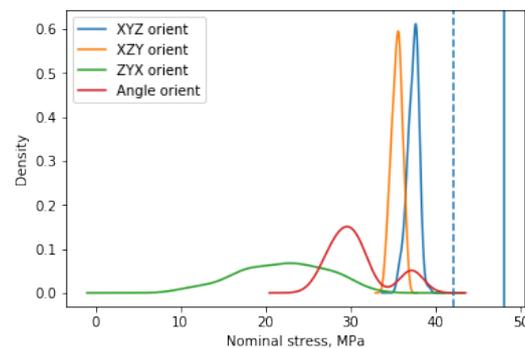


Figure 5. Distribution of nominal stress for different orientations based on kernel distribution estimation. The straight solid (48 MPa for XYZ orientation) and dashed lines (42 MPa for ZYX orientation) correspond to the value from EOS Balanced datasheet

139 Elongation at break comparing with two other mechanical properties has more similar results to
 140 the ones provided by EOS, and is illustrated in Figure 6. According to EOS datasheet, elongation at
 141 break is expected to be 4 % for ZYX orientation and 18% for XYZ orientation. The average value of
 142 elongation at break for ZYX and XYZ orientations are ca.3.5% and 13.4%, respectively (are taken from
 143 Table 4). Since there is no information from the EOS for other orientations, the observed values for
 144 XZY and Angle orientations cannot be compared with nominal ones. However, it is expected the XZY
 145 orientation should have similar results to XYZ orientation due to dominating X axis, and thus sclicing
 146 of the specimens is performed perpendicular to the direction of force load in tensile test. Similarly,
 147 ZYX and Angle orientations are sliced in such way that makes easier crack generation under tensile
 148 test.

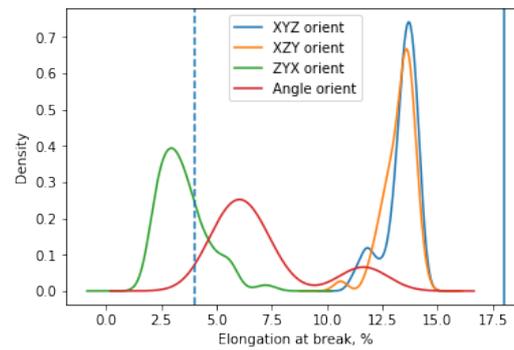


Figure 6. Distribution of elongation at break for different orientations based on kernel distribution estimation. The straight solid (18 % for XYZ orientation) and dashed lines (4% for ZYX orientation) correspond to the value from EOS Balanced datasheet

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

153 3.2. Application of machine learning techniques to predict mechanical properties without prior knowledge about 154 PA properties

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

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

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

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

180 3.2.1. Short introduction to used machine learning techniques

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

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

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

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

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

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

208 Since all of the described methods needs to be trained on the data before they can be used for
209 prediction task, the data should be divided into training and testing samples, usually with a ratio 75/25
210 % and 85/15 % when smaller data sets are used. For this purpose there is a library *training_testing_split*
211 in Skicit-Learn [34], which was used by author in this work. Training data set is used to train the
212 model (define the model), while testing data set is needed for evaluation of model generalization.
213 By comparing prediction accuracy obtained for training and testing data sets separately, one can
214 understanding whether under- or overfitting is present. Overfitting is present when model memorizes
215 input data, while underfitting means that model cannot find any patterns in the data due to small
216 number of data points. Both phenomena needs to be overcome in order to obtain robust model.

217 3.2.2. Prediction of Tensile Modulus and comparison of models' performance

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

227 However, prediction of Tensile Modulus based only on part positioning and STL model properties
228 in ZYX orientation has promising results. Model based on the gradient boost regressor algorithm

229 outperformed other models with a prediction accuracy of 0.808 out of 1 (80.8% out of 100 %) for ZYX
 230 orientation. Additionally, it can be seen that increase of number of data points (see All in Table 5,
 231 where number of data points represents number of data points used to train the model) leads to the
 232 higher prediction accuracy of 0.88 or 88 % for the developed model. This means that description
 233 of the part placement (positioning) in the build chamber in combination with part orientation and
 234 STL model properties can be used to predict Tensile Modulus especially when collected data is not
 235 divided in the groups corresponding to each orientation, but instead this information is used as an
 236 additional feature. This results show similar trend to the one Caulfield *et al.* [12] have reported in his
 237 study. Thermal distribution in the build chamber has an impact on the resulting mechanical properties,
 238 and presented results are in a good agreement with results reported in [12]. Besides, more details on
 239 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 stands for Gradient Boost Regressor, DTR - Decision Tree Regressor, and ABR - AdaBoost Regressor.

# data points	Orientation	Linear		GBR		DTR		ABR	
		R ²	MSE	R ²	MSE	R ²	MSE	R ²	MSE
110	XYZ	0.129	602.945	0.272	503.781	-0.76	1219.019	0.404	412.905
40	XZY	-0.927	1421.147	-2.297	2431.052	-2.313	2442.847	-2.102	2286.854
142	ZYX	0.48	4151.161	0.809	1524.994	0.764	1886.726	0.801	1586.234
74	Angle	0.03	1193.589	-0.159	1426.052	-0.469	1808.483	0.264	905.402
325	All	0.528	3876.678	0.888	916.721	0.819	1488.903	0.879	995.159

240 3.2.3. Prediction of Nomial Stress and comparison of models' performance

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

247 In addition, an interesting phenomena can be observed for Angle orientation. Since number of
 248 data points for this orientation is smaller than in XYZ orientation, model performance is significantly
 249 better. This can be explained by looking at the linear regression models. In this case, prediction of
 250 Nominal Stress in Angle orientation is even possible with a use of linear model, which has prediction
 251 accuracy relatively high - 0.867 out of 1. This means that combination of part positioning and STL model
 252 properties has linear correlation with Nominal Stress in Angle orientation. Therefore, application of
 253 more advanced methods results in improved model performance with higher prediction accuracy (like
 254 AdaBoost regressor in Table 6). Prediction of Nominal Stress in ZYX orientation has similar results
 255 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.

# data points	Orientation	Linear		GBR		DTR		ABR	
		R ²	MSE	R ²	MSE	R ²	MSE	R ²	MSE
110	XYZ	0.393	2.093	0.197	2.768	0.173	2.852	0.372	2.165
40	XZY	-0.645	0.827	-0.013	0.509	-0.043	0.525	0.50	0.251
142	ZYX	0.252	15.983	0.902	2.102	0.893	2.293	0.843	3.356
74	Angle	0.867	0.527	0.855	0.578	0.839	0.642	0.906	0.373
325	All	0.763	10.193	0.964	1.537	0.963	1.609	0.937	2.689

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:

$$y = -832.16 * x_1 - 6.819 * x_2 + 415.9 * x_3 + 13.639 * x_4 + 416.24 * x_5 - 6.819 * x_6 - 7.44e - 04 * x_7 + 0.823 * x_8 + 0.197 * x_9 \quad (1)$$

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.

# data points	Orientation	Linear		GBR		DTR		ABR	
		R ²	MSE	R ²	MSE	R ²	MSE	R ²	MSE
110	XYZ	0.261	0.0907	0.0146	0.121	-0.168	0.143	0.165	0.103
40	XZY	0.476	0.667	0.46	0.681	0.453	0.696	0.486	0.655
142	ZYX	0.269	0.963	0.67	0.434	0.587	0.545	0.638	0.476
74	Angle	0.889	0.500	0.795	0.927	0.749	1.129	0.903	0.439
325	All	0.965	0.739	0.987	0.284	0.985	0.326	0.971	0.616

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

$$\begin{aligned}
 y_{eb} = & 49.54 * x_1 - 2.757 * x_2 - 25.02 * x_3 + 5.516 * x_4 - \\
 & - 9.45e - 06 * x_5 - 24.52 * x_6 - 2.757 * x_7 + \\
 & + 2.497e - 03 * x_8 - 2.41e - 02 * x_9
 \end{aligned}
 \tag{2}$$

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

289 4. Discussion

290 Defining importance of the features can be done with a help of different techniques. However, each
291 of them typically provides slightly different assumptions. Therefore, in order to avoid this uncertainty,
292 the author propose to use model performance metrics, namely the coefficient of determination and
293 mean square errors (MSE) as key criteria for decision making process. Among investigated features
294 are STL model properties (surface, volume and number of mesh triangles), part orientation (angle for
295 x/y/z axes), and part placement (positioning) in the build chamber in terms of maximal, minimal and
296 central coordinates in x, y and z axes. These features were extracted from build layout prepared in
297 Magics 22.03 software (see Figure 1). More details about build layout have been provided in Section
298 2.1.

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

308 4.1. Feature importance for prediction of Tensile Modulus

309 Prediction of Tensile modulus with model prediction accuracy higher than 0.8 out of 1 was
310 considered as successful. However, when the author have made an attempt to develop model for
311 each orientation separately, models for XYZ, XZY and Angle orientation appeared to be unsatisfactory,
312 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.

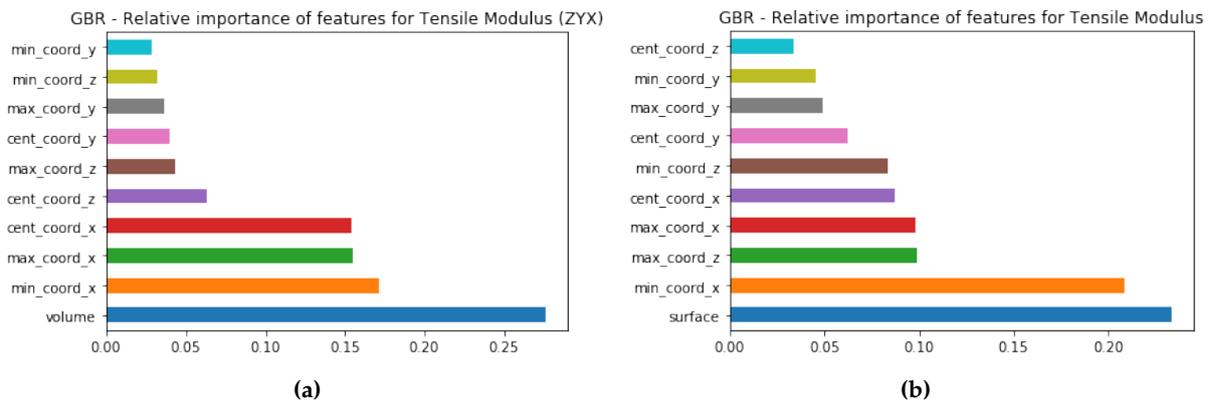


Figure 7. Feature relative importance based on the specimens orientation (a) Tensile Modulus - ZYX orientation. (b) Tensile Modulus - All orientations.

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.

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

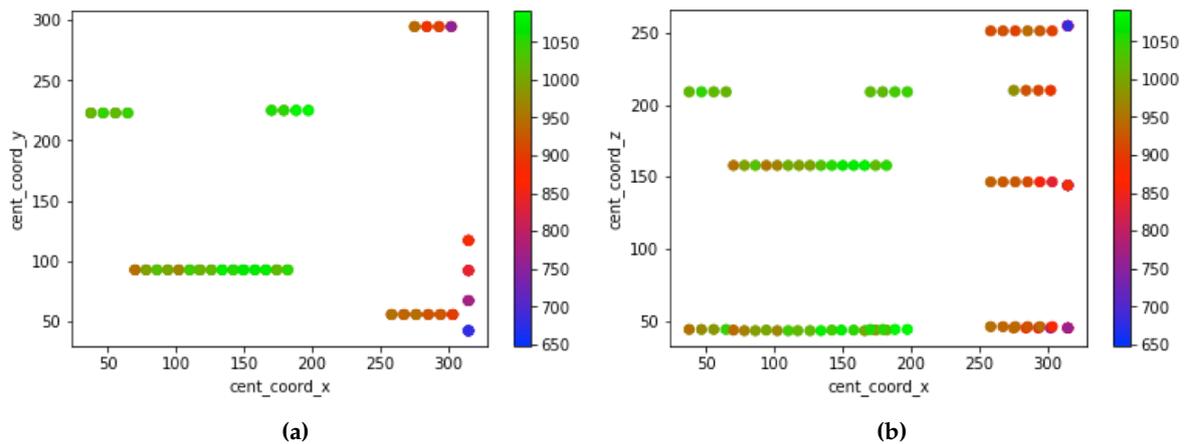


Figure 8. Visualization of Tensile Modulus for ZYX orientation (a) As a function of central coordinates in x and y axes in *mm*. (b) As a function of central coordinates in x and z axes in *mm*.

347 in the list, its relative importance is a bit higher than for ZYX orientation. Additionally, maximal
 348 coordinates in z and x axes are important to the same extent.

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

358 4.2. Feature importance for prediction of Nominal Stress

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

373 However, when it comes to the analysis of features' importance for developed model in Angle
 374 orientation, STL model properties are still in the list of being important but their contribution is less
 375 significant comparing to the ZYX/All orientations (see Figure 9b). One of the reasons why volume
 376 and surface features are among the least significant for the developed model can be the distribution of
 377 actual values for all specimens in Angle orientation. Thus surface values are in the range 1401.787 –
 378 1432.563 mm^2 , while values range for volume is even smaller (1029.925 – 1035.427 mm^3). However,

value range for surface feature for all specimens (without separation on orientations) has significant difference (e.g. $1381.555 - 1441.187\text{mm}^2$) comparing with volume values ($1029.925 - 1035.427\text{mm}^3$). 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.

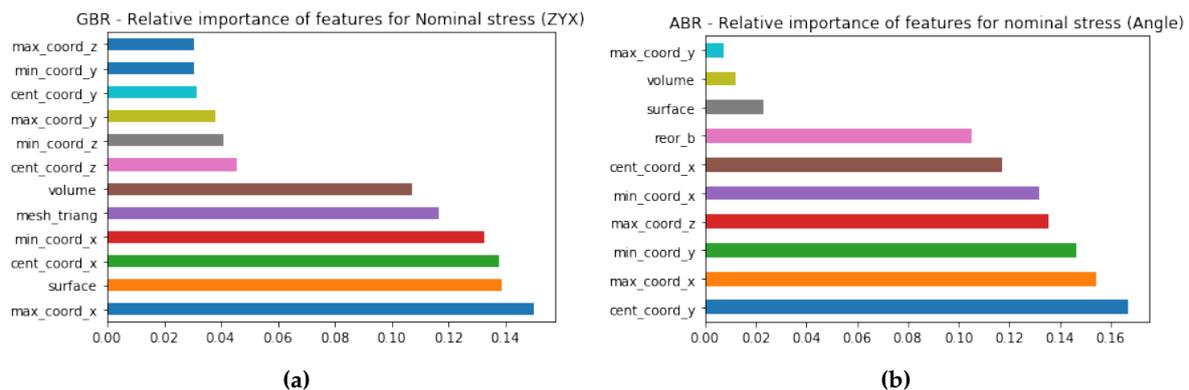


Figure 9. Feature relative importance based on the specimens orientation (a) Nominal stress - ZYX orientation. (b) Nominal Stress - Angle orientation.

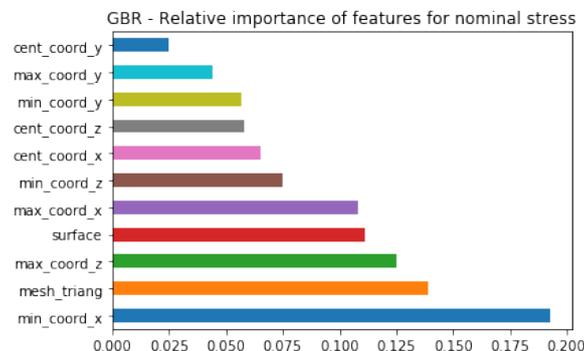


Figure 10. Feature relative importance for Nominal Stress - All orientations.

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

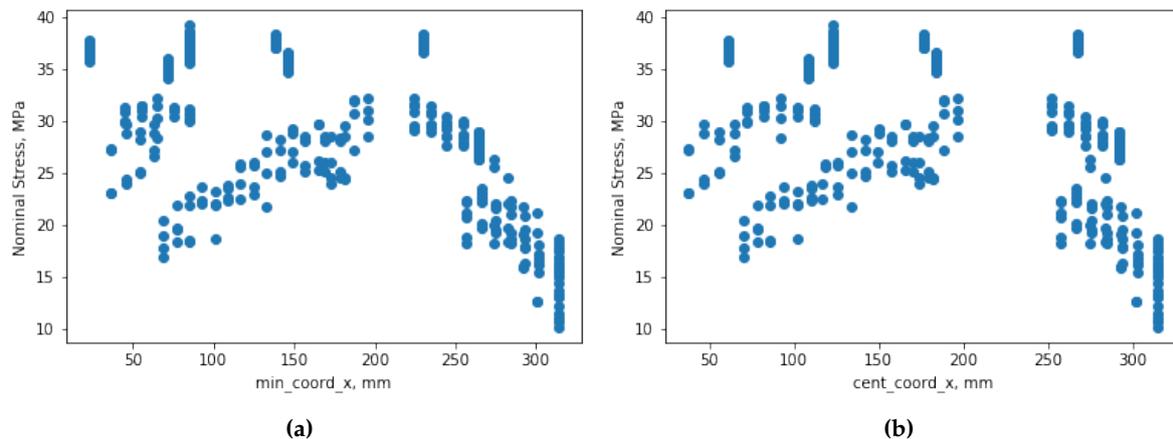


Figure 11. Comparison of the correlations between Nominal Stress and coordinates in x axis (for all data) (a) Nominal Stress vs minimal coordinate in x axis. (b) Nominal Stress vs central coordinate in x axis.

402 to develop this models. Besides the main difference between the techniques lies in the different
 403 approaches of weighting input parameters. However, analyzing feature importance for models can
 404 help in this study to rise new quations and show new direction for the experimental work in the future.

405 4.3. Feature importance for prediction of Elongation at break

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

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

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

430 Additionally, it is important to mentiona that speed under which force was loaded on the
 431 specimens has also an impact on the values of elongation at break. Since the difference between

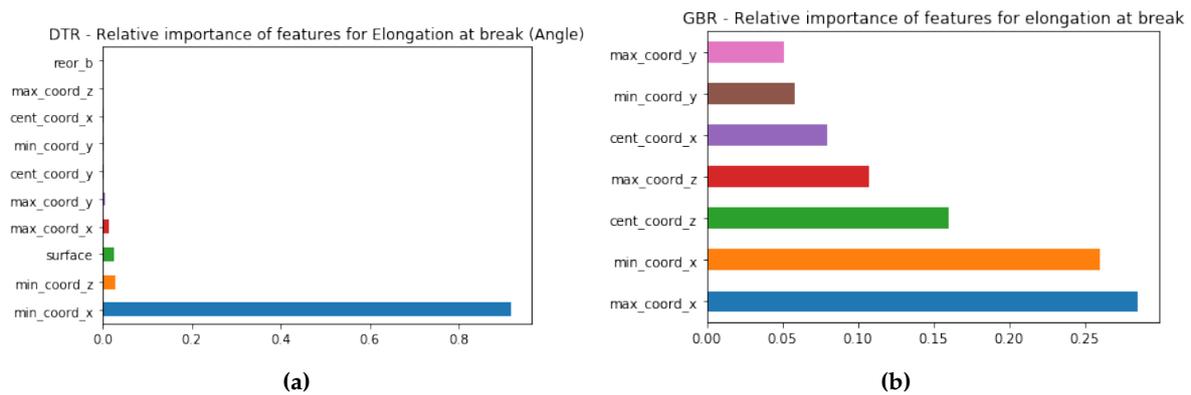


Figure 12. Relative importance of the feauters based on the specimens orientation ((a) Elongation at break - Angle orientation. (b) Elongation at break - All orientations.

432 values mentioned in EOS datasheets and obtained in the experimental work are similar, one can
 433 assume that this factor can be neglected.

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

444 5. Conclusions

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

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

459 When it comes to the prediction of mechanical properties by using traditional methods like
 460 linear regression, it can be seen from the Tables 5 - 7 that prediction accuracy for linear regression
 461 (except for Nominal Stress anf Elongation at breaks in Angle orientation) is low, and therefore more
 462 advanced techniques needs to be used. Since machine learning techniques have also been widely used
 463 in traditional manufacturing [29–32], these methods were applied in this study to develop non-linear
 464 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

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