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Research Article

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Posted Date: March 3rd, 2022

DOI: <https://doi.org/10.21203/rs.3.rs-1393827/v1>

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Prediction of Mechanical Behaviors of Additively Manufactured SS 316L via Machine Learning

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Abstract: Directed energy deposition (DED) is a rising field in the arena of metal additive manufacturing and has extensive applications in aerospace, medical and rapid prototyping. The process parameters, such as laser power, scanning speed, and layer thickness, play an important role in controlling and affecting the properties of DED fabricated parts. Nevertheless, both experimental and simulation methods have shown constraints and limited ability to generate accurate and efficient computational predictions on the correlations between the process parameters and the final part quality. In this work, data-driven machine learning models using XGBoost and Random Forest have been built and applied to predict the tensile behaviors of the stainless steel 316L parts by DED with variation in process parameters. The results suggest that both models can predict the tensile properties, e.g., yield strength, elongation, and ultimate tensile strength, of the fabricated parts and compute the significance of the factors affecting the quality of the part. The performance of the models was then compared with the Ridge Regression. XGBoost outperformed both Ridge Regression and Random Forest.

Keywords: Directed energy deposition, XGBoost, Random Forest, Ridge Regression, Tensile Properties.

1. Introduction

Additive manufacturing (AM), also called 3D printing, is a manufacturing technique where an object is created by adding material layer upon layer directly from 3D model data. AM has revolutionized the way of creating lighter, stronger parts and complex systems as it eliminates traditional manufacturing-process design restrictions. Directed Energy Deposition (DED) is a flexible type of AM process in which a focused heat source is used to melt the feedstock material and build up three-dimensional objects in a manner similar to the extrusion-based processes [1]. Holding the advantages of metallurgical bonding, controllable heat input, minimal stress and distortion, and comparable mechanical properties with traditional means, DED is now popular for effectively repairing and refurbishing defective and damaged high-tech components, e.g., turbine blades [1]. One of the major challenges in DED is the unrepeatable material properties and unpredictable microstructure. The quality of the deposited layers highly depends on the dynamic processes during material deposition, including energy absorption, melting, mass transfer, and rapid solidification. Better part quality and accuracies can be achieved by altering process parameters, such as laser power and scanning speed, but the effect mechanism is not documented. To achieve compact and reliable deposited layers and to optimize the processing parameters, the process-structure-property (PSP) relationship needs to be fully understood.

Over the past decades, both experiment-based methods and simulations are performed to investigate PSP relationships in DED. Finite Element Analysis (FEA) is commonly applied to model the mechanical behavior of printed parts. Using cohesive elements to model bonded interfaces is an advantage of FEA, but it is difficult to determine the boundary conditions at the

bonded interface [2]. Recently, researchers attempted to combine physics-based hybrid models and Artificial Neural Network to predict the mechanical properties of the printed parts, but these models faced difficulties in achieving better prediction due to the requirement of huge sets of data [3]. Conducting experiments and high-fidelity simulations are time-either consuming or expensive, there is a critical need for an effective and efficient tool for data analysis and data mining.

Machine learning (ML), being a subset of artificial intelligence (AI), has been proved to be a useful tool in modeling and simulation in AM [4]. This paper aims to perform data-driven predictive modeling with machine learning on the print quality of DED printed parts. The goal is to address the challenges arising from both experimentation and modeling methods. The experimentation section includes the design of the specimen, fabrication, strength behaviors testing, and data collection. In predictive modeling, the ML model is trained by the training data, then, the prediction is compared with the test data to analyze the accuracy of the prediction. The rest of the paper is organized as follows. In section 2, the previous research works are mentioned. Section 3 describes the methodology, including the theory of the machine learning algorithms, material selection and the detailed experimentation. In section 4, we discussed and explained the results obtained using ML. In section 5, we concluded with an explanation of the result and the future recommendation.

2. Related work

Enriched literature is available on data-driven models on various AM process parameters. Zhang et. al [5] developed a data-driven predictive model using extreme gradient boosting (XGBoost) and long short-term memory (LSTM) to estimate the melt pool temperature during DED with high accuracy. They also introduced a Data-Driven predictive modeling approach to estimate the tensile strength of polymers fabricated by the cooperative 3D printing process. The authors used Ensemble learning that combines multiple learning algorithms including Lasso, Support Vector Regression, and XGBoost, and compared the results with Ridge Regression. They claimed that the ensemble learning method outperformed the linear regression model.

Li et. al [6] presented an ensemble learning-based approach to surface roughness prediction in fused deposition modeling processes. To improve computational efficiency and to avoid overfitting, a subset (40) of the features was selected based on feature importance. The ensemble learning algorithm combined six different machine learning algorithms, including Random Forest (RF), Adaptive Boosting (AdaBoost), Classification & Regression Tree (CART), Support Vector Regression (SVR), and Random Vector Functional Link (RVFL) network. The authors claimed that the performance of the ensemble approach outperforms the individual base learners based on RMSE and RE. Scime et. al [7] worked on Inconel 718 material for flaw formation in Laser-Based Powder Bed Fusion (PBF) using Bag of Words (BoW) and Scale Invariant Feature Transform (SIFT) method. The prediction of thermal history and microhardness in the DED process were experimentally validated by a computational thermo-fluid dynamics (CtFD) model by Wolff et. al [8]. Both mentioned works demonstrated that the proposed inexpensive and well-tested computational frameworks can generate a large amount of high-quality prediction data, including temperature field, velocity field, melt pool dimensions, dilution, heating and cooling rates, solidification parameters, and microhardness. Several other algorithms have been proposed and applied in data-driven modeling in AM processes, including Ensembled Learning, Taguchi, and Discriminant Analysis, etc., as summarized in Table 1.

Table 1: Summary of data-driven models in AM process

Algorithm	AM process	Process parameters	Prediction variable	Model accuracy	Refs
Hybrid ANN & GA	DED	AM- α + β stress relieved, HIP, annealed	Tensile Properties	Deviation	[3]
XGBoost & LSTM	DED	Laser Power, Scanning Speed, Layer Height	Melt pool temperature	RMSE	[5]
Ensembled Learning	FDM	Layer thickness, Extruder temperature, Extrusion speed	Surface Roughness	R ² and RE	[6]
BoW and SIFT	PBF	Beam Velocity, Beam Power	Flaw formation	Prediction Accuracy	[7]
CtFD	DED	Laser power, Beam radius, Scan Speed	Thermal history, microhardness	-	[8]
Lasso, SVR and XGBoost	FDM	Incline Angle, Overlapping length, Number of shells	Tensile Strength	RMSE	[9]
ANN	DED	Laser power, scanning speed, powder feed rate	Height, Width, Depth	MAPE	[10]
DT, KNN, SVM, LDA, and QDA	DED	Morphological characteristics of the melt pool	Porosity	RMSE	[11]
Numerical & Analytical model	DED	Scanning Speed, Cooling rate, Laser power	Surface temperature	-	[12]
Taguchi method	DED	Laser power, Feed speed, Carrier gas, Powder flow	Tensile Strength	-	[13]
Bayesian Hybrid Model	DED	Scan Speed, Hatch Speed, Contour Speed	Tool path strategy	R ²	[14]
Ensemble learning	FDM	Layer thickness, orientation, raster angle,	Wear strength of prototype Vibration,	RMSE & MAPE	[15]
RF, SVR, Lasso	FDM	Layer thickness, Extruder temperature, Print Speed	Temperature and Melt pool temperature	R ² and RE	[16]

Note: Cross Validation = CV, Mean absolute percentage error = MAPE, Decision Tree = DT, K-Nearest Neighbor = KNN, Support Vector Machine = SVM, Linear Discriminant Analysis = LDA, Quadratic Discriminant Analysis = QDA, Genetic Algorithm = GA

Model and data collection are the most challenging aspects in data-driven modeling for DED because there are multiple parameters and a non-linear relationship existed between input variables and outputs. In addition, data collection in DED is either expensive or extremely complicated and lengthy or even both. Therefore, the data size to construct models for DED prediction is always relatively smaller and overfitting may occur in fitting predictive modeling. Few techniques can be used to reduce overfitting, e.g., random sampling, regularization, averaging across multiple

models, and data randomization. Since boosting and bagging methods perform the random sampling and averaging across multiple models, also they have regularization in their objective functions, both two ML algorithms are suitable matches for better prediction for the data which is non-linear and relatively smaller in size. Other challenges during data-driven modeling for DED include preprocessing and hyperparameter tuning. Special measures are needed to ensure the data quality in preprocessing. The hyperparameter, number of trees, shrinking rate, observation nodes, depth of trees are required to be tuned accordingly to achieve a higher prediction accuracy.

3. Methodology

3.1 Predictive Modeling

3.1.1 Extreme Gradient Boosting (XGBoost)

As an open-source and fast algorithm, extreme gradient boosting (XGBoost) is a widely recognized machine learning algorithm and a very popular choice of data scientists [17]. XGBoost is suitable for data mining challenges and tabular data types. XGBoost uses a gradient descent algorithm to minimize the loss when adding new models. It combines a set of weak learners (decision trees) and delivers improved prediction accuracy [18]. The concept of boosting is to add a new model to the ensemble [19]. After each iteration, a decision tree is added to the ensemble with the weights added from the error of the previous learner added to the model. From the mistakes/errors of the previous model, the weak learners are trained to improve the performance of the ensemble learner to function as a single strong learner. The purpose of building XGBoost is to appraise up all the computational advantages of boosting. XGBoost is an advanced implementation of Gradient Boosted Models (GBM) because GBM builds trees in series, while XGBoost follows parallel mechanism.

Tree Building: The main concept of the tree building is to predict the residuals from the prediction and test data. At every iteration, a new tree is built and then the residuals are recomputed. Tree building process keeps going until the model can fit the data well. A tree in XGBoost with a total of J leave can be expressed in Equation (1) [5].

$$T(x; \theta) = \sum_{j=1}^J \gamma_j I(x \in R_j) \quad (1)$$

Here, parameters $\theta = \{R_j, \gamma_j\}_1^J$ where γ_j is the constant assigned to the disjoint region R_j . The boosted tree model can be expressed by the sum of all trees, as shown in Equation (2), where M represents the number of trees.

$$f_M(x) = \sum_{m=1}^M T(x; \theta_m) \quad (2)$$

Loss Function: In the forward stagewise procedure, the objective function that needs to be optimized at each step can be expressed as Equation (3) where ν is the shrinkage factor while ϵ and λ are the regularization parameters to reduce overfitting.

$$objective_m = \sum_{i=1}^n L(y_i, f_{m-1}(x_i) + v \cdot T(x_i; \Theta_m)) + \varepsilon \cdot J + \lambda \cdot \sum_{j=1}^J \gamma_{jm}^2 \quad (3)$$

The first part of the objective function, $\sum_{i=1}^n L(y_i, f_{m-1}(x_i) + v \cdot T(x_i; \Theta_m))$ measures the loss for using $f_m(x_i)$ to predict y_i . The prediction $f_m(x_i)$ in XGBoost is combined by the prediction from previous trees $f_{m-1}(x_i)$ and the scaled approximation from the m -th tree $v \cdot T(x_i; \Theta_m)$. The second part of the objective function, $\varepsilon \cdot J + \lambda \cdot \sum_{j=1}^J \gamma_{jm}^2$ defines the complexity of the tree $T(x_i; \Theta_m)$ and perform regularization to reduce overfitting.

Split: XGBoost trees use binary splitting. And the split point selection starts with searching the point where the gain is maximum. During the tree pruning process, a gain function is calculated with Equation (4).

$$G = \frac{1}{2} \left[\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} \right] \quad (4)$$

where G_L , H_L , G_R and H_R represent the sum of g_i and h_i at the left and right branch after splitting, respectively. g_i and h_i are the first and second derivatives of $L(y_i, f_{m-1}(x_i))$. To make the optimal split at each node, the branch with the maximum value of gain is selected. γ is a constant assigned as a tuning factor. This is used as a stopping criterion in pruning. Pruning also works as the regularization to reduce the overfitting. If the gain function value G is higher than the γ , then the leaves are not pruned and don't check the parent node. If the gain function value G is smaller than γ , then it prunes the node. That is how XGBoost performs bottom-up pruning.

Figure 1: Flowchart of XGBoost

The flowchart for the XGBoost modeling is shown in Figure 1, includes two main phases: 1) The training phase, where the data is loaded into the model and the algorithm is trained to create the right output, and 2) The testing phase, where a set of observations is used to evaluate the

performance of the model. In the training phase, the hyperparameters need to be tuned according to the data and the problem type. The n number of trees are built where the objective values are minimized, the residuals are computed consequent, and weight is given to the errors of the previous models for the new model to learn. In this study, the training data is selected from tensile test and the split function is used to separate the test data from the training data.

3.1.2 Random Forest

Random forest regression is a supervised learning technique that uses ensemble learning to construct a group of decision trees from the bootstrap samples of a training data set [20]. It is a bagging technique that contains several decision trees on different subsets of the given dataset and takes the average to increase the accuracy of the prediction. For a given predictor, a response is created by a decision tree, where the branch denotes the outcome of the test and the leaves are the responses as the predictions. The tree is regarded as the regression tree if the response is continuous. Since tensile properties are continuous values, the regression model is performed for prediction.

For a given training data D , expressed as Equation (5), with N samples from the original training data set, for, $i = 1$ to N [16,33].

$$D_i = (x_i, y_i) \quad (5)$$

At each node, m number of variables and random split called feature bagging is selected. The data is partitioned by M number of regions, as shown in Equation (6), where R_m is the region and Y_m is a constant.

$$f_M(x) = \sum_{m=1}^M Y_m I(x \in R_m) \quad (6)$$

The splitting at node is performed to minimize the sum of the squares. The best $\hat{S}_m$ as shown in Equation (7) is the average of y_i in region R_m .

$$\hat{S}_m = y_i | x_i \in R_m \quad (7)$$

We suppose a splitting variable k and split points n , and the pair of the half planes are defined as Equation (8) and (9).

$$R_1(k, n) = x | x_k \leq n \quad (8)$$

$$R_2(k, n) = x | x_k \geq n \quad (9)$$

The objective function L to solve the splitting variables and split points can be expressed in Equation (10).

$$L_{k,n} = \min_{k,n} [\min_{c_1} \sum_{x_i \in R_1(k,n)} (y_i - S_1) + \min_{c_2} \sum_{x_i \in R_2(k,n)} (y_i - S_2)] \quad (10)$$

For any random values of k and n , the inner minimizations are solved by Equation (11) and (12) [33].

$$\hat{S}_1 = \text{average}[y_i | x_i \in R_1(k, n)] \quad (11)$$

$$\hat{S}_2 = \text{average}[y_i | x_i \in R_2(k, n)] \quad (12)$$

The stopping criterion is satisfied when the number of responses in D_i falls under the threshold. The number estimators or trees we have selected is 500 and 1000, a prediction at a new point x is made by average of all the regression trees, as shown in Equation (13). Bootstrap or bagging generates b number of new training data set D_i and V_t is the bootstrapped tree in Equation (13). The flowchart of the Random Forest model is shown in Figure 2.

$$f_b(x) = \frac{1}{b} \sum_{b=1}^b V_t(x) \quad (13)$$

Figure 2: Flowchart of Random Forest

3.2 Data Collection

3.2.1 Material Selection

Commercial gas atomized 316 Stainless Steel L (SS 316L) powder (45~105 micron) is used in this study because it has higher creep, higher tensile strength properties, and is widely used for durable and high-stress situations [21]. Low carbon steel is used as the substrate. The chemical composition of SS 316L is shown in Table 2.

Table 2: Chemical composition of SS 316 L

C	Mn	Si	Cr	Ni	Mb	P	S	N	Fe
0.08	2	0.75	16	10	2	0.045	0.03	0.1	Bal.

3.2.2 Specimen Design

Dog bone specimen is designed according to the ASTM standard [22]. To reduce the printing time and associated expenses, the standard dimensions are scaled down to length, width and height to

82.5 mm, 9.50 mm, and 3 mm respectively, as shown in Figure 3 [23]. The layer thickness is 0.54 mm with totally five layers.

3.2.3 Design of Experiment

Four process variables were selected in this work. The input of laser power was selected between 600 W to 1000 W with 100 W interval, and the scanning speed was changed from 8 to 12 mm/s. Powder feed rate (5 g/mm), laser spot diameter (2 mm), nozzle gas rate (9 L/min), shield gas rate (12 L/min), and carrier gas rate (5 L/min) are constant for all the experiments. In this study, full experimental design is applied, thereby, a total of 25 dog bone specimens are printed using 25 different distinct sets of parameters, as shown in Table 3.

Table 3: Design of Experiment with groups of parameters

Group No	Laser Power (W)	Scanning Speed (mm/s)	Average Layer Height (mm)	Energy Density (J/mm ²)
1	600	8	1.51	18.8
1	700	8	1.52	21.9
1	800	8	1.75	25.0
1	900	8	1.8	28.1
1	1000	8	1.75	31.3
2	600	9	1.32	16.7
2	700	9	1.47	19.4
2	800	9	1.34	22.2
2	900	9	1.37	25.0
2	1000	9	1.35	27.8
3	600	10	0.79	15.0
3	700	10	1.71	17.5
3	800	10	1.7	20.0
3	900	10	1.77	22.5
3	1000	10	1.83	25.0
4	600	11	1.38	13.6
4	700	11	1.41	15.9
4	800	11	1.49	18.2
4	900	11	1.62	20.5
4	1000	11	1.73	22.7
5	600	12	1.27	12.5
5	700	12	1.42	14.6
5	800	12	1.51	16.7
5	900	12	1.54	18.8
5	1000	12	1.37	20.8

3.2.4 Dog bone specimen fabrication

The experiments were performed with a customized powder based DED system (AMBIT™ core DED, Hybrid Manufacturing Technology, TX, USA). The system consists of an inert gas supply, a system chamber including the X-Y axes motion table, the deposition head and the lens system, powder hoppers, AMBIT core, operator control, a chiller, and a fume extractor, as shown in Figure 3 from [23]. SS 316 L powders are delivered to the deposition head with delivery gas (argon), the powder feeding rate is controlled with the rotational disk in the hoppers. Inert gas is supplied to the system's chamber to avoid oxidation during the print. The path of the deposition head is generated by Autodesk Fusion 360 and controlled by the AMBIT™ core. In DED, a subsequent layer is typically deposited in a different orientation than the previous layer. Common scan patterns from layer to layer are usually multiples of 30°, 45°, and 90° [1]. Layer orientations can also be randomized between layers. In this setup, the first and fifth layers are at 0°, the second layer at 45°, the third layer at 135°, the fourth layer at 45°. The scanning pattern at different layers is shown in Table 4 [23]. The variation in printing orientation from layer to layer eliminates preferential grain growth, which otherwise makes the properties anisotropic and reduces residual stresses [1]. The printing directions are demonstrated in Figure 4 from [23].

Figure 3: Schematic diagram of AMBITTM laser-based DED Hybrid System

Table 4: Infill Structure of Each layer

Layers #	1	2	3	4	5
Infill Structure

Figure 4: 3D printed SS 316L Dog bone specimens by L-DED process

3.2.5 Dog bone specimen processing

Electric discharge machining (EDM) was used to subtract the dog bones from the substrate. Each specimen was first separated with the substrate with a vertical bandsaw. Then each specimen was cut from its substrate with the height of 2 mm with a wire EDM machine (VG plus series, EXCETEC Technologies Co. Ltd, Taiwan). A brass wire with a small diameter of 0.23 mm cut the narrow width of 2 mm from the original specimen. The workpiece moved steadily around the wire so that it can have an accurate tool path. Numerical control was used during cutting to maintain the precision of the motion. During cutting, the wire continuously moved between a supply and take in reels of wire to maintain the constant diameter of the electrode. Dielectric fluid was constantly flushed to wash away all the debris.

3.2.6 Tensile Testing

The tensile test was performed on a universal testing machine (AGS-X, Shimadzu Co., Kyoto, Japan) with a 10 KN capacity load cell to evaluate the tensile properties according to ASMT E8. The gauge length was 12.5 mm, and the test speed was 1.5 mm/min. Stress and strain are calculated from the recorded tensile loads and extensions. In the beginning, the cross-sectional area of each dog bone specimen is measured. Then the specimen is mounted to both clamps of the machine tightly to avoid distortion while the load is applied. The plastic deformation is visible during the testing. The graph is originated from the Trapezium software connected to the universal testing machine. The final data set is provided by the software to calculate the tensile strengths.

The average value of the yield strength, ultimate tensile strength, and elongation (%) of the DED fabricated SS 316 L parts are compared with the similar properties of raw SS 316 L (ASTM: A240). The result in Table 5 showed that the printed parts have mechanical properties similar to those of raw material. The mechanical properties of DED fabricated SS316 L is close to the ASTM standard values [22]. The average yield strength improved 50%, and ultimate tensile strength improved 8.06% but elongation (%) is 19% less than the ASTM standard. The fabricated parts behaved less ductile than the raw material but possess more strength compared to the raw ones. The decrease in ductility might have been caused by the internal porosities inside the printed part induced by the inert gas, or by the pores that existed in the original powders.

Table 5: Comparison between the mechanical properties of printed and raw SS 316 L

Material	Yield Strength (MPa)	Ultimate Tensile Strength (MPa)	Elongation (%)
Printed SS 316L by DED	310.5	544.6	32.4%
Raw SS 316L	207	504	40%

The overall experimentation workflow starting from generating CAD files to the final state of the specimens after tensile testing is shown step by step in Figure 5.

Figure 5: Workflow of the experimentation of the Dog bone specimens by DED

4. Results and discussion

4.1 Effects of process variables on material strength behaviors

Laser power determines the amount of energy absorbed by the melt pool and, also controls the powder efficiency in DED [24]. Typically, with higher laser power, heat increases causing more powder to melt in the melt pool; hence, increases the thickness of the specimen [25]. The effects of laser power on materials' tensile behavior are shown in Figure 6. Yield strength (YS, MPa) has a descending trendline with the increase of the laser power whereas ultimate tensile strength (UTS, MPa) and elongation (%) have an ascending trendline with the increase of laser power. All three curves dropped down at the maximum laser power of 1000 W. UTS and elongation are maximum at 900 (W) at 11 mm/sec scanning speed. Lower laser power induces higher un-melted particles in the layers and on the surface which is also responsible for shrinkage. So, the graph tends to rise with the rise of power but with higher laser power, there are higher chances of gas porosity which also means there is a higher thermal gradient. It induces higher residual stress which degrades the mechanical properties.

Energy density is defined as the amount of energy absorbed by the powder and substrate during melting per unit area [26]. Energy density can be calculated by Equation (14):

$$E \text{ (J/mm}^2\text{)} = \frac{P}{vD} \quad (14)$$

Where, P is the laser power (W or J/s), v is the scanning speed (mm/sec) of the operating tool and D is the diameter (mm) of the laser spot. In our work, $P = [600, 1000]$, $v = [8, 12]$ and $D = 2$ mm (constant). As energy density is a combination of laser power and scanning speed, the graph showed a similar trend as laser power, as shown in Figure 6 (b).

Laser scanning speed directly affects the part shape and dimensional accuracy [27]. Changes in the scanning speed cause variations in the bead size because of different deposition amount at a

constant powder feed rate [27]. The higher the laser scanning speed, the better the tensile behavior but the trend goes down after a certain point [28]. With the rise of the scanning speed, the granular bainite decreases which improves the grain boundary area. Thus, the dislocation density increases but with higher speed, the grain bainite size decreases due to very poor bonding between the deposition layers causing the fall of the tensile strength [28]. The specimens are sorted into five groups based on different scanning speeds, and the graphs are plotted as the scanning speed of each group against the three other process parameters to exhibit the tensile behaviors of the specimens of a particular scanning speed group.

Both geometrical accuracies and mechanical properties of the printed parts are affected by the layer thickness, also referred as vertical resolution [26]. The average layer thickness for each specimen is calculated and considered as one of the affecting parameters. The effects of layer thickness on materials' tensile behavior are shown in Figure 6 (c). Layer thickness (mm) has a similar effect on YS, elongation (%), and UTS like the other two process parameters. It has been proved that scanning speed, laser power, and powder feed rate controls bead height, bead width, and penetration [27]. The result suggests that the bead height couldn't be maintained constant during the printing process. With the increase of scanning speed, bead height decreased and increased with the increase of powder feed rate. Laser power didn't affect the height much compared to scanning speed and powder feed rate.

Figure 6: Yield Strength (MPa), Ultimate Tensile Strength (MPa) and Elongation (%) VS. (a) Laser Power (W), (b) Energy Density (J/mm²) and (c) Layer Height (mm) respectively for 11 mm/sec scanning speed

4.2 Prediction results

YS, UTS, and Elongation (%) were collected from the tensile testing and they were considered as three separate outputs (Y_0) Yield. Four process parameters, including laser power, scanning speed, layer height, and energy density are considered as the input array (X_0). The modeling process starts from calling the built-in functions from a machine learning library, loading the data, defining the input array (X_0) and the output array (Y_0), then the training and testing split function were defined, the hyperparameter metrics were created as the param_grid. The last step is to call the prediction function and define the performance evaluation metrics.

In this work, Scikit learn was used as the library and the PyCharm 2020.2 version was used as a writing module. Both XGBoost and Random Forest have built-in functions in Scikit learn library. Hyperparameter tuning was completed using RandomizedSearch cross validation for both of the models and XGRegressor() and RandomForestRegressor() as the main fitting function were called from the sk.learn_model selection. The predictions are fitted against the randomly selected test data. The model fitted to the data by XGBoost and Random Forest is shown in Figure 7 (a~c) and Figure 7 (d~f). Smaller residuals are observed in a few points which is a good indicator of the performance accuracy of the model. To get a clearer idea of the accuracy, performance evaluation is performed on the predicted and test data.

4.3 Performance Evaluation

As mentioned before, performance evaluation is an indicator of the model's accuracy and precision of predicting the output. For regression modeling, root means square error, coefficient of determination, relative error are suitable statistical metrics for this purpose. RMSE has been a standard statistical metric to measure the model performance. The RMSE can be calculated with Equation (15). It is assumed that there is a n number of samples and unbiased errors in the prediction and test data. A smaller RMSE value indicates better performance of the model.

$$RMSE = \sqrt{\sum_{i=1}^n \frac{(\hat{y}_i - y_i)^2}{n}} \quad (15)$$

Relative error (RE), shown in Equation (16), is the ratio of absolute error and the real measurement taken. This is used to explain how accurate the prediction was compared to the real value.

$$RE = \frac{1}{n} \left| \sum_{i=1}^n \frac{\hat{y}_i - y_i}{y_i} \right| \times 100\% \quad (16)$$

Where, $\hat{y}_i$ = predicted values, y_i = observed values, $\bar{y}_i$ = mean of the observed values.

The coefficient of determination (R^2), shown in Equation (17), explains how much of the data has fitted the regression model. Usually, closer the value to 1 indicates the model has fitted the data well but not always a higher value is a good indication of the better-fitted model.

$$R^2 = 1 - \frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{\sum_{i=1}^n (\bar{y}_i - y_i)^2} \quad (17)$$

Where, $\hat{y}_i$ = predicted values, y_i = observed values, $\bar{y}_i$ = mean of the observed values.

Figure 7: The predicted and test data for (a) Yield Strength (MPa), (b) Ultimate Tensile Strength (MPa), (c) Elongation (%) by XGBoost (d) Yield Strength (MPa), (e) Elongation (%), (f) Ultimate Tensile Strength (MPa) by Random Forest

4.3.1 XGBoost & RF performance evaluation

The performance evaluation metrics of our XGBoost and RF models are computed using the `sk.learn.metrics`. For RMSE, `mean_sqaure_error`, for the coefficient of determination `r2_score` is

called from the respective library. The relative error calculation is manually imported to the metrics.

Table 6: Performance evaluation metrics for XGBoost and RF

Models	XGBoost	Random Forest	XGBoost	Random Forest	XGBoost	Random Forest
Test	RMSE	RMSE	R ²	R ²	RE	RE
Yield Strength (MPa)	6.09	12.85	0.71	0.65	1.11%	1.098%
Ultimate Tensile Strength (MPa)	11.89	28.76	0.65	0.56	3.23%	3.5%
Elongation (%)	2.64	3.54	0.73	0.68	0.83%	1.01%

The RMSEs obtained for the three outputs are summarized in the Table 6, indicating the aggregated means of the deviation of the predicted values from the test data. For XGBoost, the deviation in RMSE is highest for UTS (11.89) and lowest for elongation (%) (2.64). The coefficient of determination (R²) indicates how well the model fit the training data. The results show that the XGBoost model fitted 71% of the YS data, 65% of the UTS data, and 73% of the elongation (%) data. Similarly, the deviation in RMSE is highest for UTS (12.85) and lowest for the elongation (%) (3.54) for RF. And this model fitted 65% of the YS data, 56% of the UTS data, and 68% of the elongation (%) data. The results of relative errors suggest that the relative uncertainty of the prediction to the actual values for YS, UTS, and elongation is 1.11%, 3.23%, and 0.83%, respectively for XGBoost. And for RF, the values for YS, UTS, and elongation are 1.098%, 3.5%, and 1.01%, indicating that the XGBoost model outran the Random Forest in prediction.

4.3.2 Ridge Regression

Ridge Regression (RR) is a suitable choice for data set with multicollinearity. If there is a possibility of multicollinearity, the variance of the least square estimates gets too large to be closer to the true value though the estimates are unbiased [29]. In Ridge Regression, standardization of both dependable and independent variables is a must. Standardization is the statistical process of rescaling the mean and the standard deviation to 0 and 1 respectively. Ridge Regression is calculated on the standardized variable. But the final regression co-efficient are estimated, they are adjusted back to the original scale. The data was first standardized by using MinMaxScaler() function called from Sklearn.preprocessing. The test size kept 25% of the data using test_train_split. For the three tensile strength behavior. The predicted and test values of the three tensile properties are shown in Figure 8.

The performance evaluation metrics for Ridge Regression are summarized in Table 8. The RMSE values obtained for the three outputs meant a deviation of the predicted values from the test data. Similar to XGBoost, the deviation for RR is highest for UTS (33.25) and lowest for elongation (%) (4.59). The RR model fitted the 49% of the YS data, 56% of the UTS data, and 58% of the elongation (%) data. The relative uncertainty of the prediction to the actual values for YS, UTS, and elongation is 2.93%, 4.61%, and 1.89%. The overall performance accuracy of the model is good but still cannot surpass either of the machine learning models.

Figure 8: The predicted and test data for (a) Yield Strength (MPa), (b) Elongation (%), (c) Ultimate Tensile Strength (MPa) by Ridge Regression.

Table 8: The performance evaluation metrics for Ridge Regression

Test	RMSE	R ²	RE
Yield Strength (MPa)	21.89	0.49	2.93%
Ultimate Tensile Strength (MPa)	33.25	0.56	4.61%
Elongation (%)	4.59	0.58	1.89%

The results suggest XGBoost is a better choice for mechanical behaviors prediction. One of the possible reasons is that XGBoost first prunes the tree with a score called the “Similarity Score” before starting the prediction. It considers the gain function value of a node as the difference between the similarity score of the node and the similarity score of the children node. If the gain from a node is found to be minimal then it just stops constructing the tree to a greater depth which controls overfitting to a great extent. On the other hand, Random Forest tends to overfit the data if the majority of the trees in the forest are provided with similar samples. XGBoost can handle imbalanced data better than Random Forest. XGBoost tends to put the highest significance to the functional space while reducing the loss function when Random Forest puts maximum importance on the hyperparameter optimization. The basic mechanism which makes XGBoost faster is the

weights are calculated as the ratio of the square of the sum of the residuals to the sum of the number of residuals and the regularization factor whereas for Ridge Regression, it's the sum of the squared residuals in the denominator. Therefore, in the case of XGBoost, the sum of the residuals first neutralizes the negative values which reduces the overall values of residual. On the other hand, the squared values of the residuals in Ridge Regression are always non-negative which increases the values of residuals for Ridge Regression compared to XGBoost.

4.4 Limitations

For XGBoost & Random Forest which are capable to fit the small size of tabular data, the data size in this study is smaller for the model to train. It can be expected that with the larger data size, the prediction accuracy can be increased. The experimentation includes three extensive experimental works e.g., fabrication, preparation of the final specimens by EDM, and finally the tensile testing. Fabrication by the L-DED machine is time-consuming and expensive. Due to time and facility constraints due to COVID 19, EDM facilities were not available to the users. For future work, more experiments are recommended to perform to improve the performance accuracy of the model.

DED process is prone to rough surface finish and internal porosity [1]. The stress-strain curves obtained are similar but not identical between any two specimens. Such variation of tensile properties possibly resulted due to the variation in the layer thickness [26], which was caused by the surface and internal defects of the fabricated specimens. According to Zheng et. al [29] the internal defects were observed in 316 stainless steel specimens fabricated by the L-DED process and these defects can be divided mainly into two kinds: gas porosity and lack-of-fusion porosity. The final specimens are cut from the original one with the substrate by EDM. The final thickness was preset to 2 mm for all the specimens, but the cutting process faced difficulties due to defects of the specimens. Therefore, the thickness couldn't be maintained constant to 2 mm for all the groups, and after manual surface finishing the final layer height ranged from 0.79 mm to 1.83 mm with an average of 1.51 mm. It was observed that the first two groups with higher energy density due to their lower scanning speeds 8 mm/sec and 9 mm/sec had more constant layer thickness and was closer to 2 mm while the deviation from 2 mm and the more variation in the layer height was observed in the rest of the groups as well. It can be concluded that with higher energy density which means lower scanning speed, there are fewer defects like entrapped gas porosity and un-melted particles found in the specimen. It was observed just after the printing that with higher laser power, the powder efficiency increased. Although the higher powder efficiency is responsible for the higher thickness of the original specimen, it is evident that it could not control the un-melted particles in the melt pool

5 Conclusion

The goal of this study is to employ machine learning to predict the tensile behavior of SS 316L printed using laser-based DED process. The motivation behind our current work is to examine the tensile properties of the printed specimens by the L-DED process and, at the same time, to be able to predict the tensile behavior of the fabricated parts without performing a series of laborious experiments. The results from the tensile testing provided outstanding insights, which exhibited better mechanical properties of the printed parts compared to raw SS 316L. A total of 25

experiments have been performed with three sets of data and XGBoost and Random Forest have been selected because of their capability to predict with smaller tabular data. From this study, it can be concluded: (1) The yield strength and ultimate tensile strength of the printed SS 316 L were better than the raw materials, (2) XGBoost outperformed both Random Forest and Ridge Regression in terms of evaluation metrics.

There are a few challenges and difficulties in data-driven modeling for AM process prediction. The prospects and forthcoming investigation of this study will focus on the following issues.

- The effects of thermal behavior and solidification on print quality are not considered in our study. Due to the varied laser power and additive layer nature of the process, the specimen experienced complex thermal cycles in the different locations of the built. Thermal behaviors can add a great deal to the prediction quality of the model.
- A traversed molten pool formed by the finely focused laser beam causes a higher cooling rate and solidification. These complex thermal behaviors are responsible for microstructure complexity due to which the consistency of the tensile properties might have suffered. Therefore, the microstructure can be used as one of the outcomes along with the tensile properties to establish the correlation among them.
- The inconsistency of the tensile properties of different groups also affected the learning curve of the model during training. Therefore, multicollinearity should be avoided during data collection.
- To improve the model's accuracy, different parameters should be considered along with the current ones in terms of F score to find out the optimum combination of parameters affecting the results. Based on feature importance, more experiments should be performed while modeling to examine whether the model performs better with and without the most important factors.

Declaration

- Funding:** Not applicable.
- Conflict of Interest/ Competing interests:** The authors declare no conflict of interest or competing interests.
- Availability of Data/Materials:** Not available for publication.
- Code availability:** Not available for publication.
- Ethics approval:** The authors declare the article was constructed respecting all ethical conditions of publication.
- Consent to participate:** All authors participated in the preparation of the article. Therefore, the authors allow their names in the article.
- Consent for publication:** The authors allow for publication.

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