INTERNATIONAL JOURNAL OF INNOVATION IN MECHANICAL CONSTRUCTION AND ENERGY
Vol. 1 No. 1 (2024), 11-20

IJIMCE
https://ijimce.ppj.unp.ac.id/index.php/ijimce
University of Negeri Padang

International Journal of Innovation in Mechanical Construction and Energy

ISSN: - e-ISSN: -

Predictive Modeling For Low Alloy Steel Mechanical Properties: A Comparison Of Machine Learning Algorithms And Parameter Optimization

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Received 5 November 2023; Accepted 15 January 2024; Available online 15 February 2024

Abstract

The development of machine learning in predicting the mechanical properties of alloy steel has become an important research subject in recent years. This is due to the ability of machine learning to extract complex patterns from large and intricate data, which can be used to understand the relationship between chemical composition, microstructure, and mechanical properties of alloy steel. This research aims to design a machine learning model to predict the mechanical properties of low alloy steel, such as Yield Strength (YS) and Ultimate Tensile Strength (UTS), based on the percentage composition of chemical elements in low alloy steel and the heat treatment applied. The machine learning model in this study consists of 10 input variables and 2 target variables. The research compares the performance of 3 machine learning algorithms, namely Decision Tree (DT), Random Forest (RF), and Artificial Neural Network (ANN). The research findings indicate that the ANN algorithm model performs best in predicting the mechanical properties of low alloy steel. This model has Mean Absolute Error (MAE) values of 16.5 and 19.593 for predicting YS and UTS, Root Mean Square Error (RMSE) values of 19.111 and 22.005, and coefficient of determination (R) values of 0.964 and 0.947 for YS and UTS respectively. The modeling uses the ANN algorithm with an 80% training data and 20% testing data split, and applies the K-Fold Cross Validation method with a value of K=5. The best parameters obtained are a learning rate of 0.001, momentum of 0.1, and a hidden layer neuron count of 9. These results indicate that ANN has great potential in addressing the complexity and variability in material data. The implications of these findings are that the implementation of ANN in manufacturing and material engineering industries can enhance the accuracy and efficiency in material strength prediction processes, which, in turn, can aid in designing and developing better and more durable products.

Keywords: Modeling, machine learning, algorithms, yield strength, low alloy steel

INTRODUCTION

Low alloy steels are alloys with alloying elements content below 10% and a low carbon content. These steels possess ductile properties and high-temperature factors, making them widely used in various industrial fields such as shipbuilding, bridges, tanks, boilers, and automotive industries [1]. The rapid and diverse utilization of low alloy steels in the engineering world drives the steel industry to develop steel alloys suitable for their applications. This aims to prevent material failures, as the mechanical properties of a material play a crucial role in determining the material for modern industrial components to prevent premature component failures [2]. Mechanical properties of materials include strength, which refers to a material's ability to resist plastic deformation or fracture. Strength properties such as tensile strength and material plasticity are influenced by its chemical composition. Additionally, heat treatment processes, such as tempering and cooling rates, can effectively control microstructure, grain size, and defects, all of which are closely related to the material's tensile properties [3]. Heat treatment is a significant process in manufacturing machine parts and tools. Tempering, one part of heat treatment, applied not only to harden steel but also to improve its hardness and toughness properties [4]. Strength and toughness are the most important indices of steel [5], thus tempering processes are conducted to enhance the strength and toughness of low alloy steels. It is found that tempering treatment can increase the strength of low alloy steel; however, with further increasing temperature, the material's strength gradually decreases [6]. The combined effect of cooling rate and tempering temperature on alloy steel is nonlinear and complex, making it challenging to explain. The combined effect of cooling rate and tempering temperature can enhance secondary hardening, while further increases in tempering temperature can decrease strength [7]. Testing of mechanical properties of low alloy steels, such as tensile strength and yield strength, is generally still manually conducted using tensile testing machines.

The rapid development of computer technology in the field of material science has propelled experts and researchers to develop computational approaches to analyze and solve various material-related issues [8]. The advancement of computational technology in the field of materials allows for non-destructive testing of materials. In recent years, the complexity of engineering problems has driven the increased adoption of machine learning methods that utilize mathematical algorithms to quickly learn from previously introduced patterns. These techniques can successfully establish complex relationships between multiple parameters and rapidly predict desired outputs [9]. Machine learning is an efficient statistical analysis method for capturing internal linear or nonlinear relationships by learning from empirical data [10]. Currently, there are various types of machine learning algorithms used to determine the mechanical properties of materials based on their composition and heat treatment without damaging specimens. The utilization of machine learning algorithms such as Random Forest, Neural Network, and Decision Tree in predicting the tensile strength of steel yields good prediction results [11]. Furthermore, machine learning methods have also proven to be practical in predicting the fatigue strength of materials based on fatigue data sheets [12].

The composition of low alloy steel and tempering temperature can influence the tensile strength and yield strength of low alloy steel. The addition of small amounts of chemical elements to the composition of low alloy steel can alter its tensile and yield strengths. Besides steel composition, the temperature of the heat treatment process also affects the tensile and yield strengths. Therefore, manual testing of the mechanical properties of low alloy steel requires significant time, expense, expertise, and is environmentally unfriendly due to the production of steel waste from tensile testing. Universal Testing Machines (UTMs) are used to test steel and determine mechanical properties such as tensile and yield strengths. However, when materials need to be tested at varying high temperatures, more time is needed to calculate the mechanical properties of the material. This research aims to design a machine learning model using several algorithms such as Random Forest (RF), Neural Network (NN), and Decision Tree (DT) to predict the tensile and yield strengths of low alloy steel. The study involves varying parameters for each machine learning algorithm and comparing performance metrics such as Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and correlation coefficient (R). Smaller validation values indicate more accurate predictions from the generated model.

RESEARCH METHOD

1. Data Collection

The dataset used in this research was obtained from N.S. Reddy (2012) [7], compiled from the handbook on Standard EN Steels. The dataset consists of 140 entries comprising both input and output data. The input data include specimen numbers, the percentage composition of chemical elements such as C, Si, Mn, P, Ni, Cr, Mo, Mn/S ratio, tempering temperature (TT), and cooling rate (CR). During model training, careful selection of input variables is crucial. The model is trained on the Mn and S ratio, where concentrations are in wt%. This is because sulfur reacts with manganese and forms MnS. To avoid model bias, individual variables forming the Mn/S ratio are also included, enabling direct influence detection from each variable. The output data consist of ultimate tensile strength (UTS) and yield strength (YS). For further clarification, please refer to **Table 1.**

Table1. Low alloy steel dataset statistics

Variable	Data type	Min	Max	Mean
C (%)	Input	0.32	0.44	0.37
Si (%)	Input	0.19	0.37	0.27
Mn (%)	Input	0.33	1.51	0.91
P (%)	Input	0.22	0.042	0.033
Ni (%)	Input	0.56	1.08	0.031
Cr (%)	Input	0.21	0.57	0.82
Mo (%)	Input	0.11	0.25	0.17
Mn/s (%)	Input	7.86	150	37.27
CR (°C)	Input	2.8	118	24.9
TT (°C)	Input	400	700	588.8
UTS (Mpa)	Output	707	1284.8	923.6
YS (Mpa)	Output	542.8	1193.6	798.3

2. Comparison of Machine Learning Algorithms

This comparison of machine learning algorithms was conducted using the Python programming language running on Google Colab. Three different machine learning algorithms were employed in this study to design models for predicting the UTS and YS of low alloy steel based on input data. The algorithms used in this research are Random Forest (RF), Artificial Neural Network (ANN), and Decision Tree (DT). In this study, 80% of the data were utilized as training data, and 20% were used as testing data. The performance of the trained models was evaluated by calculating Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Correlation Coefficient (R) from the actual and predicted values of the test data.

a. Random Forest (RF):
Random forest is an ensemble learning method introduced by Leo Breiman and Adele Cutler. Random Forest (RF) (Hastie; Tibshirani; Friedman, 2009) is an ensemble learning method for classification that constructs decision trees from the training set in iterations k. In each iteration, the algorithm randomly selects a subset of samples from the training set. To reproduce decision trees from this subset, RF randomly selects a subset of features as candidate features for each node. Thus, each decision tree is built through an ensemble using independent random subsets of features and samples. In this study, the DT algorithm used 80% of the data as training data, and 20% were used as testing data. The performance of the trained model was evaluated by calculating RMSE, MAE, and R from the actual and predicted values of the test data.

b. Artificial Neural Network (ANN):
Neural networks are powerful machine learning classifiers or methods. Neural networks almost always fit various machine learning problems, making them hypotheses for various real-world problems because neural networks are formed based on how the human brain works. In this study, the DT algorithm used 80% of the data as training data, and 20% were used as testing data. The performance of the trained model was evaluated by calculating RMSE, MAE, and R from the actual and predicted values of the test data.

c. Decision Tree (DT):
Decision tree regression is one of the predictive models used in machine learning. This model is a supervised technique that performs classification and regression techniques. Decision trees work well for categorical and continuous input variables. It develops decision trees by dividing the dataset into smaller subsets. In this study, the DT algorithm used 80% of the data as training data, and 20% were used as testing data. The performance of the trained model was evaluated by calculating RMSE, MAE, and R from the actual and predicted values of the test data.

3. Cross-validation

The modeling in this research adopts an approach based on grid search and k-fold cross-validation to prevent overfitting. Therefore, selecting appropriate parameter values from machine learning methods significantly impacts its accuracy. Furthermore, optimal parameter values may vary depending on the problem at hand. Grid search is a strategy for automatically adjusting and optimizing model parameters. This technique constructs a mesh of pre-defined values for each parameter. For each possible parameter combination, a predictive model is trained with multiple data, producing a set of outputs, and the best parameter values will yield the best output set [13]. During the training step, k-fold cross-validation is employed, which divides the dataset into k sets. The model is trained on k-1 sets and validated with the remaining portion. The training and testing steps are iterated k times alternately between training and testing sets. Figure 1 illustrates the implementation of k-fold cross-validation. In this research, k = 5 is utilized.

4. Model Evaluation

The modeling in this research comprises 10 input data variables and 2 output data variables as targets. Each model generated from each algorithm is evaluated by calculating the Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and Correlation Coefficient (R) from the actual and predicted values of the test data, as shown in the following equations:

$$MAE = \frac{i}{N}\sum |y_i - z_i| \quad (1)$$

Where i is the index of data in the sample, N is the total number of samples, y_i is the actual value of the ith data, and z_i is the predicted value of the model for the ith data.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(f(X_i) - Y_i)^2}\ , \quad (2)$$

Where n is the number of data used to test the model, f(X_i) is the value predicted by the model for the ith data, and Y_i is the actual value for the ith data.

$$R = \frac{\sum_{i}^{n=1}(f(X_i)-f(X))(Y_i-Y)}{\sqrt{\sum_{i=1}^{n}(f(X_i)-f(X))^2}\sqrt{\sum_{i=1}^{n}Y_i-Y)^2}} \quad (3)$$

Where f(Xi) is the predicted value of the dependent variable (Y) based on the independent variable (X) at the ith observation, $f(\bar{X})$ is the average of all predicted values f(Xi) over all observations, Yi is the actual observation value of the dependent variable at the ith observation, $\bar{Y}$ is the average of all observation values Yi over all observations, and n is the total number.

1. Results and Discussion

The modeling was conducted on Google Colab using the Python programming language. The first step involved examining the correlation between variables using a correlation heatmap, as depicted in **Fig. 2**. The correlation results indicate that yield strength (YS) strongly correlates with ultimate tensile strength (UTS) in low alloy steel. The input variable Mn/S shows a correlation of approximately 0.35, followed by CR and Mo with 0.33 each, while TT does not exhibit significant correlation with YS and UTS. This aligns with previous research [7], which stated that tempering temperature at higher temperatures results in a decrease in UTS values.

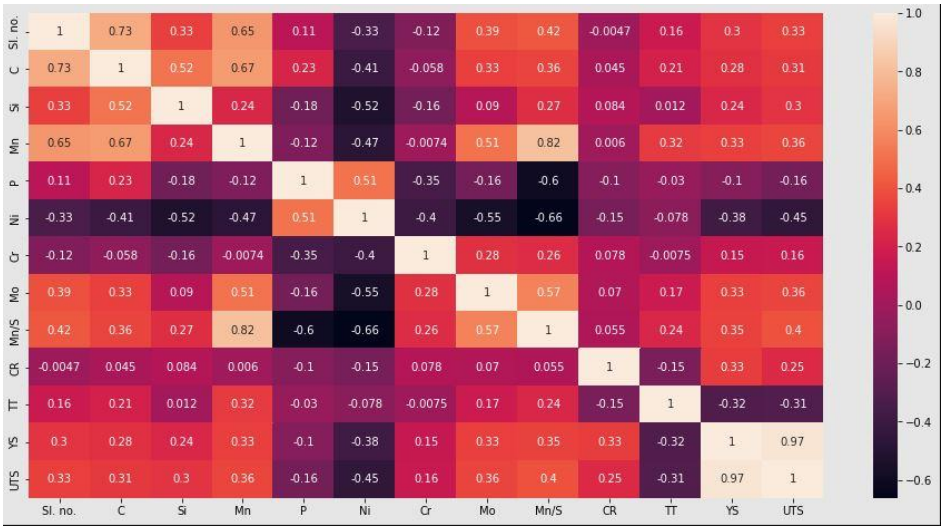

Fig. 2. Correlation between variables

The modeling was designed with three machine learning algorithms: Random Forest (RF), Artificial Neural Network (ANN), and Decision Tree (DT). For each algorithm, the best parameters were sought by varying each parameter, as shown in the treatment of parameters in **Table 2**. In the first column of Table 2, the three algorithms used, namely DT, RF, and ANN, are listed. The second column shows the names of the parameters that will be given different variations, and the third column indicates the parameter settings for each algorithm.

Table 2. Treatment of parameter variations to find the best parameters.

Algorithm	Parameter	Parameter Settings
DT	Depth	1,2,3,4,5,6,7,8,9,10,15,20,25,30
RF	Number of tree	20,50, 80, 110, 140,150
	Maximal depth	5,10,15,25,30
ANN	Training cycle	10.000, 20,000, 30.000, 40,000
	Learning rate	0,001, sd 0,1
	Momentum	0.1 sd 1
	Size hiden layer	1 sd 9

2. Decision Trees (DT)

Variations in parameter treatment in Decision Trees (DT) modeling yielded the best parameters with a number of trees set to 10, resulting in MAE of 20.195, RMSE of 23.423, and R of 0.956 from the actual and predicted values of the test data. Increasing the number of trees above 10 to 20 resulted in constant values for MAE, RMSE, and R, while the number of trees above 20 led to an increase in performance values. The best performance is indicated by the smallest values of MAE, RMSE, and R. In **Fig. 3**, a comparison of actual values against predicted Yield Strength obtained from modeling using the DT algorithm is illustrated.

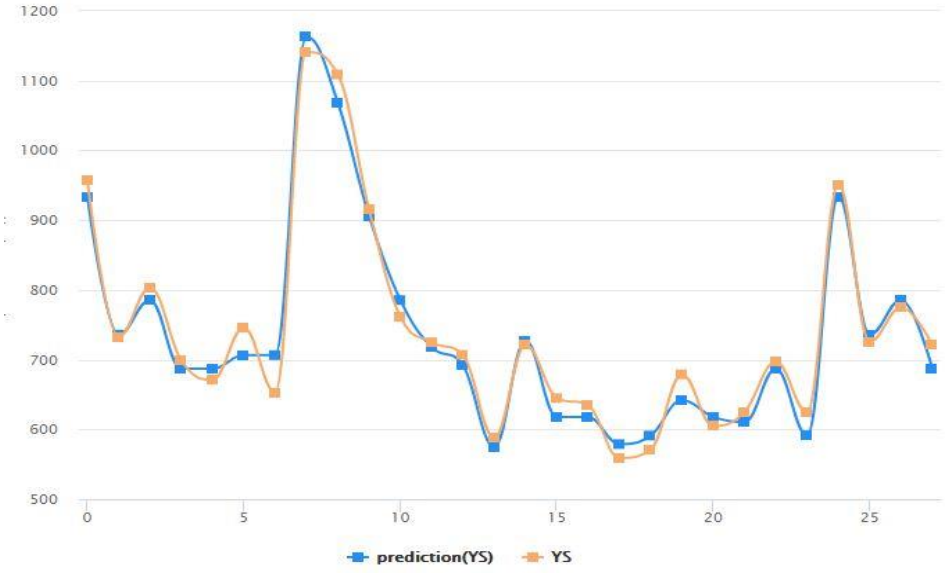

Fig. 3. Comparison of predicted YS results and actual values using DT

On the other hand, for the prediction of Ultimate Tensile Strength (UTS), the DT model achieved MAE of 20.324, RMSE of 23.941, and R of 0.941. **Fig. 4** shows the comparison between predicted and actual values.

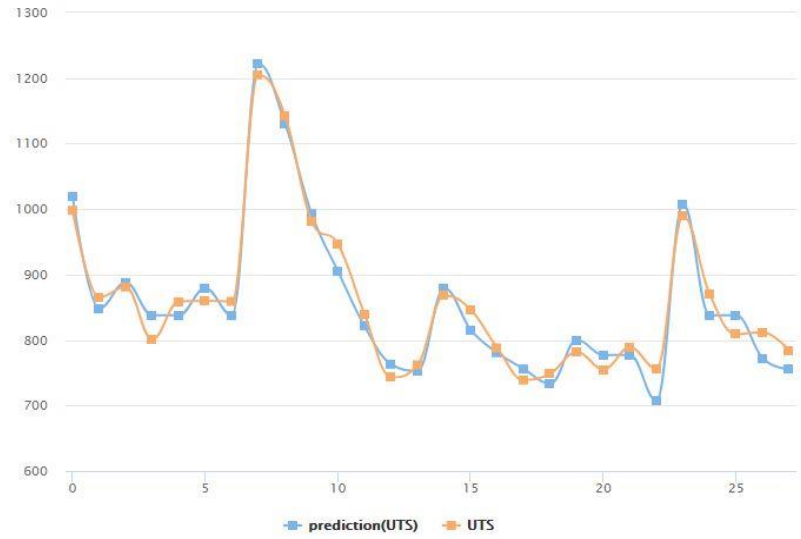

Fig. 4. Comparison of predicted UTS results and actual values using DT

3. Random Forest (RF)

In the modeling using the Random Forest (RF) algorithm, two parameters were varied: the number of trees and the maximal depth, as shown in **Table 2**. The modeling with the RF algorithm yielded the best parameters: a number of trees of 20 and a maximal depth of 10, resulting in MAE of 21.673, RMSE of 26.949, and R of 0.951 from the actual and predicted values of the test data. **Fig. 5** illustrates the comparison between predicted Yield Strength (YS) results and actual values.

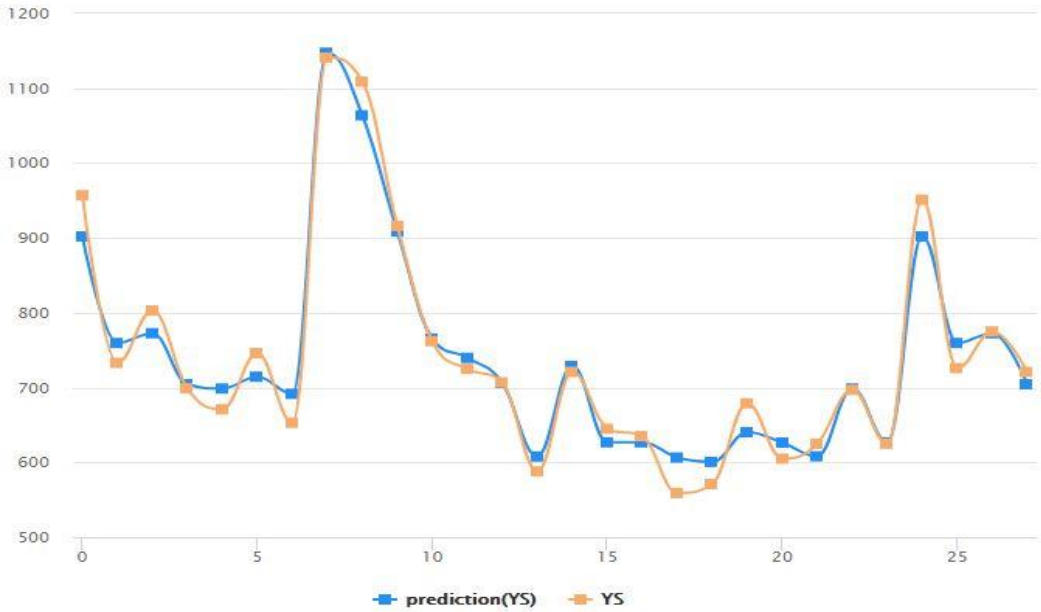

Fig. 5. Comparison of predicted YS results and actual values using RF

The RF model also obtained MAE of 21.669, RMSE of 28.342, and R of 0.935 from the actual and predicted values of the test data. In **Fig. 6**, the variation of actual values against predicted Ultimate Tensile Strength (UTS) can be observed.

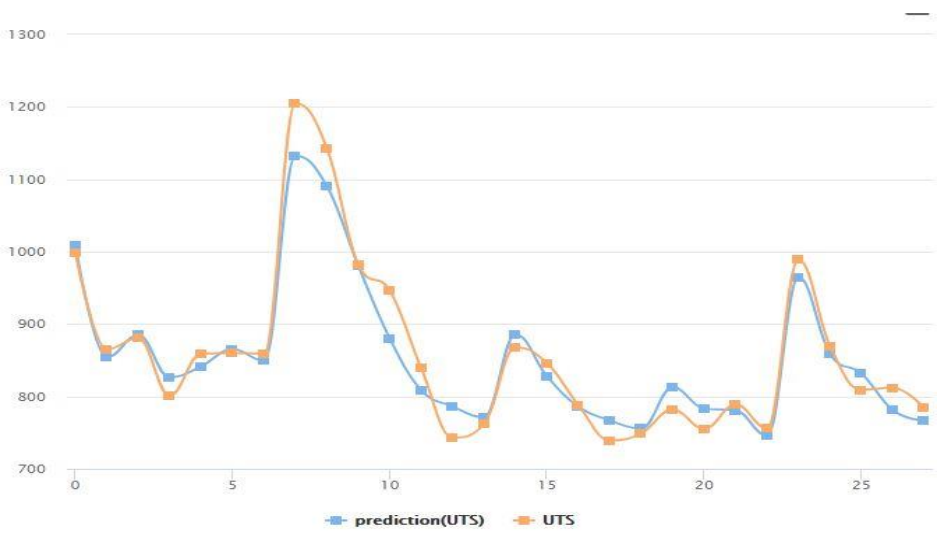

Fig. 6. Comparison of predicted UTS results and actual values using RF

4. Artificial Neural Network (ANN)

In modeling using the ANN algorithm, there are 4 parameter variations consisting of training cycles, learning rate, momentum, and hidden layer size. The ANN modeling yielded the best parameters with a training cycle of 10,000, learning rate of 0.001, momentum of 0.1, and a hidden layer size of 9, resulting in MAE of 16.5, RMSE of 19.111, and R of 0.964 from the actual and predicted values of the test data. **Fig. 7** illustrates the comparison between predicted Yield Strength (YS) results and actual values.

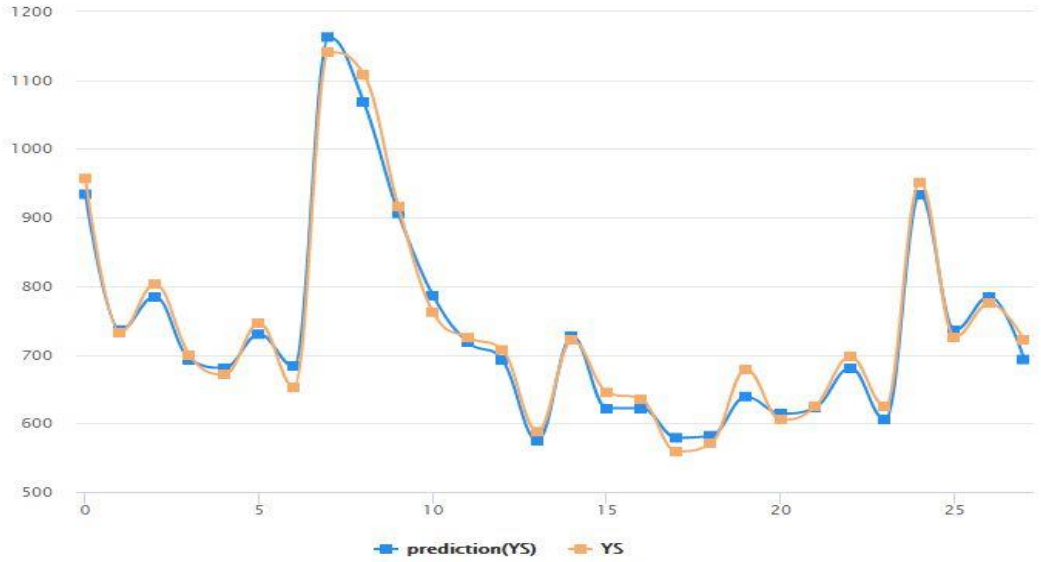

Fig. 7. Comparison of predicted YS results and actual values using ANN

The ANN modeling also obtained MAE of 19.593, RMSE of 22.005, and R of 0.947 from the actual and predicted values of the test data. In **Fig. 8**, the variation between actual and predicted values of Ultimate Tensile Strength (UTS) can be observed.

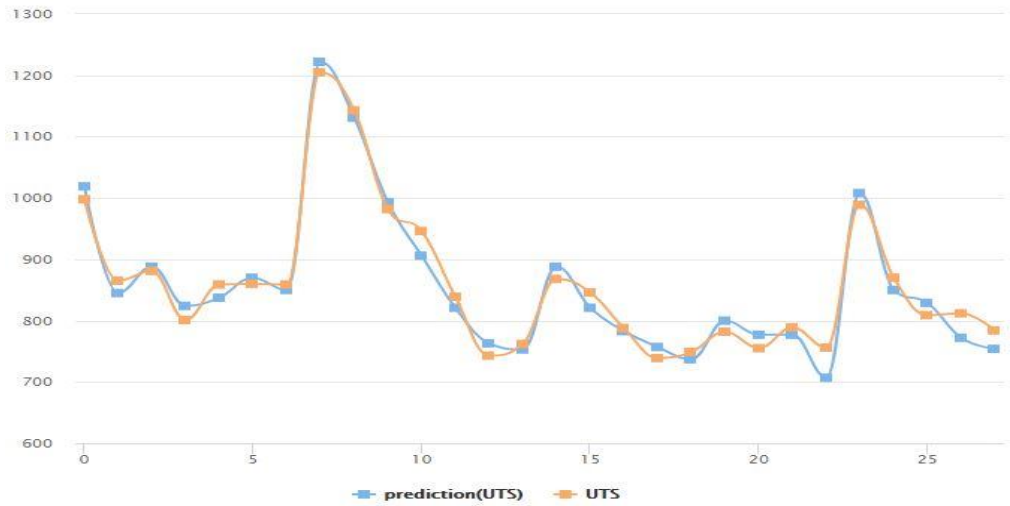

Fig. 8. Comparison of predicted UTS results and actual values using ANN

Machine learning modeling with various algorithms has been conducted with an 80% training data split and 20% testing data, implementing K-Fold with K=5. Comparison of machine learning algorithms such as Decision Tree (DT), Random Forest (RF), and Artificial Neural Network (ANN) with various parameter treatments for each algorithm has been performed. The ANN algorithm yielded the best modeling performance, producing the highest R value. Additionally, ANN also resulted in the smallest MAE and RMSE values compared to the DT and RF algorithms. The comparison of these three algorithms can be seen in **Fig. 9** for predicting YS, while the performance comparison for predicting UTS can be observed in **Fig. 10**.

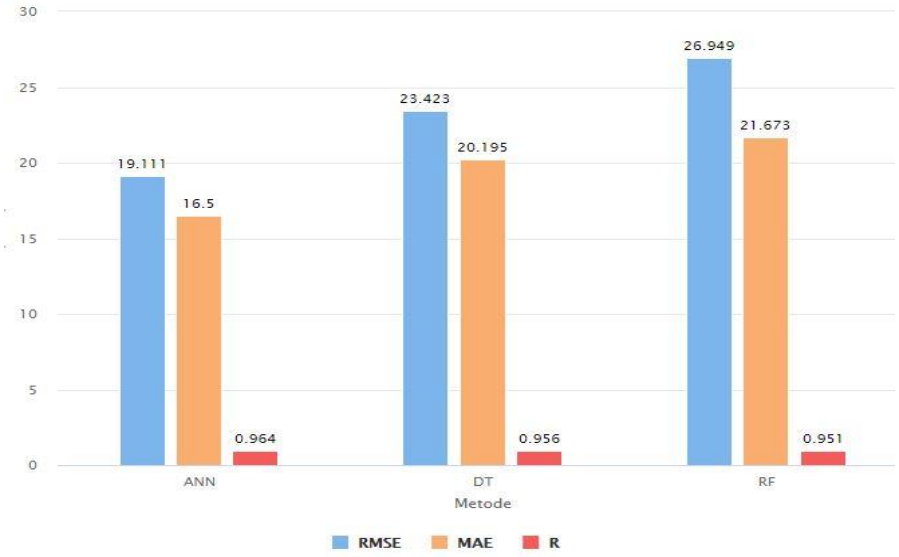

Fig. 9. Results of YS evaluation metrics

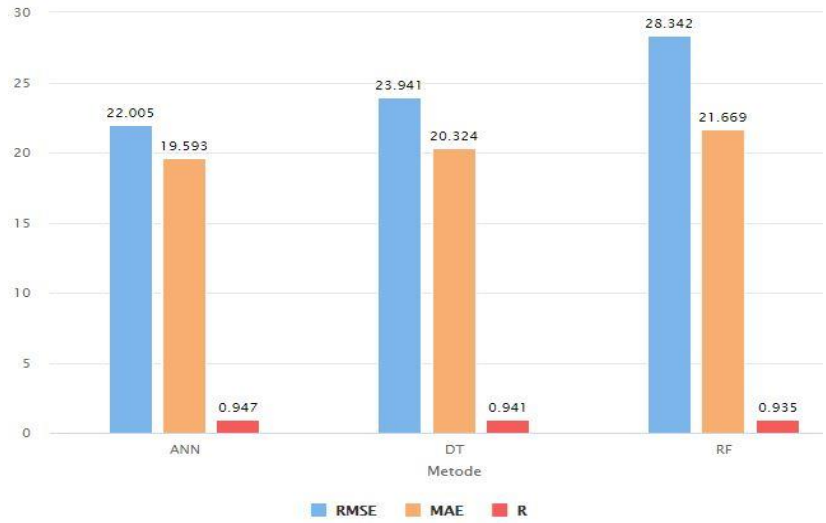

Fig. 10. Results of YS evaluation metrics

CONCLUSION

In this study, three machine learning algorithms were compared, namely DT, RF, and ANN, where the ANN algorithm outperformed DT and RF. This research resulted in a machine learning modeling to predict the tensile strength (UTS) and yield strength (YS) of low alloy steel using the Artificial Neural Network (ANN) algorithm with the best parameters: training cycle of 10,000, learning rate of 0.001 , momentum of 0.1, and hidden layer size of 9. This yielded MAE of 16.5, RMSE of 19.111, and R of 0.964 for predicting YS values, while for predicting UTS values, MAE of 19.593, RMSE of 22.005, and R of 0.947 were obtained from the actual and predicted values of the test data. These results indicate that ANN has great potential in addressing the complexity and variability in material data. The implications of these findings are that the implementation of ANN in manufacturing and material engineering industries can enhance the accuracy and efficiency in material strength prediction processes, which, in turn, can aid in designing and developing better and more durable products. Additionally, this study also provides insights into the optimal best parameters for training ANN models, which can serve as guidelines for researchers and practitioners in the utilization of ANN for similar problems in the future.

REFERENCES

[1] D. Leni, F. Earnestly, R. Sumiati, A. Adriansyah, and Y. P. Kusuma, "Evaluasi sifat mekanik baja paduan rendah bedasarkan komposisi kimia dan suhu perlakuan panas menggunakan teknik exploratory data analysis (EDA)," *Din. Tek. Mesin*, vol. 13, no. 1, p. 74, Apr. 2023, doi: 10.29303/dtm.v13i1.624.

[2] A. A. Morini, M. J. Ribeiro, and D. Hotza, "Early-stage materials selection based on embodied energy and carbon footprint," *Mater. Des.*, vol. 178, p. 107861, Sep. 2019, doi: 10.1016/j.matdes.2019.107861.

[3] R. Šmak, J. Votava, and A. Polcar, "The Cooling Media Influence on Selected Mechanical Properties of Steel," *Acta Technol. Agric.*, vol. 23, no. 4, pp. 183–189, Dec. 2020, doi: 10.2478/ata-2020-0029.

[4] N. M. Ismail, N. A. A. Khatif, M. A. K. A. Kecik, and M. A. H. Shaharudin, "The effect of heat treatment on the hardness and impact properties of medium carbon steel," *IOP Conf. Ser. Mater. Sci. Eng.*, vol. 114, p. 012108, Feb. 2016, doi: 10.1088/1757-899X/114/1/012108.

[5] Y. Zhang, J. Yang, D. Xiao, D. Luo, C. Tuo, and H. Wu, "Effect of Quenching and Tempering on Mechanical Properties and Impact Fracture Behavior of Low-Carbon Low-Alloy Steel," *Metals*, vol. 12, no. 7, p. 1087, Jun. 2022, doi: 10.3390/met12071087.

[6] B. Hutchinson *et al.*, "Microstructures and hardness of as-quenched martensites (0.1–0.5%C)," *Acta Mater.*, vol. 59, no. 14, pp. 5845–5858, Aug. 2011, doi: 10.1016/j.actamat.2011.05.061.

[7] N. S. Reddy, J. Krishnaiah, S.-G. Hong, and J. S. Lee, "Modeling medium carbon steels by using artificial neural networks," *Mater. Sci. Eng. A*, vol. 508, no. 1–2, pp. 93–105, May 2009, doi: 10.1016/j.msea.2008.12.022.

[8] L. Qiao, Z. Wang, and J. Zhu, "Application of improved GRNN model to predict interlamellar spacing and mechanical properties of hypereutectoid steel," *Mater. Sci. Eng. A*, vol. 792, p. 139845, Aug. 2020, doi: 10.1016/j.msea.2020.139845.

[9] N. Amiri, G. H. Farrahi, K. R. Kashyzadeh, and M. Chizari, "Applications of ultrasonic testing and machine learning methods to predict the static & fatigue behavior of spot-welded joints," *J. Manuf. Process.*, vol. 52, pp. 26–34, Apr. 2020, doi: 10.1016/j.jmapro.2020.01.047.

[10] D. Leni, "Prediction Modeling of Low Alloy Steel Based on Chemical Composition and Heat Treatment Using Artificial Neural Network," *J. Polimesin*, vol. 21, no. 5, pp. 54–61, Oct. 2023, doi: 10.30811/jpl.v21i5.3896.

[11] D. Leni, Y. P. Kusuma, M. Muchlisinalahuddin, F. Earnerstly, R. Muharni, and R. Sumiati, "PERANCANGAN METODE MACHINE LEARNING BERBASIS WEB UNTUK PREDIKSI SIFAT MEKANIK ALUMINIUM," *J. Rekayasa Mesin*, vol. 14, no. 2, pp. 611–626, Aug. 2023, doi: 10.21776/jrm.v14i2.1370.

[12] A. Agrawal, P. D. Deshpande, A. Cecen, G. P. Basavarsu, A. N. Choudhary, and S. R. Kalidindi, "Exploration of data science techniques to predict fatigue strength of steel from composition and processing parameters," *Integrating Mater. Manuf. Innov.*, vol. 3, no. 1, pp. 90–108, Dec. 2014, doi: 10.1186/2193-9772-3-8.

[13] Ade Usra Berli, Desmarita Leni, and Helga Yermadona, "Analisis Pengaruh Komposisi Kimia dan Suhu Perlakuan Panas Terhadap Sifat Mekanik Baja Tahan Karat untuk Aplikasi Konstruksi," *J. Surya Tek.*, vol. 10, no. 2, pp. 811–819, Dec. 2023, doi: 10.37859/jst.v10i2.6059.