

# Prediction of Mechanical Properties of Steel using Data Science Techniques



N. Sandhya, Valluripally Sowmya, Chennakesava Rao Bandaru, G. Raghu Babu

**Abstract:** *Stainless steel is most extensively utilized material in all engineering applications, house hold products, constructions, because it is environment friendly and can be recycled. The principal purpose of this paper is to implement different data science algorithms for predicting stainless steel mechanical properties. Integrating Data science techniques in material science and engineering helps manufacturers, designers, researchers and students in understanding the selection, discovery and development of materials used for various engineering applications. Data science algorithms help to find out the properties of the material without performing any experiments. The Data Science techniques such as Random Forest, Neural Network, Linear regression, K- Nearest Neighbor, Support vector Machine, Decision Tree, and Ensemble methods are used for predicting Tensile Strength by specifying processing parameters of stainless steel like carbon content, sectional size, temperature, manufacturing process. The research here is developed as part of AICTE grant sanctioned under RPS scheme [19] and it aims to implement different data science algorithms for predicting Tensile strength of steel and identifying the algorithm with decent prediction accuracy.*

**Index Terms:** *Data Science algorithms, Material Science, Mechanical properties of steel, process parameters of steel, Statistical measures of accuracy.*

## I. INTRODUCTION

The designers, manufacturers, researchers of material sciences and engineering have habitually contingent on results obtained from the experiments that are conducted in testing laboratory to identify the mechanical properties of any material. So, to obtain the desired properties for a material they need to customize composition of material and process parameters of the material prior of conducting the experiment. But these procedures demand massive expenditure and time to figure out the properties of materials. Different types of materials in material science and engineering includes ceramics, Biomaterials, Composites, Concretes, Electronic and Optical materials,

Glasses and Metal alloys. This paper on the whole focuses on Steel which is a metal alloy and prominent material used in wide variety of applications like construction, infrastructure, automobiles, machine appliances, ships, cars, weapons, vessels, household purposes, surgical instruments, etc. Steel is predominantly accustomed in many applications due to its elevated tensile strength and recyclability without dropping down the mechanical property values. To meet the modern market requirements and to withstand the competitiveness many industries emphasized to produce high precision and good quality steel products. But using the traditional approach of conducting tensile tests using UTM (universal tensile testing machine) and some other tests are not effective in terms of cost and time consumed for tests for finding out mechanical properties of steel. There is a lot of progress in the recent years by using Data Science techniques in material sciences and engineering for discovering the design, structure, physical and mechanical properties of any material. The main goal of data science is to diminish cost and reduce time mechanical properties prediction to help the manufacturers and designers of advanced material science and engineering. Accurate prediction of material mechanical properties and its behavior based on existing data has been the persistent effort of many material researchers. Data Science has succeeded in adding value to business models with the help of statistics, machine learning and deep learning. The main aim of the Data Science is to develop novel approaches, algorithms, tools, methods and the associated infrastructure to extract the high value information based on the available data and resources. The Data Science techniques are widely classified into machine learning, regression, logistic regression, pattern recognition, Feature selection, Text mining, Attribute modelling, k-means clustering, Association analysis, Anomaly detection, Social network analysis, collaborative filtering, Time series forecasting, Model fitting, cross validation, LTV and RFM Analysis, etc. This paper aims to implement data science techniques to predict tensile strength of Stainless steels.

## II. RELATED WORK

Titus Thankachan.et.al [1] proposed method predicts tensile strength, yield strength of hydrogen charged aluminum alloys using artificial neural network by considering composition of alloy and various processing parameters as an input to the model. GH Senussi.et.al [2] presented an approach for predicting stainless steel micro hardness using artificial neural network, where micro hardness of six different types of stainless steel is predicted based on the distance from the base surface.

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Raghuram Karthik Desu.et.al [3] predicted Tensile strength, yield strength of Austenitic stainless steel 304L and 316L using feed forward back propagation neural network. The composition of steels is kept constant while predicting the properties at varying strain rates and at elevated temperatures. Yang Weng.et.al [4] implemented Single Index model that predicts Tensile strength, Yield strength of hot rolled strips of C-Mn steels concerning its chemical composition and processing parameters. Vandana Somkuwar.et.al [5] proffered a solution which predicts hardness of low carbon steel by employing RBF and back propagation models. Jun Huang.et.al [6] intended model predicts impact toughness of E4303 Electrode by considering the coating formula of electrode as input. The model developed in this approach is a non-linear combination of back propagation, radial basis function and adaptive fuzzy neural network that combines the predicted results of all the three models to acquire accurate predicted value.

P. SaravanaKumar.et.al [7] recommended an approach of predicting tensile strength, yield strength, Elongation of hot rolled low carbon steel using feed forward back propagation (FFBP) algorithm. The composition of steel remains standard where as the model predicts the properties based on various temperatures like dispatch temperature, transfer-bar or rolling temperature, coiling temperature, finishing temperature, and carbon equivalent. A. Anita Lakshmi.et.al [8] trained feed forward back propagation algorithm which predicts tensile strength, yield strength, strain hardening coefficient, elongation percentage, strength coefficient of Austenite Stainless Steel 304 with respect to rolling direction, three different strain rates and at various temperatures (0 -900°C) of the steel. Xu Liujie.et.al [9] has projected a technique for predicting hardness, impact toughness in line with quenching, tempering temperatures of High-Speed Steel using back propagation algorithm of artificial neural network model. Bilal M. Zahran.et.al [10] recommended approach predicts hardness of the aluminum alloy based on the alloying elements such as Silicon, Iron, Manganese, Magnesium, Copper using back propagation algorithm of Artificial neural network. M.Hanief.et.al [11] implemented artificial neural network model and regression analysis for predicting surface roughness during turning of red brass using high-speed steel. The inputs of developed models will be cutting speed, feed rate, depth of cut and output is surface roughness. LI Xincheng.et.al [12] employed partial least square prediction model which predicts thermal-fatigue of hot working steel at 600°C by considering material properties yield strength, impact toughness, elongation, oxidation resistance, plasticity, hardness, contraction of area of hot working steel as inputs to the model.

### III. MATERIALS AND METHODOLOGY

#### 3.1 Material used for Investigation

In the recent times, the study of steel is much requisite as it is extensively used among all the materials which can be manufactured in huge quantity for a better price. In this research, we have exploited British standard stainless steels for our investigation of mechanical properties prediction using data science techniques. Steel is a resourceful and adaptable material to tune its composition, structure to mould its properties as per the requirements. Steel is mixture of iron, carbon made from iron ore that is mined from the

ground and smelt in blast furnace to efface the impurities and add carbon. Carbon content in steel is minimum of 0.05% and maximum of 2.1% weight. Classification of steels based on their chemical composition, physical and mechanical properties shown in the figure 1.

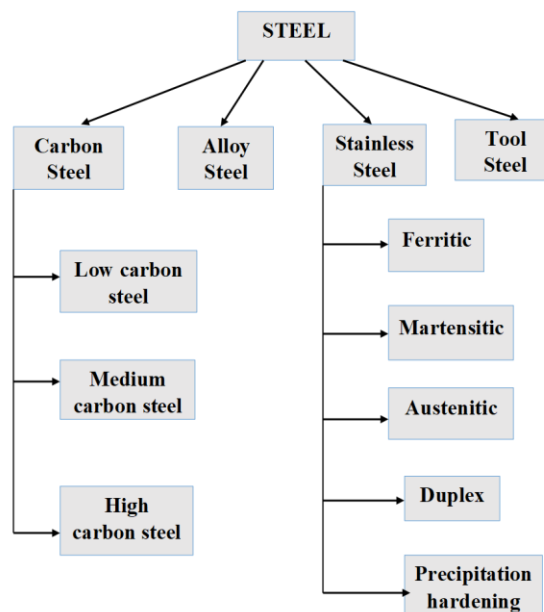


Fig 1: Classification of steels

Carbon Steels composes of iron, carbon and alloying elements like manganese, silicon, and copper. Based on the carbon content in the steels they are further classified as low carbon steel contains 0.04 - 0.3% carbon, medium carbon steel contains 0.31 - 0.6% carbon, high carbon steel contains 0.61 - 1.5% carbon. Tool steels composes carbon (0.5 - 1.5%), cobalt, vanadium, tungsten, molybdenum in differing amounts. There six types of tool steels: hot-work, cold-work, shock-resistant, water-hardening, special purpose and high-speed steels. Alloy steels include nickel, copper, aluminum, manganese, titanium, chromium along with carbon. Stainless steels are very strong and can withstand to elevated temperatures. Other than carbon alloying elements in stainless steel are chromium, nickel and molybdenum. In accordance with the crystalline structure of stainless steels are five types austenitic, ferritic, martensitic, duplex, precipitation hardening.

The appropriate selection of Steel in any kind of application is done only when there is a good knowledge on some basic mechanical properties of steel. Mechanical properties of steels help to know the behavior of steels under various load conditions, and decides whether manufacturing process is suitable for application or not. Mechanical properties of steel are: Tensile Strength, Yield Point, Elongation, Hardness, Toughness, Ductility, Flexibility, Mealibility, Density, Thermal Expansion, Thermal Conductivity, Electric Resistivity, and Specific Heat Capacity, etc. Among all the listed mechanical properties tensile strength of British standard Stainless Steels is predicted in this research. Tensile Strength is defined as capacity of a material resisting maximum stress applied on it. It is the point where materials are plastically deformed but not broken.

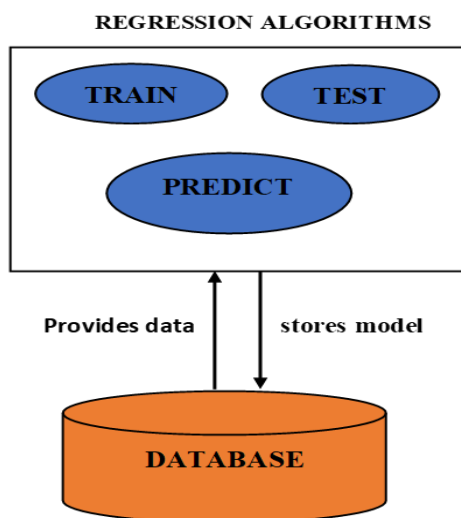


These different types of steels are separated by Steel Grades based on their physical, chemical and mechanical properties of steels. National and International standard organizations have categorized different types of steels into different steel grades. Engineers, researchers, manufacturers, etc. rely on these standards to use steel in their applications. Some of the most commonly used grading systems: International Organization of Standardization (ISO), Society of Automotive Engineers (SAE), British Standards (BS), European Standards (EN), German Standards (DIN), Japanese Industrial Standards (JIS), and Chinese Standards (GB) American Society for Testing and Materials (ASTM). All types of steels are graded by the above grading systems, but the only variation is the grade number of steels differs from one grading system to another grading system.

**3.2 Proposed Methodology:**

In advance material science and engineering in order to identify the mechanical properties of any metal researchers, manufacturers and practitioners of material science and engineering have standardly relied on conventional testing methods which consume time, money and manpower. In case of Steels, Universal Tensile Testing Machine (UTM) is used for testing the steels and determining mechanical properties of steel like tensile strength, yield strength, etc. But when the material has to be tested at elevated temperatures it consumes more time to figure out the properties of material. The main objective of this paper is to implement different data science techniques or algorithms and present which algorithm accurately predicts tensile strength of Stainless steel.

In the proposed method data collected from Steel manufacturing company is used for training the models. The inputs for the trained models are Carbon content in the steel, Sectional size, Temperature, Process of Manufacture, here three manufacturing processes are considered they are: Acid Open Hearth (AOH), Basic Open Hearth (BOH), Basic Electric Arc (BEA). The Targeted output of the models is Tensile Strength of Stainless Steel. The below figure 2 explains the system view of the proposed system where the working of the proposed system



**Fig 2: System view of steel property predictor**

Initially the collected dataset which is stored in database, here database represents local storage in computer is divided into train data and test data where the models are trained with train data and trained models are validated with test

data. The developed trained models are saved in database and used for further predictions. Further, the accurate data science algorithms predict tensile strength of steel for given input details like carbon content in the steel, sectional size, temperature, manufacturing process.

**IV. DATA SCIENCE TECHNIQUES**

Different regression based predictive methods are employed to build models to predict Tensile Strength for the given input parameters carbon content, sectional size, temperature and process of manufacture. The regression-based algorithms selected for predicting the mechanical properties are Random forest, Support Vector Machine (SVM), Artificial Neural Network (ANN), Decision Tree, Ensemble Method – boosting, linear regression, K-Nearest Neighbor(K-NN).

**4.1 Random Forest:**

A supervised machine learning algorithm which is an extension for decision trees and similar to ensemble method called bagging. It can be used for both classification and regression tasks. It creates multiple decision trees during training phase where each data point is fed to all trees and yields mean predictions from all trees and combines all the predictions to give its own prediction. It also avoids over fitting problem in trees. In this approach of predicting mechanical properties random forest regression is opted to train the model and predict the target variables. In the collected data 85% of data is used for training the models and 15% of the data for testing models. The trained model performance is evaluated by calculating the correlation coefficient of actual values and predicted values of test data.

**4.2 Support Vector Machine (SVM):**

SVM performs classification and regression tasks and a supervised technique that handles multiple continuous and categorical variables. In regression, there are two types of SVM models they are: epsilon-SVM regression, nu -SVM regression. The different types of SVM kernels are sigmoid, radial basis function (RBF), polynomial and linear. To train SVM models 85% of collected data is used and the trained SVM models are tested using 15% of collected data. In the proposed approach nu - SVM regression model with radial kernel is selected. Coefficient of Correlation is calculated for actual test data values and predicted test data values for trained model performance evaluation.

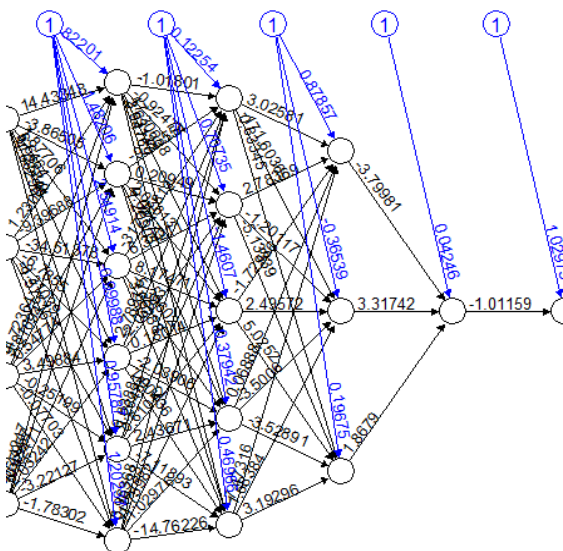
**4.3 Decision Tree:**

This is a supervised technique performs both classification and regression techniques. Decision trees work well for categorical and continuous input, output variables. It develops a associated decision tree by dividing the dataset into smaller subsets. The multiple algorithms to develop a decision tree model are ID3, C4.5, CART, CHAID, MARS, conditional inference trees, etc. which can be used to solve the problem characteristics. In the proposed approach 85% of data is used for training the decision tree model and 15% of data is used to test the trained decision tree model. Further the trained and tested decision tree model is evaluated by correlation coefficient of test data values and predicted data values.



**4.4 Artificial Neural Network (ANN):**

Neural networks have been evolved from the functioning of human brain which is adopted from the simplified models of biological neural network. In human nervous system neuron is the basic functional unit and in neural networks node is the basic computational and functional unit. Nodes are interconnected in layers and form an interconnected network to provide output. Nodes have three components they are weight, bias and activation function. Neural Network algorithm is used for both classification and regression techniques [13-17]. The Architecture of neural network entails three layers input layer, hidden layer and output layer. The model developed to predict tensile strength values has been trained with 85% of data and tested with 15% of data, It consists of one input layer with 4 neurons i.e. (carbon content, sectional size, temperature, process of manufacture), and 4 hidden layers. 6 neurons in first layer, 5 neurons in second layer, 3 neurons in third layer, 1 neuron in fourth layer. 1 neuron in output layer i.e. target variable tensile strength. The below figure 3 gives clear picture of proposed ANN model.



**Fig 3: ANN Architecture of model predicting tensile strength**

**4.5 Ensemble Method (boosting):**

Ensemble methods are the combination of multiple models to improve the prediction accuracy and yields better results. This model is mainly used to decrease variance and increase bias. The various methods in ensemble methods are: Bagging, Boosting, stacking, simple average, weighted average, majority voting, weighted voting. In this proposed method to predict the mechanical properties tensile strength boosting method is employed. Boosting is the method which boosts up the performance of the weak models. It converts weak models to strong models. There are three different types of boosting techniques: Ada Boost (Adaptive Boosting), Gradient Boosting, XGBoost. The Gradient Boosting Machine algorithm is trained with 85% of data and tested with 15% of data with Gaussian distribution. For predicting tensile strength 15,000 trees are used Further, performance of the algorithm is tested by using correlation coefficient for test data and predicted data.

**4.6 K-Nearest Neighbor (K-NN)**

K-NN is the algorithm which is used for both classification and regression. In regression K-NN algorithm will avail all

the suitable cases to predict numerical target based on similarity measure. This algorithm is widely used in applications like pattern recognition and statistical estimation. The K-NN regression calculates average of numerical targets of k-nearest neighbors. K-NN uses three types of distance functions they are: Euclidean, Manhattan, Minkowski. The developed model is trained with 85% of experimental data and validated with 15% of data.

**4.7 Linear Regression**

Linear regression finds relationship between continuous variables i.e. between dependent and independent variables by fitting a linear equation for the data. Usually the relationships between variables be either linear or non-linear. Linear relationships between the variables are represented by using straight lines and non-linear relationships between the variables are represented by curved lines. Two types of linear regression are simple linear and multiple linear regressions. When a single independent predicts a dependent variable then it is called as simple linear regression. When two or more independent variables predict a dependent variable then it is called as multiple linear regression. As part of this research 85% of data trains the developed linear regression model and 15% of data is used to validate the developed linear regression model

**V. RESULTS**

The performance of developed models predicting tensile strength will be evaluated in this section. Efficiency of developed models are evaluated by validating the predictions done by the models on the test data. The statistical parameter used to evaluate developed Random Forest, ANN, SVM, Decision tree, Ensemble models is correlation coefficient(R) which evaluates the strength of linear relationship among two variables. Correlation coefficient measures how targets explain variation in output. R value between two variables is between -1 to +1. -1 represents strong negative correlation between two variables. If there is no association between two variables then R value is 0, strong positive correlation between two variables is denoted as 1. The fitted models using regression analysis in the proposed method are evaluated using coefficient of correlation(R). The coefficient of correlation is mathematically calculated using the below equation 1.

$$R = \frac{\sum_{i=1}^N (x_e^i - \bar{x}_e)(x_p^i - \bar{x}_p)}{\sqrt{\sum_{i=1}^N (x_e^i - \bar{x}_e)^2 \sum_{i=1}^N (x_p^i - \bar{x}_p)^2}} \quad (1)$$

In the equation (1)  $x_e$  is experimental value,  $\bar{x}_e$  is mean of all the experimental values  $x_e$ ,  $x_p$  is predicted value and  $\bar{x}_p$  is mean of all predicted values. N is number of values.

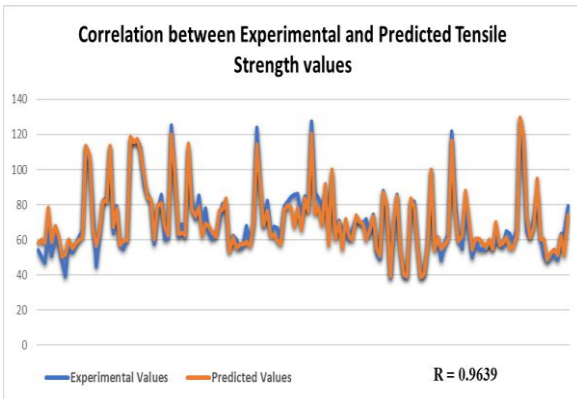
The collected experimental data is splitted as train data and test data. 85% is train data to train developed model and rest 15% of data is used as testing set which is used to test the trained model. The trained model predicts the outputs for the test data which are called as predictions done by the trained model. Now the correlation coefficient is calculated between test data and predicted values on test data to see how accurate trained model predicts tensile strength.



The developed model's random forest, SVM, ANN, ensemble and decision tree are evaluated using statistical metric correlation coefficient(R). The plot shown below represents how predicted values are related to experimental values.

**5.1 Random Forest:**

Developed Random forest model predicts tensile strength of stainless steel. Below figure 4 depict coefficient correlation between experimental and predicted values.

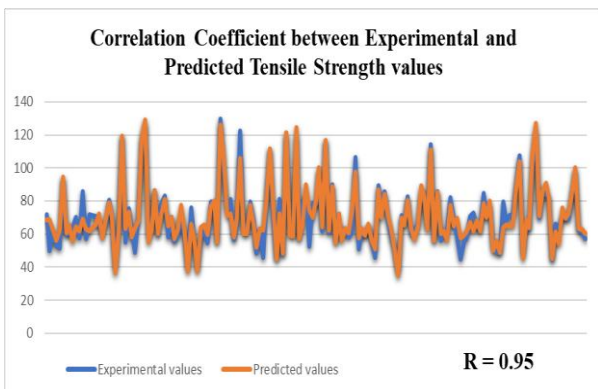


**Fig 4: correlation of tensile strength experimental and predicted values**

The above figure 4 represents variation among predicted and experimental values and the correlation coefficient R is 0.9639 which depicts model predicts mechanical properties accurately. Therefore, the trained random forest model is accurate in predicting tensile strength of stainless steel.

**5.2 Support Vector Machine (SVM):**

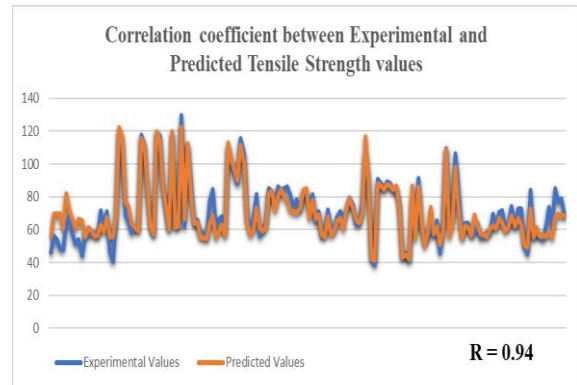
The regression plot graphs of SVM models trained to predict tensile strength. The below figure 5 shows coefficient of correlation between the experimental, predicted values of tensile strength is 0.95



**Fig 5: correlation between experimental and predicted values of tensile strength**

**5.3 ANN:**

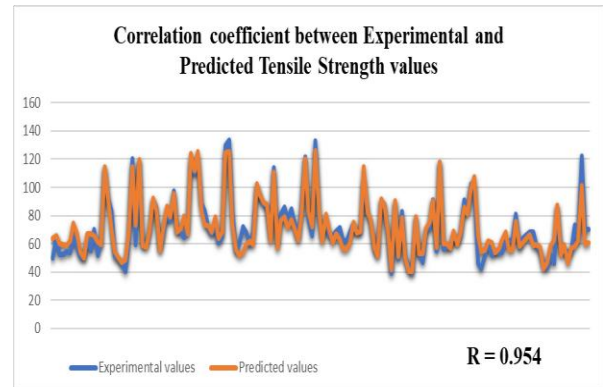
The performance of developed ANN models is validated by using correlation coefficient. The coefficient of correlation of collected experimental and predicted tensile strength is shown in below figure 6. The correlation coefficient R for the tensile strength values is 0.94.



**Fig 6: – correlation between predicted and experimental tensile strength values**

**5.4 Ensemble (boosting):**

The ensemble technique boosting models are developed for predicting tensile strength which is evaluated using correlation of coefficient. The correlation coefficients for experimental and predicted values are given below in figure 7:

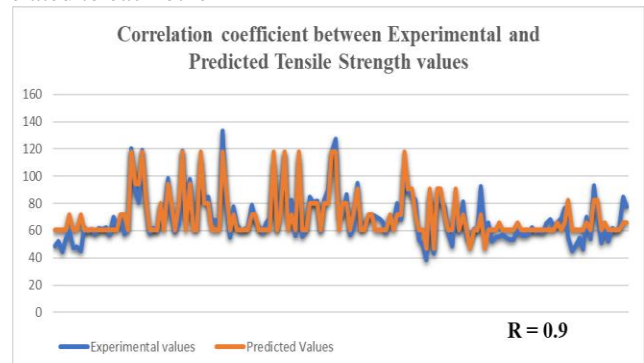


**Fig 7: correlation of predicted, experimental tensile strength values**

The boosting model is successful in predicting tensile strength with correlation coefficients 0.95.

**5.5 Decision Tree:**

The below presented figure 8 represents how well decision tree models predicted tensile strength and shows how experimental and predicted tensile strength values are related to each other

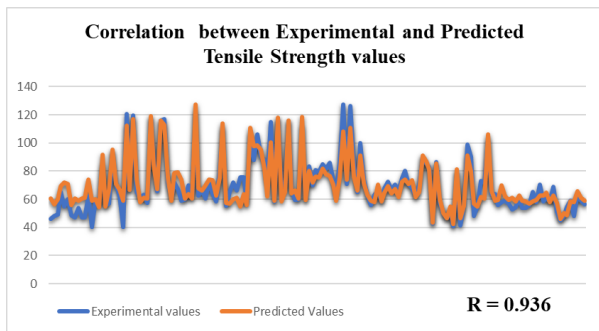


**Fig 8: correlation of predicted vs experimental tensile strength values**

From the above graphs it is known that the correlation coefficient R value for tensile strength is 0.9.

**5.6 K-Nearest Neighbor (K-NN):**

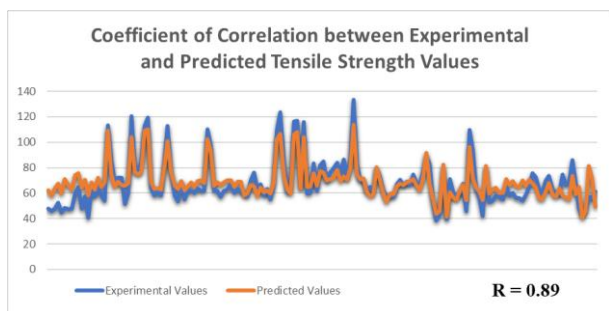
K-NN models predict tensile strength values with an accuracy of 93.6%. The correlation of predicted and experimental tensile strength values is given as 0.936 as shown in the below figure 9



**Fig 9: correlation of predicted vs experimental tensile strength values**

**5.7 Linear Regression:**

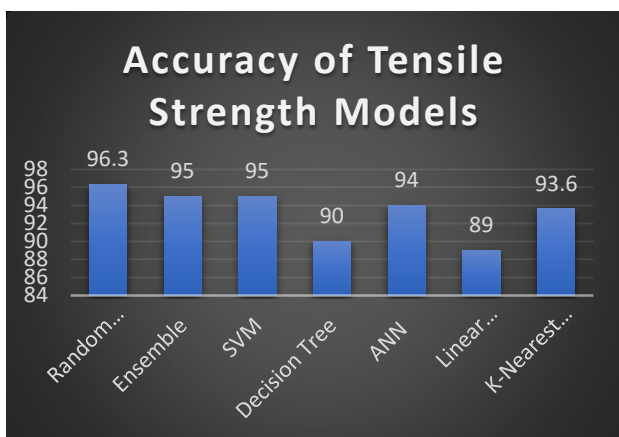
The correlation coefficient for experimental and predicted tensile values by using linear regression model is 0.89 shown in below figure 10 which represents it predicts tensile strength values with an accuracy of 89%.



**Fig 10: correlation of predicted vs experimental tensile strength values**

**5.8 Comparison of developed models**

The below figure 11 shows the performance analysis of developed models and shows which algorithm accurately predicts tensile strength of steel. From below figure it is proved that Random forest model is accurately predicting mechanical properties of steel. The developed random forest model predicts tensile strength values with an accuracy of 96.3%.



**Fig 11: Accuracy comparison of the data science techniques predicting tensile strength**

From the above figures it is proved that Random Forest model accurately predicts tensile strength of stainless for the given processing parameters. The below table represents performance and accuracy of data science algorithms in predicting tensile strength values.

Algorithm	Accuracy
Random Forest	96.3
Ensemble	95
SVM	95
Decision Tree	90
ANN	94
Linear Regression	89
K-Nearest Neighbor	93.6

**Table I: Accuracy of various data science algorithms predicting tensile strength**

**VI. CONCLUSION AND FUTURE SCOPE**

The current material sciences will definitely be affected by Data science and analytics by exaggerating accuracy and reliability in predicting mechanical properties using large ensemble of datasets from different material databases and by using different data science algorithms. In this paper a total of 7 different algorithms were implemented on the dataset and the accurate model is identified. The proposed idea will be a breakthrough for conventional approach of conducting tensile tests using Universal Tensile Test machine (UTM) to know mechanical properties of steel. The developed regression-based models' random forest, SVM, ANN, decision tree, linear regression, K- Nearest Neighbor and ensemble method(boosting) predicted tensile strength values with an accuracy of 96.3%, 95%, 94%, 90%, 95%. The developed data science algorithms predict mechanical properties of stainless steel i.e. tensile strength for given input processing parameters carbon content, sectional size, temperature, process of manufacture by reducing time and money.

In future this research will be enhanced by predicting various other mechanical properties like yield point, elongation rate, work hardening, extreme rate sensitivity index etc. A user-friendly GUI (Graphical User Interface) will be developed by integrating data science algorithms which accurately predicts mechanical properties based on their composition and processing parameters. Therefore, this research can be used for predicting mechanical properties of steel without performing traditional experiments and tests.

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