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A Machine Learning Approach to Predict the Tensile Strength of Aluminum Alloys

Md. Tanbir Hasan, Mahmudul Hasan Rohan, Md Mahfuzur Rahman, Shahriar Islam Sium, Abdullah Mohammad Khaled, Md. Tanvir Hossain, Chaity Dey and Akteruzzaman Nadim
Department of Industrial & Production Engineering
Jashore University of Science & Technology
Jessore-7408, Bangladesh
tanbirhasan.mail@gmail.com, rohanovro756@gmail.com, mrahman.ipe@just.edu.bd, sium.ipe.just@gmail.com, abdullahmdkhaled7@gmail.com, mdtanvirhossain.ai@gmail.com, chaitydeyctg@gmail.com, akhteruzzamannadim@gmail.com

Abstract

This Studies explores a comprehensive machine learning (ML) framework for predicting the tensile strength of aluminum alloys using chemical composition and processing without the high cost of endless, trail-and-error experiments. An Extreme Gradient Boosting (XGBoost) algorithm, trained on a 1145 sample dataset we compiled from Mendeley data repository. The data is a mix of chemical inputs (wt.% of Al, Cu, Zn) and processing history (like "Strain hardened" or Artificial Aged"). The goal was to see if the model could determine the complex, non-linear relationships that govern an alloy's final strength. The results were very strong. On unseen data the model achieved an R^2 of 0.9416, and the error (RSME) 37.30 MPa on the test set, demonstrating very good prediction accuracy across a wide range of tensile strength values (100-800 MPa). We were run a permutation importance analysis to see what it learned. We found the most three influential alloying elements were Copper (Cu), Aluminum (Al), and Zinc (Zn) respectively in determining tensile strength. We also run diagnostic check to confirmed the model statically sound and unbiased. The study yields significant insights into composition-property correlation and offers a reliable tool for accelerate aluminum alloy design and optimization.

Keywords

Aluminum Alloys, Tensile Strength, Machine Learning, Extreme Gradient Boosting and Alloy Design.

1. Introduction

Aluminum alloys are a cornerstone of modern engineering, used as fundamental structural elements in aerospace, automotive, and construction industries due to their excellent strength-to-weight ratio, corrosion resistance, recyclability, low maintenance and manufacturing cost (Hu et al. 2021).Therefore, there is constant hunt for new aluminum alloy with higher tensile strength. The main problem is that developing new alloys with specific properties is a slow, expensive process due to trial-and-error method. An alloy's strength is not just about its chemical composition it also depends on how it's processed. Tensile strength is a critical mechanical property, determines the alloy's ability to withstand under external forces without failure. Empirical formulas, physical testing, and constitutive models are used in traditional methods for predicting tensile strength, which are time consuming, costly and limited in accuracy due to the complex interplay of alloy composition, and processing methods. Recent developments in machine learning (ML) have transformed materials science with the possibility of data driven prediction of material characteristics. ML models can understand non-linear relationships between input features like alloy compositions, processing conditions, and tensile strength with a fast and more accurate alternative for traditional methods(Hu et al. 2021). Several studies have proven the potential of ML for the prediction of the

mechanical properties of aluminum alloys. For instance, prior work achieved a 0.914 R^2 value for estimation of tensile strength using an application of XGBoost algorithm (Fu et al. 2023). Our study set out to build and test ML framework to do accurately predict the tensile strength of aluminum alloys. We believe this ML framework can be accelerate the design and screening of new, high strength aluminum alloy (S. K. Mishra et al. 2021) .

1.1 Objectives

Our main goal is to train and fine-tune a gradient boosting ML model to get most accurate tensile strength productions and making sure to capture chemical compositions and processing details. Then checking the model performance based on standard metrics and statistical diagnostic plots. And, finally figuring out which features had the biggest impact on tensile strength.

2. Literature Review

Aluminum alloys get their strength from different strengthening mechanisms including solid solution strengthening, precipitation hardening, grain refinement, and work hardening (Zheng et al. 2022). The tensile strength prediction is very difficult because of the intricate interactions between these systems. The lattice deforms when alloying elements like Mg, Cu, and Zn dissolve in the aluminum matrix, these makes it much difficult for dislocations to move and resulting solid solution strengthening. Precipitation hardening, particularly in heat-treatable alloys like the 2xxx, 6xxx, and 7xxx series, involves the formation of fine precipitates that strengthen the material. Researches have used both empirical equations and computational thermodynamics to learn the correlation between alloying compositions and mechanical property. However, these conventional approaches are often failed to figuring out the nonlinear relationship and interactions between multiple alloying elements.

In recent years, the application of machine learning in materials science has grown exponentially. Agrawal and Choudhary (Agrawal & Choudhary, 2016) conducted a thorough assessment for machine learning applications in material science, highlighted the process optimization, materials discovery, and property prediction. Several machine learning techniques have been studies for aluminum alloy in particular.

Ward et al. (Ward et al. 2016) used random forests to predict mechanical properties of steel and aluminum alloys, achieving reasonable accuracy but with limited dataset size. Yu et al. (2021) applied deep learning to forecast the characteristics of aluminum alloys but faced challenges with interpretability and required large datasets. XGBoost has demonstrated potential in materials applications due to its ability to managing complex feature interactions and provide feature importance metrics (Wen et al. 2022). Other works include explainable ML for tensile in Al for 3D printing (Shah et al. 2025), predictive modelling with various algorithms (Fu et al. 2023), ML for 5083 alloy (Sundaram et al. 2025).

3. Data collection and preprocessing

we put together a dataset with 1154 samples, 30 features from a public repository (Ninad Bhat 2023). We removed all samples that have missing value in tensile strength and dropped the physical property features: Elongation and Yield strength, since we want to predict only the tensile strength based on alloying composition and processing information. The final dataset shape was 1121 samples and 26 features. Numerical features are chemical composition features including 25 alloying elements data (wt.%), namely Ag, Al, B, Be, Bi, Cd, Co, Cr, Cu, Er, Eu, Fe, Ga, Li, Mg, Mn, Ni, Pb, Sc, Si, Sn, Ti, V, Zn, Zr and processing information is the only categorical features. There is total 10 difference type of processing condition. Table 1 shows processing information and their counts.

Table 1. Processing information of aluminum alloy

Processing Information	Count
Solutionised + Artificially peak aged	375
Solutionised + Artificially over aged	214
Strain Hardened (Hard)	197
No Processing	141
Solutionised + Naturally aged	86
Solutionised + Cold Worked + Naturally aged	57
Strain hardened	41
Artificial aged	21
Naturally aged	18
Solutionised	4

In data preprocessing numerical features missing values are filed with the medians. We used LabelEncoder to turn the categorical data into numbers that model could understand and split the dataset into 80 /20 for training and testing. The training set and test set include 896 and 225 samples respectively. Table 2 shows the descriptive statistic for chemical composition used in this study.

Table 2. Descriptive statistics of chemical composition of aluminum alloys

Element	Count	Mean (wt.%)	Std. Dev. (wt.%)	Min (wt.%)	25th Percentile (wt.%)	Median (wt.%)
Al	1,121	94.21	4.09	74.95	92.2	94.65
Si	1,121	0.9	2.76	0	0	0.1
Mg	1,121	1.5	1.33	0	0.5	1
Cu	1,121	1.34	1.87	0	0	0.25
Mn	1,121	0.25	0.32	0	0	0.1
Fe	1,121	0.15	0.2	0	0	0.08
Zn	1,121	0.17	0.6	0	0	0
Cr	1,121	0.07	0.19	0	0	0
Ni	1,121	0.02	0.15	0	0	0
Li	1,121	0.17	0.6	0	0	0
Ag	1,121	0.008	0.056	0	0	0
Sc	1,121	0.015	0.095	0	0	0
Er	1,121	0.007	0.046	0	0	0
Pb	1,121	0.003	0.04	0	0	0
Co	1,121	0.005	0.054	0	0	0
Bi	1,121	0.003	0.04	0	0	0
Cd	1,121	0.001	0.012	0	0	0
B	1,121	0.0002	0.0014	0	0	0
Ga	1,121	0.0001	0.0016	0	0	0
Eu	1,121	0.00008	0.00075	0	0	0

4. Methods

4.1Feature Correlation Analysis

Before training of the model, a corelation analysis was conducted to understand the relationship between different alloying elements and target feature tensile strength. The feature correlation heatmap (Fig. 1) shows several important relations that informed about feature selection. Absolute value of correlation coefficient near to one means strong correlation between features. Coefficient greater than zero results positive correlation and less than zero indicate negative correlation (Mo et al. 2025). Fig 1. Highlights positive correlation with Zn, Cu, Zr, Li, Mg to tensile strength means increasing one of these elements leads to increase in tensile strength and negative correlation with Al, Si, B indicating increase one of these elements results decrease in tensile strength or vice-versa. Any two features, Pearson correlation coefficient calculated by Eq. (1):

$$r = \frac{\Sigma[(x_i - \bar{x}) \times (y_i - \bar{y})]}{\sqrt{\Sigma(x_i - \bar{x})^2 \sqrt{\Sigma(y_i - \bar{y})^2}}} \quad (1)$$

Hear x_i *and* y_i are any two feature values, $\overline{x}$ and $\overline{y}$ are denoting the average value of x_i and y_i respectively.

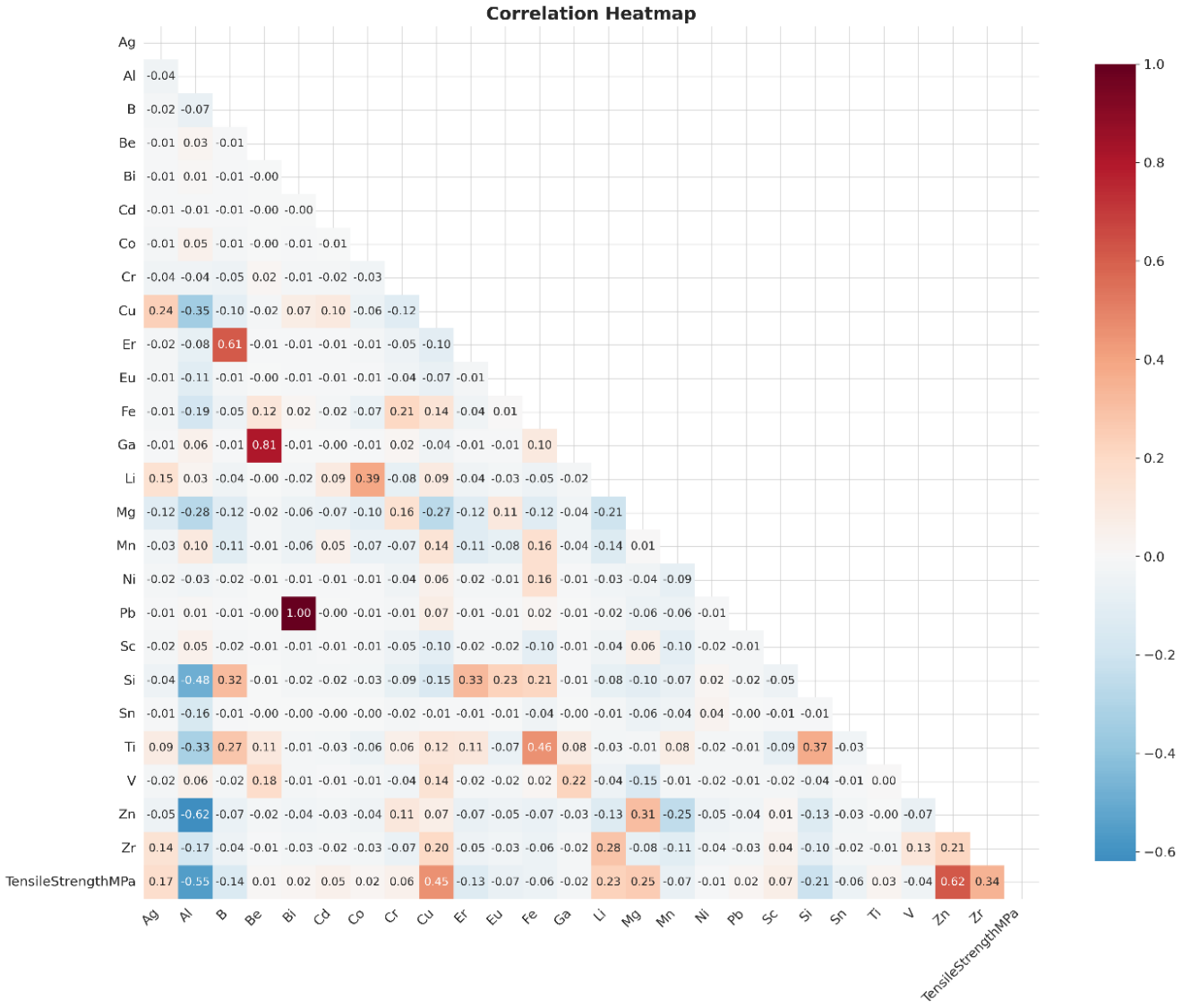

Figure 1. Feature correlation heatmap

4.2 Model Selection

We followed a "composition-process-property" machine learning pipeline. The main idea is to train a model that takes material composition and processing details as input and gives a predicted tensile strength as the output. But the relation between alloy's chemical composition, its processing history, and the final output tensile strength is highly complex and non-linear. A simple linear model won't work as they are unable to capture the intricate, non-additive interactions between features. We went with advanced ensemble model, XGBoost (Extreme Gradient Boosting), because it has a great track record in materials science(Fu et al., 2023; Lu et al., 2024). XGBoost is a really smart version of a Gradient Boosting Machine (GBM). XGBoost algorithm has been widely used in many fields and well tested (Chen and Guestrin 2016; Lee and Lee 2022). Its capable to handles a mix of numerical (element weight percentages) and categorical features (processing labels). Xgboost builds trees sequentially to fix errors, with regularization (Chen and Guestrn 2016), meaning it builds a series of decision trees, where each new tree is trained to correct the errors of the ones that came before it. As an ensemble of decision trees, XGBoost is not sensitive to the

distribution of the numerical features thus no scaling required. This allowed us to use the raw feature data without a scaling step like StandardScaler. It includes built-in regularization L1 (reg_alpha) and L2 (reg_lambda) regularization to prevent the model from memorizing the training data and failing to overfitting.

4.3 Model Tuning and Configuration

After selecting XGBoost model, we carried out a comprehensive optimization check to find the best hyperparameters. We used a 5-fold-cross-validated grid search, which tested 2304 unique parameter combinations. We were found a model through exhaustive search that ensure our model's high accuracy with strong generalization. Our model's optimized hyperparameters were:
n_estimators = 200, max_depth = 5, learning_rate = 0.1, subsample = 0.7, colample_bytree = 0.8, min_child_weight = 5, reg_alpha = 5, and reg_lambda = 1.

4.3 Feature analysis

The permutation importance and partial dependence techniques was used to analyze the rank and score of the feature importance and to understand what was going on inside the model. Permutation importance basically shuffles the input data for one feature (like 'Cu') and then sees how much the model's accuracy drops. It's a great way to see what the model really relies on. The result showed the relative of features in the model(Wen et al., 2022). On the other hand, partial dependence let us to see the effect of just one feature (like 'Cu') on the predicted tensile strength, holding everything else steady. This is excellent way to observing the non-linear relationships that the model learned.

4.4 Model validation

We selected three evaluation metrics to evaluate the performance of XGBoost model that used in this study. These are determination of coefficient (R^2), root mean square error (RMSE) and mean absolute error (MAE). The statistical equations for these metrics are given in Eq. (2)-(4).

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

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y_i})^2} \quad (3)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \widehat{y_i}| \quad (4)$$

Among these, y_i is the actual value from dataset, $\widehat{y_i}$ is the predicted value from the model, $\overline{y}$ is the mean value of y_i, and i is the number of samples taking part in the assessment (i = 1,2,…..,n).
R^2 described the interpretability of Machine Learning regression models, which is used to characterise interpretability of data. Generally, R^2 ranges from 0 to 1, with values close to 1 denoting input features and output results are better interpreted. However, only this criterion is insufficient to measure the model's performance. Therefore, RMSE and MAE are used together to evolute predictive errors of the model. The model's prediction error can be more accurately represented by RMSE and MAE, and the closer these metrics are to zero, the more accurate the model's predictions will be (Wang et al. 2023).

5. Results and Discussion

5.1 Numerical Results

In this study we used a dataset that contain 1,121 samples of aluminum alloy and 26 features. Aluminum (Al) showed the highest average composition at 94.21%, while other elements like Cu, Mn, Si, Mg, and Zn had lower proportions, yet they played a significant role for strengthening mechanisms. At first the model was validated using 5-fold cross validation on the training set that results a stable performance with Mean CV R^2 = 0.9272 accuracy, which told us we were on the right track. Then the final model was trained on the full 80% training set and 20% data used to test and evaluated the model, Table 3 shows the results of performance matrices as follows:

Table 3. Performance Matrices of the Model

Results	R^2	RMSE	MAE
Training	0.9521	32.78 MPa	23.47 MPa
Testing	0.9416	37.30 MPa	28.51 MPa

R^2 of 0.9416 on test set is outstanding and it means our model can explain almost 94.2% of the variance in tensile strength, even for the data it has never seen. A small gap between training and testing data ($\Delta R^2 = 0.0105$) ensures good generalization and no overtraining or overfitting. Moreover, the RMSE is higher (37.30 MPa) than the training data set also with lower error indicates that the model is highly precise with lower maximum error. Since, the tensile strength in our dataset ranged from under 100 MPa to Over 800 MPa, an average error of ~30 MPa is very precise result. The variables determined to have high importance in the analysis of the tensile strength property with respect to composition were Cu, Al, Zn and Mg. These elements particularly have a high role in the precipitation and solid-solution strengthening processes. In Conclusion, the accuracy, robustness, and physically consistent nature of the XGBoost model made it a convenient tool for precisely predicting the value of the tensile strength with given the composition and processing parameters of the alloy. This method can be used for a quick and intelligent alternative for experimental tests.

5.2 Graphical Results

Here all the performance matrices result shown in a graphical approach by indicating model accuracy. The analysis includes model performance evaluation, feature importance interpretation, and Partial Dependence Plots (PDPs). Figure 2. Comparison of actual and predicted tensile strength values for the (a) training set and (b) test set.

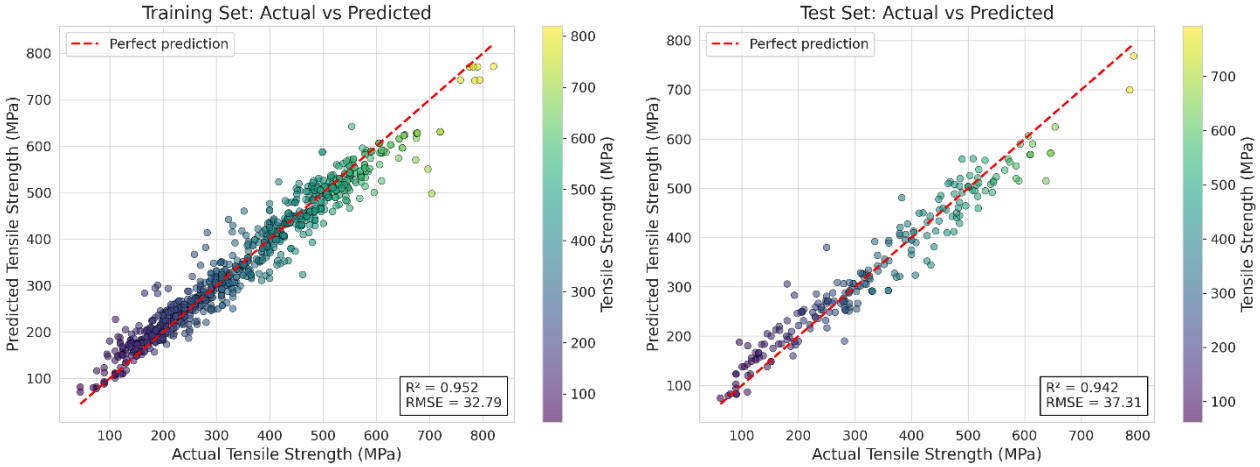

Figure 2. compares the actual and predicted tensile strength values for both training and test datasets by showing R^2 and RMSE values.

The red dashed line indicates perfect prediction, demonstrating strong agreement between model predictions and experimental data. The red dashed line, representing and ideal prediction, is surrounded by a dense cluster of data points in both graphs. Here the High R^2 scores are confirmed visually. The graphs show our model works well for both low-strength (purple dots) and high-strength (yellow dots) alloys, therefore our model may use to a wide variety of situations. run a permutation significance analysis to understand the model's focus. The outcome shown in Figure 3. We can see processing is the most important feature (importance 0.3710) in the prediction of tensile strength. It confirms that it's very difficult to predict strength from chemical composition alone. The alloy's history, how it was heated, worked etc. is critical (A. Mishra et al. 2021). After processing, the most important chemical composition that influence the tensile strength are Cu (importance 0.2339), Al (0.1599), Zn (0.1152) and Mg (0.0335)

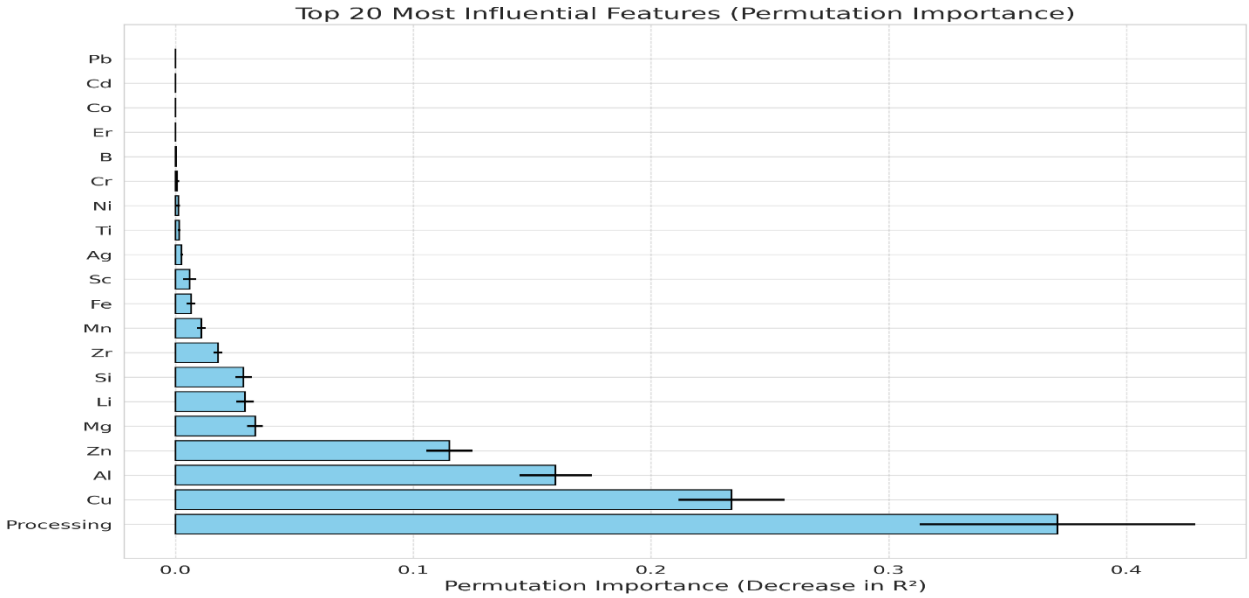

Figure 3. Permutation feature importance showing the top 20 features influencing tensile strength prediction.

Processing, Cu, Al, and Zn exhibit the highest contributions to model performance.

Figure 4 presents Partial Dependence Plots (PDPs) for Processing, Cu, Al, and Zn. The PDP for processing is non-linear, with a decreasing and then a sharply increasing trend with a peak at mid-level processing intensity. This indicates that moderate processing conditions can be ideal for grain refinement and precipitation-hardening reactions to take place effectively. For Cu and Zn, Tensile strength increases sharply with Cu content up to ~0.04 wt.% and stabilizes thereafter. Zn also shows a similar positive effect up to ~0.08 wt.%. For Al the partial effect plot reveals a small rise in the tensile strength with increasing concentrations of aluminum, followed by a fall. This could be due to dilution

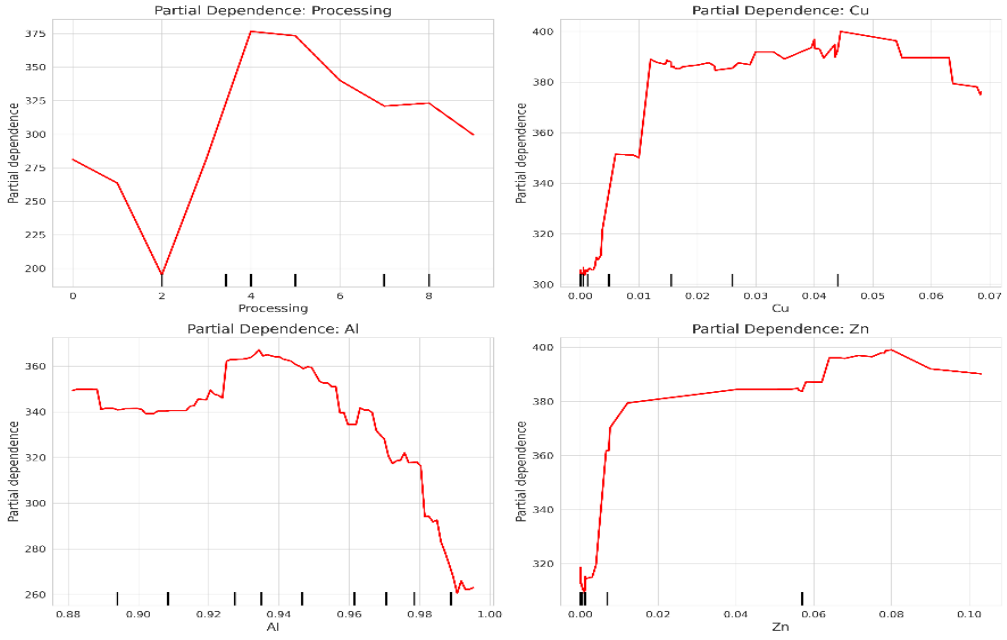

Figure 4. Partial Dependence Plots (PDPs) for (a) Processing, (b) Cu, (c) Al, and (d) Zn, illustrating the marginal effect of each variable on predicted tensile strength.

5.3 Model validation

Model validation was performed using residual analysis, Q–Q (Quantile-Quantile) plots, and learning curves to show the reliability and generalization of the proposed model.

Figure 5 shows the residual plot for both training and test set by indicating residual are randomly scattered around zero without any visible structure means the model does not suffer from any kinds of systematic bias and maintains stable error behaviour across the full prediction range. Only a few outliers appear at high tensile strength values, which is expected due to limited samples in that region.

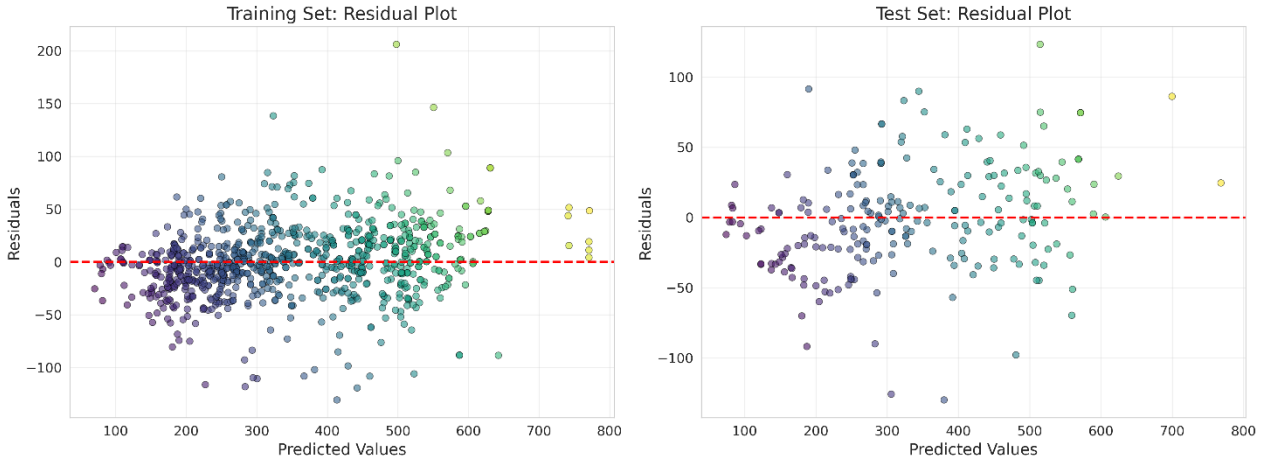

Figure 5. Residual plots for (a) the training set and (b) the test set

Figure 6 for the Q–Q (Quantile-Quantile) plots demonstrate that most residuals closely follow the reference line by confirming that the residuals follow an approximately normal distribution. Here most data points lie close to the theoretical quantile line by indicating that there are no heavy-tail or skewed features found in the prediction error.

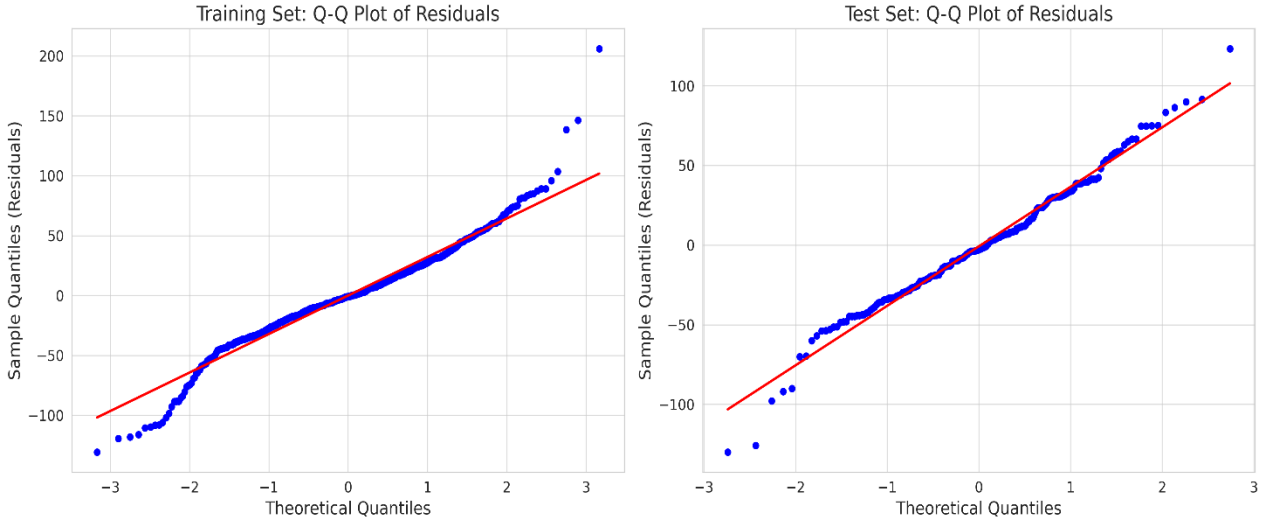

Figure 6. The Q–Q (Quantile-Quantile) plots demonstrate that most residuals closely

It the most important validation plot. The training score (red line) remains consistently high (near $R^2 = 1$), while the cross-validation score (green line) steadily increases as the number of training samples grows. The gap between these two lines is minimal, which denoting our model is not overfitting and maintains good generalization performance. As we add more data to the model the both curves flatten out, which tells us that 1121 samples were

sufficient enough for the model to learn the patterns. Figure 7 is to learning curve analysis provides additional evidence of model robustness.

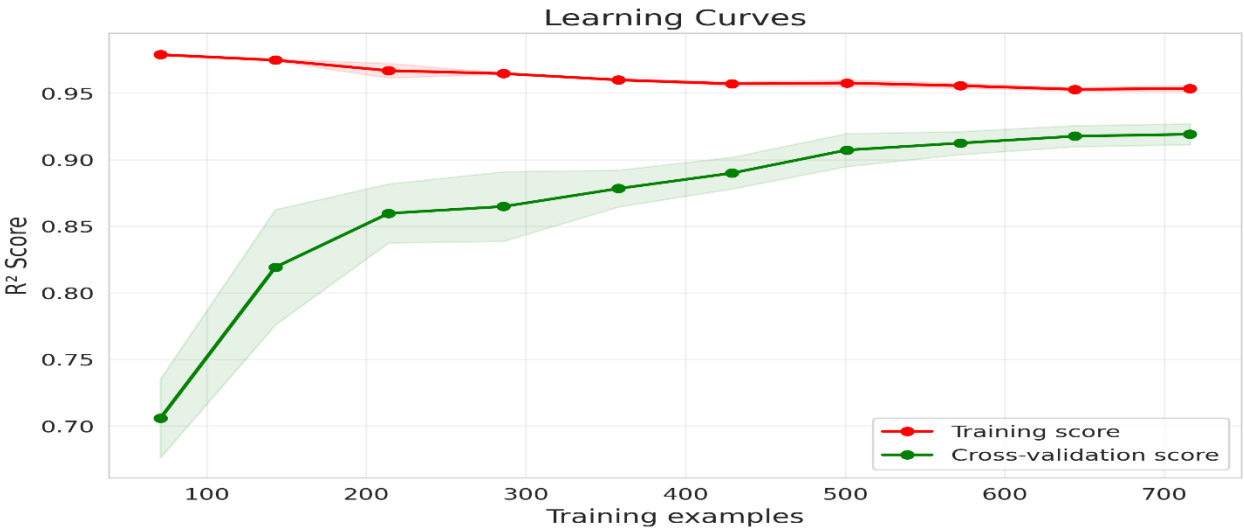

Figure 7. Learning curve of the XGBoost model showing training and cross-validation R2

5.4 Proposed Improvements

Our model's accuracy is quite good, but we see paths to make it even better. The model is only as good as the data we feed the model. In the future, we could improve the "composition- property' link by adding more detailed data instead of just encoded labels.

- As Fu *et al.*, (2023) showed, adding microstructural features like grain size and hardness could really boost the model accuracy. These properties are the physical link between composition and final strength.
- Instead of a simple "T6" label, we could feed the model processing parameters like the actual numbers for aging temperature and aging time like Wang *et al.* (2023) did. We could also try advanced feature engineering, POD method to capture more processing details like Hu *et al.* (2021b).
- There is no reason this ML framework can't be used to predict other key properties, like elongation, yield strength and fatigue life.

6. Conclusion

In this study, it has been proven that it is possible to accurately predict the tensile strength values of aluminum alloys with the aid of an XGBoost machine learning algorithm utilizing composition and process data alone. The results presented robust accuracy and excellent generalization capabilities, with importance and PDP results pointing to Processing, Cu, Al, and Zn as the key factors that determine alloy strength. Validation tests with respect to residual plots, Q-Q plots, and learning curves proved that the model was reliable, free from bias, and perfectly well generalized. In summary, it can be seen that machine learning models are viable in extracting complex metallurgical relations and that the application of these models holds tremendous potential in expediting alloy development.

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Biographies

Md. Tanbir Hasan is an undergraduate student in Industrial & Production Engineering at Jashore University of Science and Technology (JUST). Passionate about applied research and innovation, focusing on the application of AI and computational tools in modern industrial systems. His core interests are Artificial Intelligence (AI) and AI-Driven Industrial Systems, Computational Fluid Dynamics (CFD), Computer Aided Design (CAD). Mr. Tanbir utilize tools such as SolidWorks, NX, and ANSYS.

Mahmudul hasan Rohan is an undergraduate student in Industrial & Production Engineering at Jashore University of Science and Technology (JUST). His academic interests include machine learning, system dynamics simulation, materials science, artificial intelligence and aerodynamics, with a focus on applying these fields to optimize manufacturing and industrial systems.

Dr. Md. Mahfuzur Rahman is an Assistant Professor in the Department of Industrial and Production Engineering at Jashore University of Science and Technology (JUST). His research focuses on circular manufacturing, decision analysis, supply chain barriers, and sustainability. He also works in advanced materials and manufacturing, including graphene, CNTs, plasmonic nanoparticles, carbon-based composites, electromagnetic shielding, supercapacitors, and capacitive deionization (CDI).

Md. Shahriar Islam Sium is an undergraduate student in Industrial & Production Engineering at Jashore University of Science & Technology. His professional focus encompasses advanced 3D CAD design, engineering simulation and applied research. Mr. Sium utilizes tools such as SolidWorks and CATIA for sophisticated part, assembly, surface modeling and employs ANSYS for Finite Element Analysis and Computational Fluid Dynamics to guide design optimization.

Abdullah Mohammad Khaled is an undergraduate student in Industrial & Production Engineering at Jashore University of Science and Technology (JUST). His academic interests include machine learning, system dynamic simulation, machine design and their application on the manufacturing and industrial system for better efficiency.

Md. Tanvir Hossain is currently pursuing a Bachelor of Science in Industrial and Production Engineering (IPE) at Jashore University of Science and Technology (JUST). His academic interests focus on machine learning, system dynamics, and their applications in improving industrial processes, automation, and decision-making.

Chaity Dey is an undergraduate student in Industrial & Production Engineering at Jashore University of Science and Technology (JUST). Her core interests center on supply chain optimization, including demand forecasting, logistics network design, and inventory management. She is particularly focused on how data-driven methods such as operations research, and system simulation can enhance end-to-end supply chain performance and resilience.

Akteruzzaman Nadim is an undergraduate student in Industrial and Production Engineering at Jessore University of Science and Technology (JUST), Bangladesh. His academic interests include manufacturing engineering, materials processing, and the application of machine learning in industrial systems. He aims to pursue advanced studies in manufacturing and build a career in sustainable industrial engineering.