



## **Strength analysis of sugarcane bagasse ash and rice husk based subgrade material with natural soil using different machine learning**

**Khushboo Uniyal<sup>1</sup>, Bheem Pratap<sup>2</sup>, Pramod Kumar<sup>3</sup>, Keerat Kumar Gupta<sup>4</sup> and Rahul Vaishnava<sup>5</sup>**

<sup>1</sup>Assistant Professor, Department of Civil Engineering, Graphic Era (Deemed to be University), Dehradun, Uttarakhand-248002, India. Email: [khushboouniyal29@gmail.com](mailto:khushboouniyal29@gmail.com)

<sup>2</sup>Assistant Professor, Department of Civil Engineering, Graphic Era (Deemed to be University), Dehradun, Uttarakhand-248002, India. Email: [bheempratapbind009@gmail.com](mailto:bheempratapbind009@gmail.com)

<sup>3</sup>Assistant Professor, Department of Civil Engineering, Mohan Babu University (SVEC), Tirupati, Andhra Pradesh, India-517102. Email: [chaudharypramod600@gmail.com](mailto:chaudharypramod600@gmail.com)

<sup>4</sup>Professor, Department of Civil Engineering, Graphic Era (Deemed to be University), Dehradun, Uttarakhand-248002, India. Email: [kkguptafce@geu.ac.in](mailto:kkguptafce@geu.ac.in)

<sup>5</sup>Assistant Professor, Department of Civil Engineering, Graphic Era (Deemed to be University), Dehradun, Uttarakhand-248002, India. Email: [rahulvaishnav@geu.ac.in](mailto:rahulvaishnav@geu.ac.in)

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## Abstract

Sugarcane bagasse ash (SBA) is a waste product that is left over after the sugar and alcohol industries. Rice husk ash (RHA) is a byproduct of rice husk burning. A helpful soil stabilizer for road building is terrazyme, a liquid enzyme that enhances the engineering properties of soil. In this study, natural soil, SBA and rice husk were combined in different proportions along with different concentration of terrazyme. This study uses measures like root mean square error (RMSE), mean absolute error (MAE),  $R^2$ , and standard deviation to examine the performance of six predictive models across training and testing datasets: artificial neural network (ANN), XGBoost, random forest, M5P, linear regression, and non-linear regression. The ANN model exhibits overfitting as it performs poorly on unseen data ( $R^2 = 0.589$ ) but well on training data ( $R^2 = 0.971$ ). Nearly flawless training results ( $R^2 = 0.999$ , RMSE = 0.005) are obtained using XGBoost, while modest generalization (testing  $R^2 = 0.798$ ) indicates diminished but still respectable performance on fresh data. Although Random Forest performs well during training ( $R^2 = 0.977$ ), there is a discernible decline in generalization ( $R^2 = 0.853$  during testing). The M5P model exhibits extreme overfitting; its testing  $R^2$  drops to 0.229 from its training  $R^2$  of 0.983. Although linear regression consistently produces RMSE and MAE between training and testing, its explanatory ability is limited by a significant reduction in  $R^2$  (0.872 to 0.233).

**Keywords:** Sugarcane bagasse ash, Unconfined compressive strength, Artificial neural network, XGBoost and Random Forest.

## 1. Introduction

There is minimal application of SBA and RHA for rural roads. From a sugarcane production perspective, India ranks second globally. In 2010, India produced 292.3 MMT of sugarcane (Kishor et al., 2022). Following the extraction of sugarcane juice, sugarcane bagasse with high calorific values is produced. Cogeneration uses it as a fuel to generate electricity and steam because of its high calorific value. 750–1000 °C was the temperature at which the sugar cane bagasse burned. SBA is the end product of this process and the last waste product in the sugar manufacturing cycle (Kumar Yadav et al., 2017). It contains a significant amount of quartz ( $\text{SiO}_2$ ) (Anupam et al., 2017). There have been reports of SBA's effectiveness as a

stabilizer for pavement subgrade dirt. There have also been attempts to extract sodium silicate from sugarcane bagasse ash in an attempt to create silica particles (Boonmee and Jarukumjorn, 2020). These silica particles can be used as a replacement for binder materials like cement which contain high concentration of silica in their composition. This residue of sugarcane, when burnt, leaves behind about 8-10% ash known as SBA (Aigbodion et al., 2010). Osinubi and Thomas (2007) conducted various tests such as Atterberg limit test, moisture-density relation, UCS and CBR on samples of black cotton soil treated with SBA and found an increase in the unconfined compressive strength of soil with proportional increase of the SBA content and concluded that SBA can be used as an admixture with binders like lime and cement (Osinube and Thomas, 2008).

The combustion of rice husk, a readily accessible by-product of industrial waste, produces RHA. 20-25% of the rice's weight is made up of rice husks (Camargo-Pérez et al., 2023). When rice husk is burned, silica ash is left behind after cellulose and lignin are eliminated. Numerous investigators have examined the molecular and physical characteristics of RHA. When burned at a regulated temperature of 600–800 °C, RHA is chemically composed of 82–95% silica (Emdadi et al., 2017). It is a pozzolanic substance (Detphan and Chindaprasirt, 2009; Getahun et al., 2018; Kim et al., 2014). The effects of rice husk ash on geotechnical properties of lateritic soil and found that rice husk ash helps in raising the optimum moisture content of the soil but at the same time reduced maximum dry density and plasticity of the soil. It also improved the strength property and volume stability of lateritic soil (Tiwari et al., 2025). In a similar study conducted by Ewa et al., (2018) on the variability of RHA on geotechnical properties of soil subgrade, they concluded that addition of RHA as soil stabilizer increased the optimum moisture content of the soil and decreased the maximum dry density (Ewa et al., 2018). Further an all-around improvement in the UCS values of the samples was also noticed.

Complex pattern oriented problems can be dealt with the help of Artificial Neural Networks (ANN). De et al., (2007) used ANN to develop models to accurately forecast performance of a power plant's steam process (DE et al., 2007). Reddy et al., (2003) used ANN models to estimate monthly mean daily and hourly values of solar global radiation from 13 different stations across India (Reddy and Ranjan, 2003). The results were compared with other regression models and were found to be in good agreement with them. Li et al., (2024) in their study on Performance-oriented road structure and material design method used a long term pavement performance database to train a prediction model using XGBoost algorithm (Li et al., 2024). This helped them to create an automated design model that included the required

properties i.e. subgrade material, pavement thickness and pavement material. This study confirmed the satisfactory performance of XGboost algorithm by the results of high coefficient of determination ( $R^2$ ) and mean absolute percentage error achieved from ML regression. Behnood et al., (2017) used M5P model tree to predict the compressive strength of high performance concrete (Behnood et al., 2017). Data collected from literature was used to develop the model. Their study showed that the model had an accuracy of over 80%. Lei et al., (2016) proposed a combined M5P tree and M5P model to predict accident durations (Lin et al., 2016). The model demonstrated superior prediction accuracy and had lowest overall mean absolute percentage error.

### **1.1 Research gap and objectives**

There has no any research which developed the subgrade materials using sugarcane bagasse and rice husk along with terrazyme. Ultimate objective is to construct a subgrade that satisfies specifications related to unconfined compressive strength, and meets the requirements related to the pavement subgrade. It can be fabricated using sugarcane bagasse ash and rice husk ash along with terrazyme and soil to study the UCS using ANN, XGBoost, random forest, M5P, linear regression, and non-linear regression.

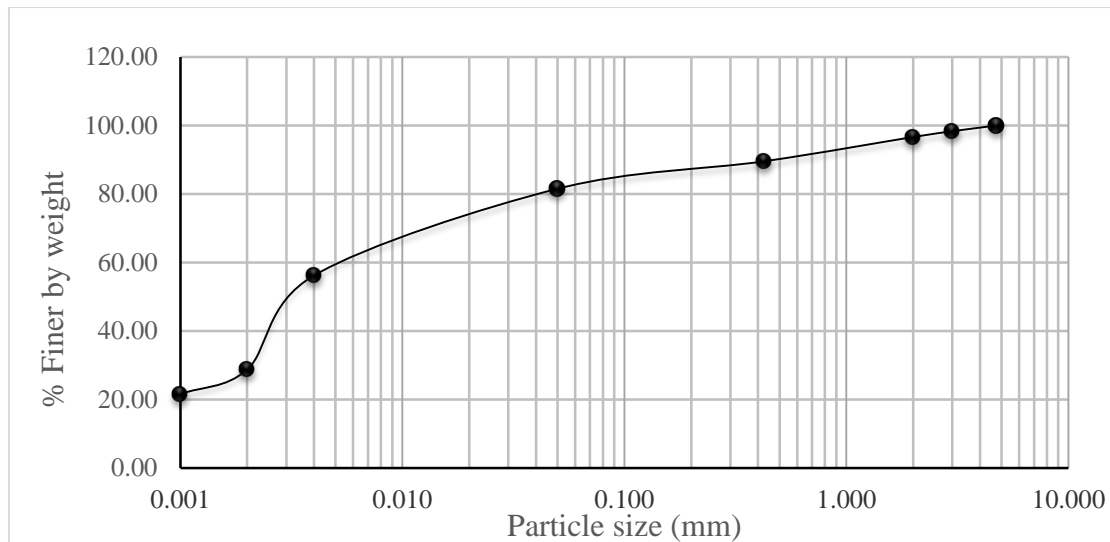
## **2. Materials**

### **2.1 Sugarcane bagasse ash**

SBA is a waste product that is left over after the sugar and alcohol industries. After the sugar cane is harvested, the pulp that remains is recycled and utilized to generate heat in boilers, leaving approximately 8%–10% ash as waste. Due to residual carbon and other unwanted substances, the ash usually referred to as sugarcane bagasse ash (SBA) is typically black in color.

### **2.2 Natural soil**

Natural soil collected from the Dehrahun, India. Its initial properties were thoroughly characterized before stabilization to ensure accurate assessment of the stabilization effects. Grain size analysis of the natural soil has been depicted in Fig. 1. Natural soil contained 60.78% of silt, 10.46% of sand and 28.76% of clay; it is a fine grained soil. Liquid limit, plastic limit and plasticity index of the soil were 50.13, 28.63 and 21.50, respectively.



**Fig. 1** Gradation curve of natural soil

### 2.3 Rice husk ash

RHA is a byproduct of rice husk burning. Silicates are the main leftovers left over after burning rice husk, since the majority of its evaporable components gradually disappear. During the milling process, the hard protective coverings known as rice husks are removed from the grains. The husks are removed from the raw grain during a standard milling procedure, revealing complete brown rice.

### 2.4 Terrazyme

A helpful soil stabilizer for road building is Terrazyme, a liquid enzyme that enhances the engineering properties of soil: A natural, non-toxic liquid called terrazyme modifies the chemical and physical characteristics of soil. It enhances the soil's structural qualities by catalyzing organic chemical processes in the soil.

### 2.5 Test methodology

The natural soil, rice husk terrazyme and sugarcane bagasse ash have been collected from the Uttarakhand. The materials were dry and sieved before used. The chemical composition of the raw materials have tabulated in Table 1. The material proportions for SBA, RHA, and terrazyme were selected based on a combination of preliminary experimental trials. Initially, a series of trial mixes were prepared to evaluate the influence of varying proportions on the soil's properties. In this study, natural soil, SBA and rice husk were combined in different proportions along with different concentration of terrazyme and presented in Table 2.

The test for unconfined compressive strength (UCS) was conducted using IS 2720 (Part X)-1991 as a guide (IS: 2720 (Part 10):1991, 1991). The specimens were cured for a period of 28 days under controlled laboratory conditions. During the curing process, the temperature was maintained at approximately  $27 \pm 2^{\circ}\text{C}$  with relative humidity around 90%, ensuring consistent hydration and strength development. These conditions were carefully monitored to maintain uniformity across all test samples.

**Table 1** XRF results of raw materials

Chemical composition	Percentage content (%)		
	SBA	RHA	Soil
CaO	12.16	18.14	10.36
SiO <sub>2</sub>	64.65	51.43	55.28
Al <sub>2</sub> O <sub>3</sub>	4.74	5.17	18.65
Fe <sub>2</sub> O <sub>3</sub>	4.62	3.67	6.56
MgO	0.15	1.61	3.14
K <sub>2</sub> O	0.76	11.75	0.52
TiO <sub>2</sub>	0.80	0.16	0.04
LOI	12.12	8.07	5.45

**Table 2** Mix design

SN	Soil	SBA (%)	RHA (%)	Terrazyme (ml/m <sup>3</sup> )	UCS (KPa)
1	40	60	0	10	1510.88
2	40	50	10	10	1524.57
3	40	40	20	10	1535.38
4	40	30	30	10	1542.56
5	40	20	40	10	1546.53
6	40	10	50	10	1544.21
7	40	60	0	20	1512.46
8	40	50	10	20	1528.55
9	40	40	20	20	1539.35
10	40	30	30	20	1545.36

11	40	20	40	20	1550.27
12	40	10	50	20	1547.44
13	40	60	0	30	1520.82
14	40	50	10	30	1535.52
15	40	40	20	30	1546.18
16	40	30	30	30	1552.37
17	40	20	40	30	1557.39
18	40	10	50	30	1554.38
19	40	60	0	40	1530.82
20	40	50	10	40	1544.58
21	40	40	20	40	1555.22
22	40	30	30	40	1561.74
23	40	20	40	40	1566.59
24	40	10	50	40	1564.63
25	40	60	0	50	1537.53
26	40	50	10	50	1551.72
27	40	40	20	50	1562.28
28	40	30	30	50	1567.47
29	40	20	40	50	1573.38
30	40	10	50	50	1570.28
31	40	60	0	60	1566.58
32	40	50	10	60	1578.71
33	40	40	20	60	1589.83
34	40	30	30	60	1595.25
35	40	20	40	60	1624.52
36	40	10	50	60	1610.34

## 2.6 Artificial Neural Networks

ANNs are the networks that use machine learning to replicate decision making of a human brain. The neural network is made up of units which replicate neurons in a human brain (Unis et al., 2022). These units can be of any number depending upon the complexity of the problem. These are arranged in two layers called the input layer and an output layer. Mimicking a human

brain, these input units gathers data from the surrounding world and uses it to learn and analyse according to the requirements of the neural network(Choudhary et al., 2024). When a problem of a similar nature is then presented to this ANN, it uses this gathered data to analyse it and transfers this data from one unit to another and gives an output through the output layer in the form of a response. This interconnected network helps it learn more and more with the variety of situations presented to it(Bebana et al., 2019).

## **2.7 XGBoost**

A scalable distributed gradient-boosted decision tree machine learning toolbox is called Extreme Gradient Boosting, or XGBoost(Mustapha et al., 2024). It provides parallel tree boosting and is useful machine learning tool for works such as regression, classification, and ranking. In such an algorithm, a model is created and trained in such a way that it identifies certain patterns in a dataset containing features and labels. This model is then used to predict labels on features in any further given dataset. Further, decision trees help in forecasting a continuous numerical value or classification to predict a category. By analysing a decision tree and calculating the bare minimum of questions required to determine the likelihood of selecting the right choice, decision trees provide a model that predicts the label(Zhang et al., 2024). Gradient boosting helps in formalizing the additive development of weaker models using a gradient descent method. It outlines the required outcomes for next models in order to minimize errors. The phrase "gradient boosting" refers to the fact that the intended results for each case are determined by the gradient of the error with respect to the forecast(Li et al., 2024).

## **2.8 Random Forest**

Random forest is a machine learning technique which combines the outputs of multiple decision trees to generate a single result. Its adaptability and simplicity of usage have promoted its use because it can handle both regression and classification problems(Mohamed et al., 2017). The algorithm of random forest is an extension of the bagging approach, it combines feature randomness and bagging to create decision trees(Chun et al., 2020). Primary difference between decision trees and random forests is that decision trees consider every conceivable feature split whereas random forests only select a subset of the features(Chun et al., 2020; Li et al., 2022; Sahour et al., 2021; Sun et al., 2023).

## **2.9 M5P model**

Quinlan first found the M5 algorithm, which has now been developed into the M5P algorithm(Ali, 2024). The ability of model trees to effectively handle numerous data sets with a high number of features and high dimensions is one of its primary benefits. They also have a reputation for being resilient in the face of missing data(Ali, 2024). The input space is first divided into many sub-spaces using the M5 method, so that each sub-space has data records with common characteristics. To reduce the variance inside a certain sub-space, linear regression models are employed in this procedure(Ali, 2024). The data gathered from the preceding stage is then utilized to generate several nodes where the splitting procedure is carried out based on a specified property. This stage enables the construction of a tree-like structure with the leaves at the bottom and the root at the top. A fresh data record begins at the tree's root and travels through the nodes until it reaches a leaf. Each node has a mathematical logic that lets the data record navigate down to a leaf by comparing a certain value of the provided data record with that of the split value(Mahmood et al., 2024). The input area is initially divided into a number of smaller regions in order to construct a tree. Utilizing the splitting criterion, the intra-subspace variability is reduced from the root to the node.

### **2.10 Linear regression**

Investigating the connections between two or more variables is a common task in scientific and engineering challenges is linear regression(Maabreh and Almasabha, 2024). The optimal link between a dependent variable and many independent variables may be predicted with the help of linear regression. Sometimes, the independent variables are referred to as predictors, and the dependent variable as the predicted(Habib and Okayli, 2024).

### **2.11 Non-linear regression**

Non-linear regression sought to investigate, using statistical models, the possible link between strength and input factors(Mouli et al., 2024). In addition to the traditional linear regression model, this study suggested non-linear models to enhance the determination coefficient when forecasting UCS using factors relevant to mixture design(Zhou et al., 2024).

## **3. Results**

### **Effects of SBA and RHA on soil**

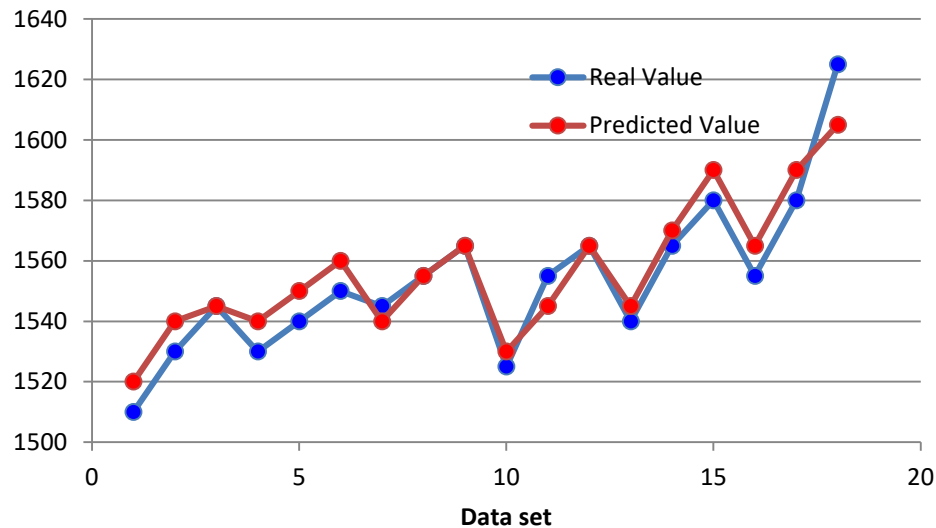
Table 2 reveals that the UCS of the soil increases with higher proportions of RHA and Terrazyme, while SBA has a comparatively lesser effect. With soil content fixed at 40%,

substituting SBA with RHA leads to a consistent rise in UCS, indicating that RHA's higher silica content promotes more effective pozzolanic reactions, forming stronger cementitious bonds(Kumar Yadav et al., 2017). terrazyme, a biochemical stabilizer, further enhances UCS by improving soil particle bonding and reducing moisture sensitivity. As terrazyme dosage increases from 10 to 60 ml/m<sup>3</sup>, UCS also rises steadily across all mix combinations, showcasing its strong role in boosting soil strength. The maximum strength of 1624.52 KPa is attained at 20% SBA, 40% RHA, and 60 ml/m<sup>3</sup> of terrazyme. The highest UCS values are obtained when 20–30% SBA, 40–50% RHA, and 60 ml/m<sup>3</sup> of terrazyme are combined. Rich in amorphous silica, which is essential for pozzolanic reactions, are SBA and RHA(Kumar Yadav et al., 2017). Cementitious chemicals such calcium silicate hydrates (C-S-H) are created when these ashes are combined with soil and water and react with calcium (Ewa et al., 2023). By strengthening the bonds between soil particles, these substances promote cohesion, decrease flexibility, and eventually raise UCS. The physical characteristics of SBA and RHA, such as their tiny particle size and high surface area, help improve soil gradation and densification in addition to the chemical processes, which further increases strength and stability(Camargo-Pérez et al., 2023; Hidalgo et al., 2020). RHA and terrazyme are especially useful in enhancing soil stabilization for engineering applications, highlighting the synergistic effect of pozzolanic materials and enzymatic treatment.

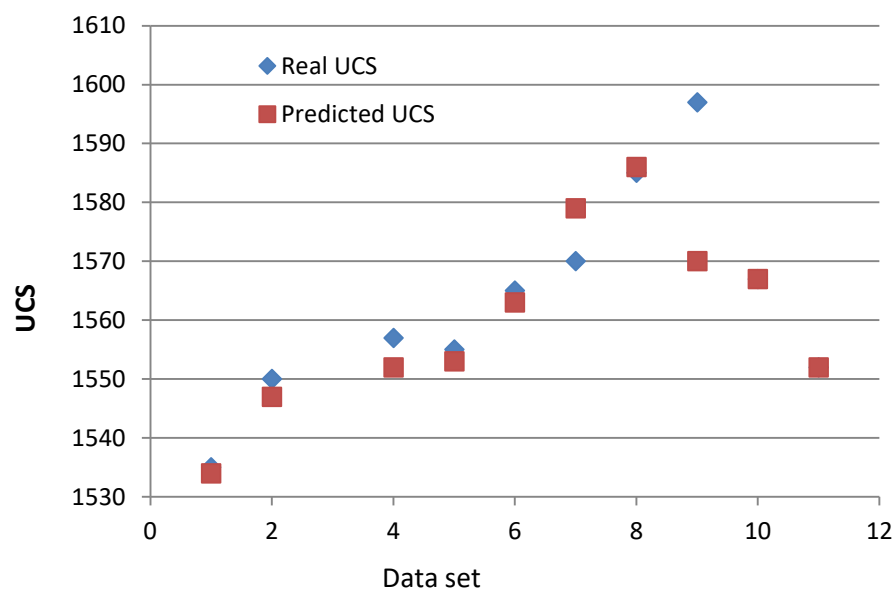
### **3.1 Artificial neural networks(ANN)**

RHA and terrazyme demonstrate the synergistic effect of pozzolanic materials and enzymatic treatment, and are particularly helpful in improving soil stabilization for engineering applications. Which shown in shown in Figs. 2 and 3 respectively. For the training dataset, the ANN achieves an impressive R<sup>2</sup> score of 0.971, signifying that the model captures 97.1% of the variance in the training data. This high value reflects the ANN's ability to learn complex patterns and relationships in the data during training, showcasing its suitability for capturing non-linear and intricate dependencies(Pratap, 2024). Such a strong performance on the training set suggests that the model architecture, including the choice of layers, activation functions, and training parameters, is well-tuned for fitting the training data(Alsulaili and Refaie, 2021). still, the testing R<sup>2</sup> score of 0.589 is considerably lower, indicating that the model explains only 58.9% of the variance in unseen data. This drop in interpretation points to a significant generalization gap, recommends that the ANN may be overfitting the training data(Tiryaki and Aydin, 2014). Overfitting happen when the model comes to be too specialized to the training dataset, learning noise or unrelated patterns that don't transfer well to new information. The

difference between the training and testing  $R^2$  scores highlights this issue, as the model struggles to follow its training success when faced with unseen scenarios (Kazemi and Gholampour, 2023).



**Fig. 2** Training of ANN model



**Fig. 3** Testing of ANN model

On unseen data, the ANN still has considerable predictive power and captures a sizable amount of variance, even with the lower testing  $R^2$  value. (Kaveh and Khavaninzadeh, 2023). However, the relatively low score suggests that improvements are needed to enhance its applicability in real-world settings where unseen data is more prevalent. Strategies to address

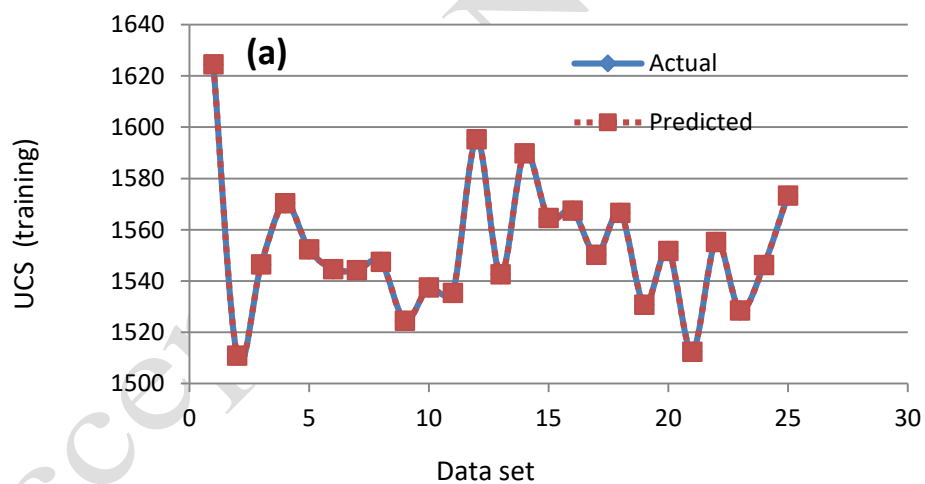
this could include simplifying the model architecture, increasing the diversity and size of the dataset, or employing techniques like early stopping during training to prevent overfitting(Kaveh, A Bakhshpoori, 2018).

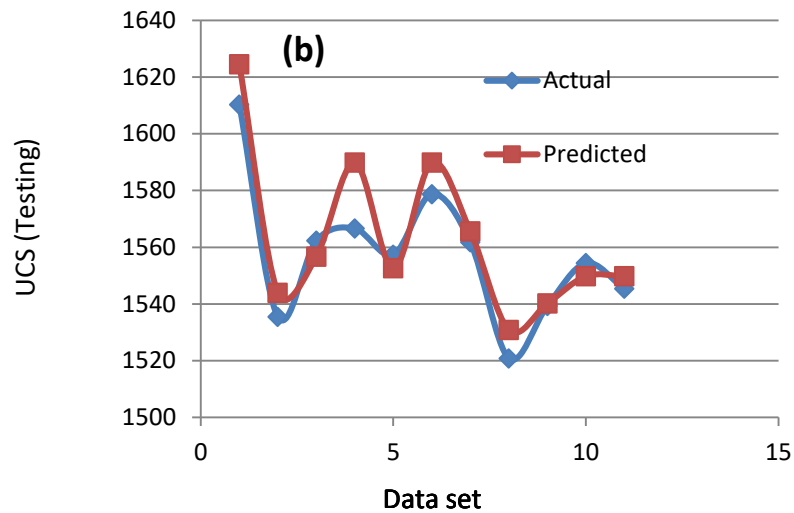
### 3.2 XGBoost

Table 3 represent the performance metrics of an XGBoost model evaluated on training and testing datasets. Each metric provides insight into the model's accuracy, error, and consistency.

Table 3 XGBoost results for training and testing

Parameters	Training results	Testing results
RMSE	0.005	10.208
MAE	0.002	8.275
Standard deviation	35.496	34.810
R <sup>2</sup> score	0.999	0.798





**Fig. 4** (a) Training and (b) testing of XGBoost

Fig. 4 presents the training and testing of the XGBoost model. The extremely low value of training of RMSE is 0.005 suggests that the model fits the training data almost perfectly, with negligible error. The much higher value of testing RMSE is 10.208 indicates that the model's performance on unseen data is significantly worse than on the training data. This discrepancy suggests potential overfitting, where the model captures the training data too well but struggles to generalize to new data(Sun et al., 2024). Training value of MAE is 0.002, a very low value indicates excellent predictive accuracy on the training set. Testing value of MAE is 8.275 presents the higher testing MAE compared to training reflects a reduction in accuracy when the model is applied to new data, reinforcing the likelihood of overfitting(Chen et al., 2024). The low error metrics of training of standard deviation is 35.496; the high standard deviation suggests variability in the model's training predictions. This could be due to the dataset's inherent characteristics. The slightly lower value in testing of standard deviation indicates similar variability in predictions on unseen data. However, the difference is small, implying that prediction inconsistencies persist across both datasets(Abdullah et al., 2024). Training value of  $R^2$  of 0.999 nearly perfect score suggests the model explains almost all the variability in the training data. Testing value of  $R^2$  of 0.798 indicates the model still performs reasonably well on unseen data, it is significantly lower than the training  $R^2$ , again pointing to overfitting(Thapa and Ghani, 2024).

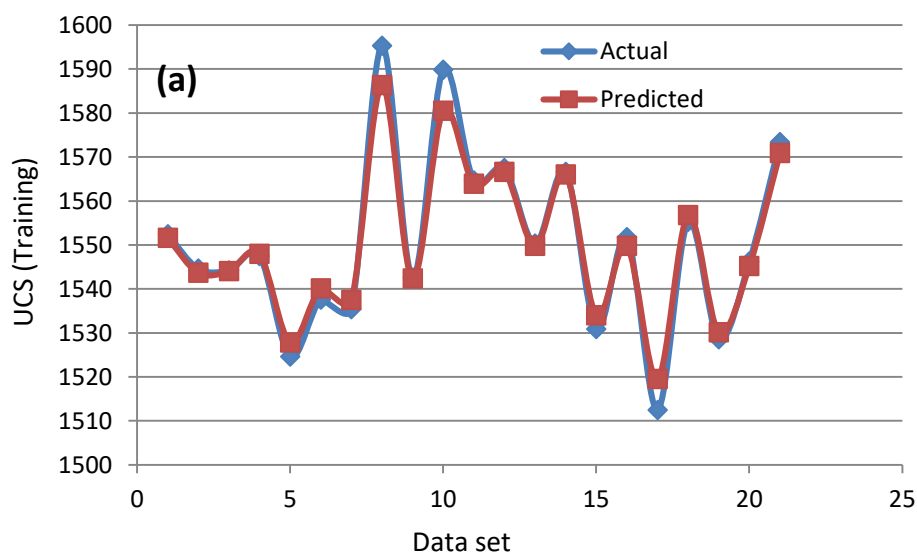
### 3.3 Random forest

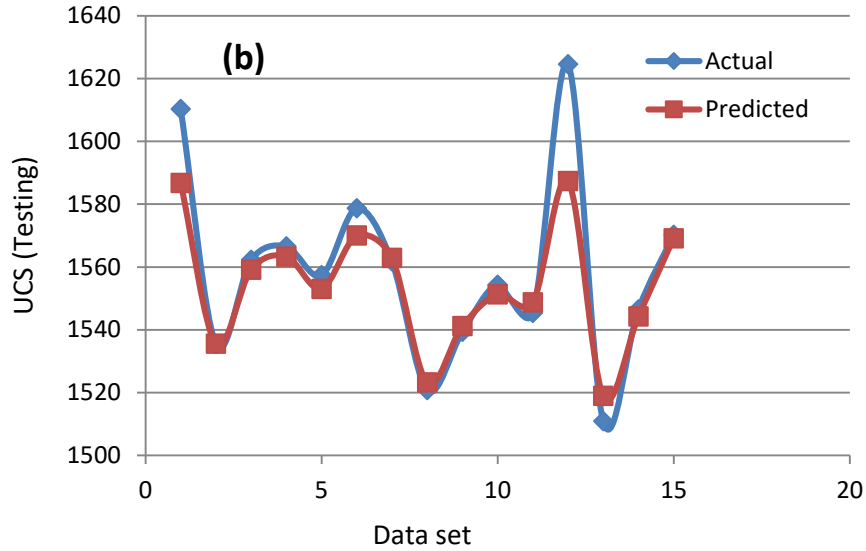
The results include RMSE, MAE, Standard Deviation, and  $R^2$  Score plotted in Table 4 for random forest.

Table 4 Random forest results for training and testing

Parameters	Training results	Testing results
RMSE	2.995	11.075
MAE	2.026	6.338
Standard deviation	17.379	20.664
$R^2$ score	0.977	0.853

The RMSE, a measure of the average magnitude of prediction errors, the training RMSE of 2.995 indicates that the model performs very well on the training dataset, with low error(Choudhary et al., 2024). However, the testing RMSE of 11.075 suggests a noticeable increase in error when the model is applied to unseen data. This disparity hints at potential overfitting, where the model might be too tailored to the training data, leading to reduced generalizability(Chen et al., 2024). The MAE, which represents the average absolute error without squaring, complements the RMSE by showing the typical magnitude of prediction errors.





**Fig. 5** (a) Training and (b) testing of RF

The graph of the Random Forest model has been plotted in Fig. 5 for training and testing datasets. The training MAE of 2.026 confirms low errors during training, while the testing MAE of 6.338, though higher, is still within a reasonable range relative to the testing RMSE. The difference between training and testing MAE supports the observation of potential overfitting. The standard deviation of the prediction errors reflects the variability in the model's errors. A training standard deviation of 17.379 compared to a higher testing value of 20.664 indicates that error variability is greater in the testing phase (Mohamed et al., 2017). This increased variability in unseen data further reinforces concerns about the model's consistency and robustness when faced with new scenarios. Finally, the  $R^2$  score, or coefficient of determination, highlights how well the model explains the variance in the target variable. A training  $R^2$  score of 0.977 signifies that the model captures nearly all the variance in the training data, demonstrating excellent fit. But, the testing  $R^2$  score of 0.853, while still well, reveals a drop in performance when generalizing. This gap between the training and testing  $R^2$  scores again points to overfitting, as the model excels on the training data but loses some predictive power on unseen data. The Random Forest model establish strong performance on the training dataset, as indicated by low RMSE and MAE, low error variability, and a near-perfect  $R^2$  score. But, the testing results indicate higher errors, more variability, and a reduced  $R^2$  score, signaling challenges with generalization. To improve the model's generalizability, techniques such as cross-validation, parameter tuning, or reducing model complexity could be employed (Huang et al., 2020; Sahour et al., 2021; Sun et al., 2023). These results underscore the significance of

balancing training performance with testing robustness to reach reliable and consistent predictive models(Chun et al., 2020).

### 3.4 M5P model

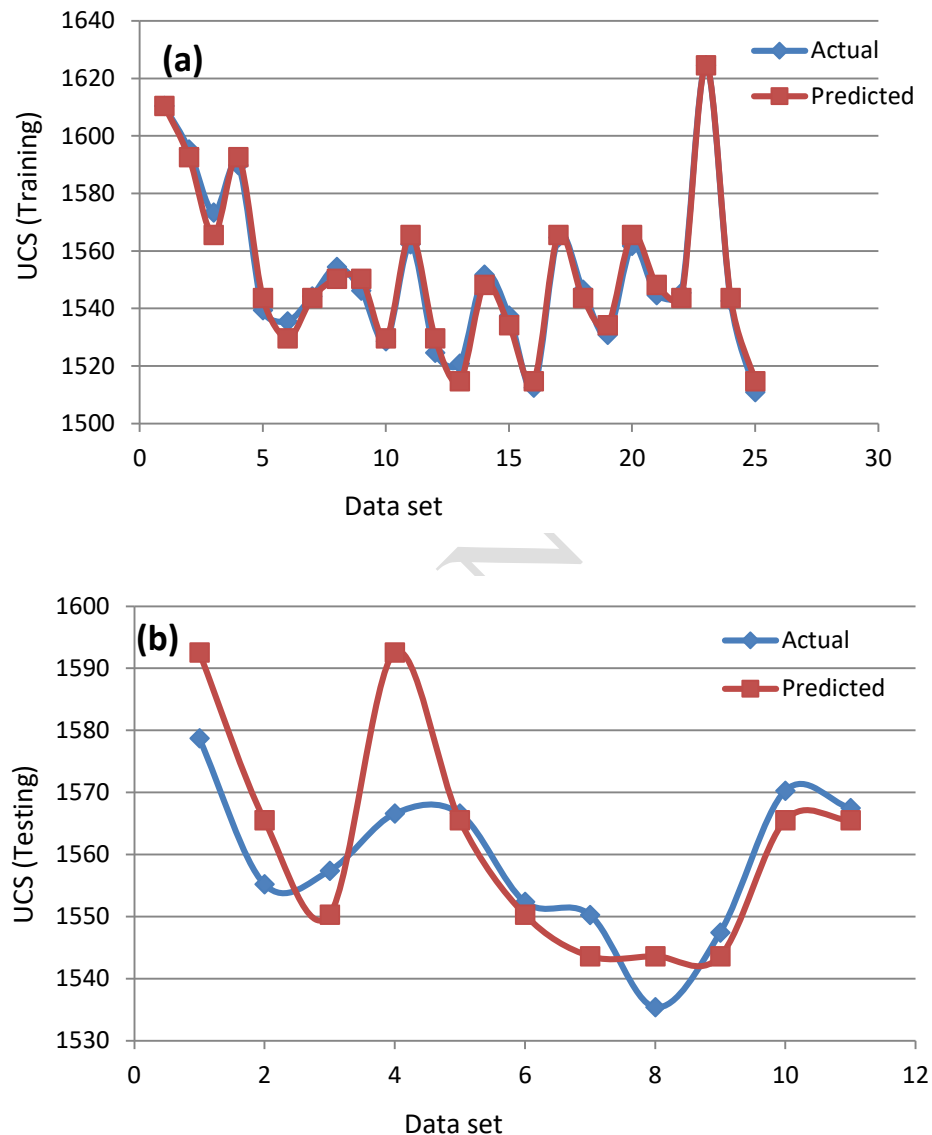
The performance metrics of the M5P model contribute valuable insights into its effectiveness in predicting result for both training and testing datasets plotted in Table 5. The result of the M5P model has been plotted in Fig. 6. The training RMSE of 3.652 show that the M5P model performs well on the training dataset, developing relatively small prediction errors. Even though, the testing RMSE of 10.360 reveals a significant increase in error magnitude when applied to unseen data. This difference suggests that the model may struggle to generalize to new observations, pointing to potential overfitting to the training data. The MAE, which represents the average absolute error, shows a similar trend. The training MAE of 3.118 is relatively low, indicating good predictive accuracy during training. However, the testing MAE of 7.802 highlights a notable increase in the average error for unseen data. This larger error in testing further underscores the model's limited generalization capability and aligns with the RMSE results.

Table 5 M5P model results for training and testing

	Training metrics	Testing metrics
RMSE	3.652	10.360
MAE	3.118	7.802
Standard deviation	39.549	20.747
R <sup>2</sup> score	0.983	0.229

The standard deviation of errors provides insight into the variability of the prediction errors. A training standard deviation of 39.549 suggests that while the model performs accurately on average, there may be occasional large deviations from actual values during training. For the testing dataset, the standard deviation drops to 20.747, which might indicate reduced error variability in testing. However, this reduction is accompanied by higher average errors, suggesting that the model's predictions for unseen data may cluster more tightly around a less accurate mean. The R<sup>2</sup> score, which measures the proportion of variance in the target variable explained by the model, provides the most striking observation. The training R<sup>2</sup> score of 0.983 indicates that the model almost perfectly captures the variance in the training data,

demonstrating excellent fit. In contrast, the testing  $R^2$  score of 0.229 is significantly lower, showing that the model explains only a small fraction of the variance in the testing dataset. This dramatic drop indicates poor generalization and suggests that the model's structure might overfit the training data patterns, rendering it ineffective at capturing the underlying relationships in new data.



**Fig. 6** (a) Training and (b) testing of M5P model

The M5P model indicate strong performance on the training dataset, as proof by low RMSE and MAE, relatively high error variability, and a near-perfect  $R^2$  score. but, its performance on the testing dataset is markedly weaker, with higher RMSE and MAE, a lower standard deviation, and a significantly reduced  $R^2$  score. These results highlight the model's overfitting to the training data, leading to limited effectiveness in predicting unseen data. To enhance the

model's generalizability, steps such as pruning the decision tree, optimizing parameters, or using additional regularization techniques should be considered. Balancing the model's complexity to enhance both training fit and testing accuracy is essential for achieving robust and reliable predictive performance.

### 3.5 Linear regression

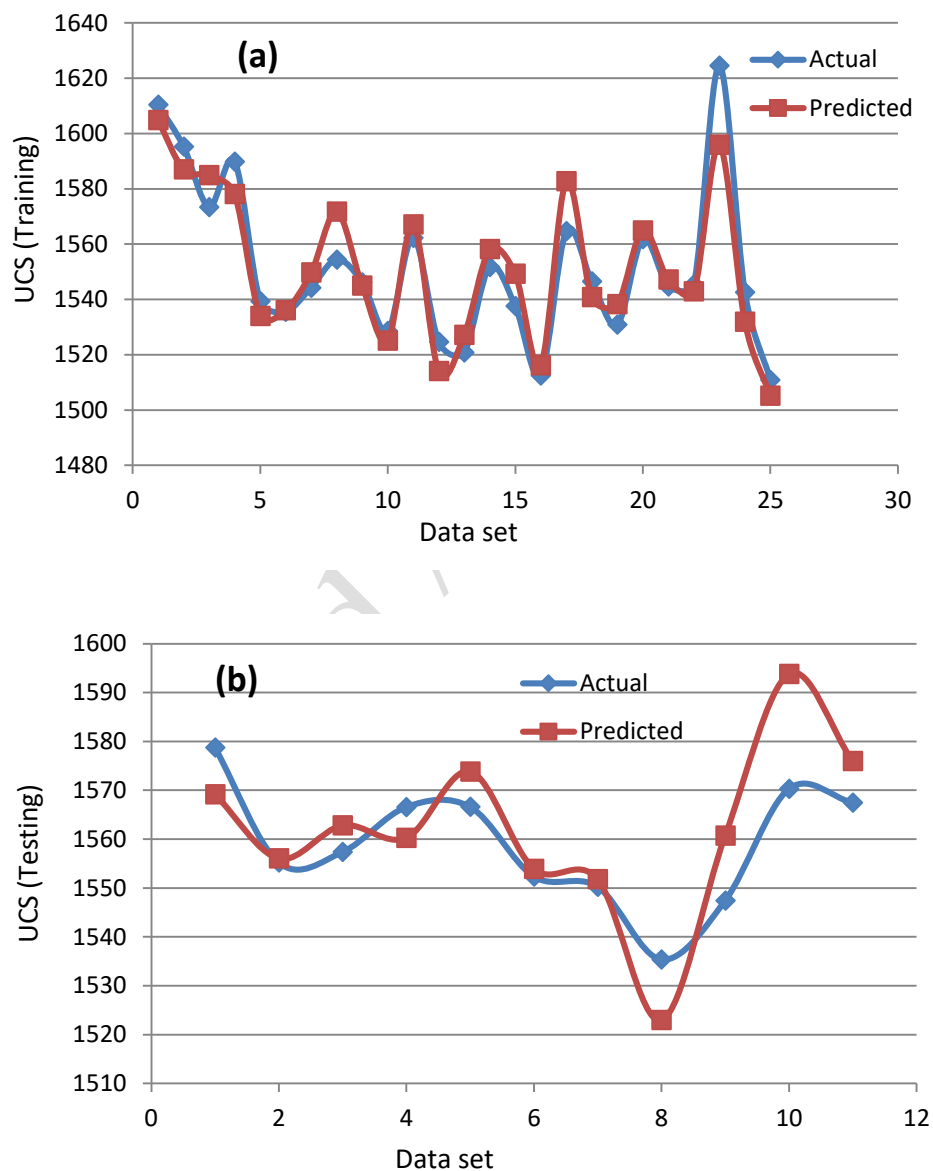
The performance metrics of the Linear Regression Forest model highlight its capability to foretell outcomes on both the training and testing datasets, offering insights into its accuracy, consistency, and generalizability. The evaluation metrics include Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Standard Deviation of errors, and the  $R^2$  score (Table 6).

Table 6 Linear regression model results for training and testing

	Training metrics	Testing metrics
RMSE	10.029	10.332
MAE	7.942	8.197
Standard deviation	10.029	9.868
$R^2$ score	0.872	0.233

Fig. 7 shows a plot of the linear regression model's outcome. The training (10.029) and testing (10.332) datasets have comparable values for the RMSE, which calculates the average magnitude of prediction errors. This closeness indicates that the model maintains consistent performance across both datasets, without a significant increase in error when applied to unseen data. At the same time the RMSE values indicate moderate prediction preciseness they also suggest room for improvement in minimizing errors. The average absolute error, or MAE, has a comparable pattern. The model's constant performance during the training and testing phases is further highlighted by the near value of the training MAE of 7.942 and testing MAE of 8.197. These MAE values indicate that the model's average prediction error is relatively stable, although slightly higher than desired for precise predictions. The standard deviation of errors, which reflects the variability in prediction errors, provides additional insight into the model's consistency (Behnood et al., 2017). The training standard deviation of 10.029 and the testing standard deviation of 9.868 are nearly identical, recommending that the error variability is similar in both phases. This consistency shows that the model does not exhibit extreme changes in

error across datasets, contributing to its robustness (Ali, 2024). The  $R^2$  score, or coefficient of determination, reveals the model's ability to explain the variance in the target variable. The training  $R^2$  score of 0.872 shows that the model captures a substantial portion of the variance in the training data, shows a good fit. However, the testing  $R^2$  score drops significantly to 0.233, indicating that the model explains only a small fraction of the variance in the testing dataset. This decline in  $R^2$  score suggests that while the model performs well on the training data, it struggles to generalize and capture the underlying relationships in unseen data.



**Fig. 7** (a) Training and (b) testing of linear regression model

The Linear Regression Forest model demonstrates regular error metrics across the training and testing datasets, as evidenced by similar RMSE, MAE, and standard deviation values. This

consistency recommend that the model does not overfit the training data. However, the sharp drop in the  $R^2$  score between training and testing indicates a challenge in explaining the variance in unseen data. This reduced descriptive power points to potential limitations in the model's structure or feature selection that hinder its ability to generalize effectively (Lin et al., 2016).

### 3.6 Non-linear regression

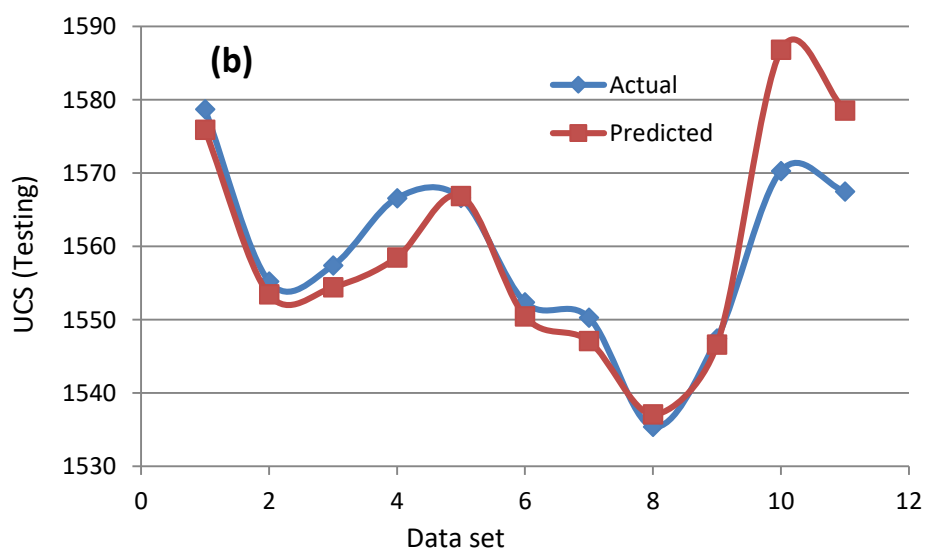
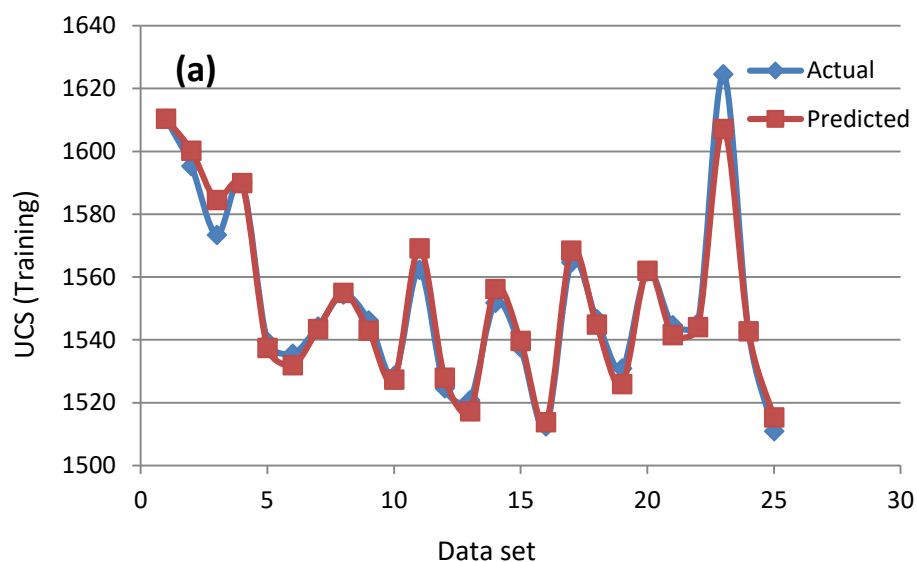
The performance metrics of the non-linear regression model give a detailed understanding of its forecasting accuracy and competency to generalize across training and testing datasets. Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Standard Deviation of errors, and the  $R^2$  score are shown in Table 7.

Table 7 Linear regression model results for training and testing

	Training metrics	Testing metrics
RMSE	5.095	6.729
MAE	3.439	4.647
Standard deviation	5.095	6.689
$R^2$ score	0.967	0.675

The result of the linear regression model has been plotted in Fig. 8. The RMSE, which measures the average magnitude of prediction errors, the training RMSE is 5.095, indicating that the model predicts outcomes with relatively low error during training. The testing RMSE of 6.729 is slightly higher, reflecting a modest increase in error when applied to unseen data. This difference suggests that while the model generalizes reasonably well, there is some loss of accuracy outside the training dataset (Zhou et al., 2024). The values show a good balance between fitting the training data and maintaining performance on new data. The MAE, which represents the average absolute error, complements the RMSE by focusing on the magnitude of errors without squaring them. A training MAE of 3.439 shows that, on average, the model's predictions are close to actual values in the training set. The testing MAE of 4.647, while a little larger, remains within a reasonable range. The relatively small difference between training and testing MAE indicates that the model's predictions are consistent and not significantly pretented by overfitting. The standard deviation of errors, reflecting the variability of prediction errors, offers additional context. The training standard deviation of 5.095 and the

testing standard deviation of 6.689 show a slight increase in error variability for unseen data. This difference recommend that while the model is consistent, there may be more fluctuations in its predictions for the testing set compared to the training set. Though the standard deviation values remain manageable, pointing to an overall reliable predictive performance. The  $R^2$  score, or coefficient of determination, is a critical metric for assessing how well the model explains the variance in the target variable. The training  $R^2$  score of 0.967 indicates that the model captures a significant portion of the variance in the training data, explaining an excellent fit. However, the testing  $R^2$  score of 0.675, though considerably lower, still reflects a strong ability to explain variance in unseen data(Zhou et al., 2024). This drop in  $R^2$  score between training and testing suggests that while the model generalizes reasonably well, there is room for improvement in capturing the underlying patterns in new data.



**Fig. 8** (a) Training and (b) testing of non-linear regression model

The non-linear regression model exhibits strong performance on the training dataset, as demonstrated by low RMSE and MAE values, low error variability, and a high  $R^2$  score. Its testing performance, while a little weaker, remains robust, with manageable increases in RMSE and MAE and a respectable  $R^2$  score. These results show that the model strikes a good balance between fitting the training data and generalizing to new observations, although further refinements, such as feature optimization or regularization techniques, could improve its predictive accuracy (Zhou et al., 2024).

### 3.7 Comparative discussions

The comparative study of the ANN, XGBoost, Random Forest, M5P, Linear Regression Forest, and Non-linear Regression models provides insights into their predictive capabilities, strengths, and weaknesses when applied to training and testing datasets. The results are assessed using key performance metrics such as RMSE, MAE, Standard Deviation, and  $R^2$  scores, alongside visualization tools like the Taylor diagram for model assessment. The ANN model indicates strong training performance with an  $R^2$  score of 0.971, indicating excellent fit and its ability to capture complex patterns. However, the testing  $R^2$  score of 0.589 reveals overfitting, where the model struggles to generalize effectively to unseen data. At the same time it captures some variability in the test dataset, significant improvements, such as regularization or architecture simplification, are needed to reduce the generalization gap. XGBoost exhibits near-perfect training results with an  $R^2$  score of 0.999 and minimal errors (RMSE: 0.005, MAE: 0.002). However, the testing  $R^2$  score drops to 0.798, and RMSE increases to 10.208, highlighting overfitting (Zhou et al., 2024). The model retains relatively strong predictive power on the testing dataset, but the discrepancy between training and testing metrics underscores the need for strategies like cross-validation or parameter tuning to enhance generalizability. Random Forest achieves robust training performance with an  $R^2$  score of 0.977 and low errors (RMSE: 2.995, MAE: 2.026). The testing  $R^2$  score of 0.853 indicates that it generalizes better than ANN and XGBoost. However, higher testing errors (RMSE: 11.075, MAE: 6.338) and increased error variability suggest overfitting. Its relatively consistent performance between training and testing phases makes it a reliable option, though further optimization could improve testing accuracy (Maabreh and Almasabha, 2024). The M5P model captures training variability well, with an  $R^2$  score of 0.983, low RMSE (3.652), and MAE (3.118). However, its testing  $R^2$  score plummets to 0.229, and errors increase significantly (RMSE: 10.360, MAE: 7.802), signaling

poor generalization. The stark contrast between training and testing metrics highlights severe overfitting(Habib and Okayli, 2024). Simplifying the model or implementing pruning techniques could enhance its applicability to unseen data. Linear Regression Forest maintains consistent performance between training and testing datasets, with close RMSE (10.029 vs. 10.332) and MAE (7.942 vs. 8.197) values. However, the sharp decline in  $R^2$  from 0.872 (training) to 0.233 (testing) indicates limited explanatory power for unseen data. This suggests that while the model avoids overfitting, it may lack the complexity to capture the underlying relationships in the data effectively. The Non-linear Regression model strikes a balance between training ( $R^2$ : 0.967, RMSE: 5.095) and testing performance ( $R^2$ : 0.675, RMSE: 6.729). It generalizes better than ANN and M5P, with relatively small differences in error metrics across datasets. The model effectively captures non-linear relationships and offers strong generalizability, making it a robust choice.

#### 4. Statistical analysis

Analysis of variance (ANOVA) results shows prime model fit. The R-Square value of 0.9991 recommend that 99.91% of the variability in the dependent variable is describe by the model, implying a nearly perfect correlation between the predictors and the response variable. The coefficient of variation (CV) of 0.0461 (or 4.61%) show low relative variability, indicating high precision and consistency in the model's predictions. The RMSE of 19.4788 represents the average prediction error, and while its significance depends on the scale of the data, it is quite low in relative terms given the high  $R^2$ . Lastly, the degrees of freedom (DF) of 3 typically corresponds to the number of predictors or groups being compared, suggesting that the model includes three explanatory factors or comparisons. Overall, these results demonstrate a highly reliable and accurate model.

Table 8 ANOVA outcomes

R-Square	Coefficient of variance	RMSE	DF
0.9991	0.0461	19.4788	3

#### 5. Conclusions

This study compares the performance of six predictive models: ANN, XGBoost, Random Forest, M5P, Linear Regression, and Non-Linear Regression using metrics such as RMSE, MAE,  $R^2$ , and standard deviation across training and testing datasets.

- The ANN model performs well on the training data ( $R^2 = 0.971$ ) but struggles with unseen data ( $R^2 = 0.589$ ), indicating overfitting.
- XGBoost achieves nearly perfect training results ( $R^2 = 0.999$ , RMSE = 0.005) but generalizes moderately (testing  $R^2 = 0.798$ ), reflecting reduced but still acceptable performance on new data.
- Random Forest shows strong training performance ( $R^2 = 0.977$ ) but a noticeable drop in generalization (testing  $R^2 = 0.853$ ).
- The M5P model demonstrates severe overfitting; its training  $R^2$  is 0.983, but the testing  $R^2$  plunges to 0.229.
- Linear Regression achieves consistent RMSE and MAE between training and testing but has a substantial drop in  $R^2$  (0.872 to 0.233), limiting its explanatory power.
- Non-Linear Regression strikes a good balance, with testing RMSE and  $R^2$  (6.729, 0.675) indicating reasonable generalization despite slightly reduced accuracy.

The Taylor diagram visually compares models using RMSE, standard deviation, and correlation, highlighting overfitting trends and generalization challenges. Non-linear regression and XGBoost emerge as robust contenders, while ANN and M5P require modifications for improved generalizability. Regularization, parameter tuning, or expanded datasets are suggested for enhancing performance.

## 6. Limitations

The study was conducted on a limited number of samples due to time and resource constraints, which may affect the generalizability of the findings. Long-term performance, including durability under environmental stressors, was not assessed in this phase. All tests were performed under controlled laboratory conditions. Techniques such as SEM and XRD, which could offer deeper insights into the stabilization mechanisms, were not conducted. ANN requires large datasets and is prone to overfitting, with interpretability being a major challenge. XGBoost, although accurate and robust, can be computationally intensive and sensitive to hyperparameter tuning. Random Forests offer good generalization but can become unwieldy with large numbers of trees and lack transparency in feature influence. M5P, a model tree algorithm, may not scale well with complex, high-dimensional data and can be sensitive to noise. Linear Regression assumes a linear relationship between variables, which oversimplifies many real-world problems and makes it ineffective for capturing complex patterns. Non-Linear

Regression, while more flexible, often involves complex equations and can struggle with convergence and overfitting, especially in the presence of noise or outliers.

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## Declarations

**Conflict of interest:** The authors declare that there is no conflict of interest regarding the publication of this paper.

**Data availability:** Data will be made available on request from the corresponding author.

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