IUBAT Review—A Multidisciplinary Academic Journal, 7(1): 90-122
https://doi.org/10.3329/iubatr.v7i1.74329

A Comparative Analysis of Machine Learning Approaches for Evaluating the Compressive Strength of Pozzolanic Concrete

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Keywords:
Compressive strength; pozzolanic concrete; machine learning; artificial neural networks; random forest; gradient boosting regressor.

Abstract
This study leverages machine learning techniques to predict pozzolanic concrete's compressive strength accurately. Using artificial neural networks (ANN), random forest (RF), and gradient boosting regressor (GBR) models trained on a dataset of 482 samples, the study divides the data into 70% training and 30% testing subsets with seven input parameters. Model performance is assessed through metrics like coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE). The RF model excels, achieving R^2 values of 0.976 in training and 0.964 in testing, along with the lowest RMSE (2.84 MPa) and MAE (2.05 MPa) during training and RMSE values of 7.81 MPa and MAE values of 5.89 MPa during testing, demonstrating superior predictive accuracy. Sensitivity analysis highlights the pivotal role of cement as an input parameter, contributing significantly to the model's accuracy. Employing K-fold cross-validation confirms the RF model's robustness with an average R^2 value of 0.959. This research underscores the RF model's reliability and effectiveness in forecasting pozzolanic concrete compressive strength, with practical applications for concrete optimization and construction practices, establishing it as the preferred choice compared to other machine learning models.

1. Introduction

Concrete is the second most widely used material in the world's construction industry (Gagg, 2014). Today, the most significant component of the industry business is concrete, which has a high variability of material owing to being composed of a variety of different materials (de-Prado-Gil *et al.*, 2022; Zaid *et al.*, 2022). Concrete is a crucial construction material due to its well-established mechanical properties, e.g., compressive strength (Rout, Biswas, & Sinha, 2023;

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Article received: November. 03, 2023 Revised and accepted: May 04, 2024 Published: June 30, 2024

Ziyad Sami *et al*., 2023). The construction industry has witnessed significant utilization of cement, with approximately 3.5 billion tons being employed. Furthermore, it is projected that cement usage will experience a considerable increase of 25% over the next decade in the context of concrete applications, and it is not sustainable due to carbon dioxide (CO_2) production (Meng *et al*., 2022). The increased cement usage may raise concerns regarding its environmental impact. It highlights the importance of implementing sustainable practices, such as using alternative sustainable cementitious materials to reduce emissions during production (Rout *et al*., 2023).

The use of pozzolanic and chemical admixtures in concrete offers numerous benefits, ranging from improved strength and durability to enhanced workability and reduced environmental impact on the construction industry in terms of constructing long-lasting and sustainable structures (Hossain *et al*., 2021; Sata *et al*., 2007). Pozzolanic materials, such as fly ash, silica fume, or slag, are commonly used as supplementary cementitious materials to enhance concrete properties (Juenger *et al*., 2012). These materials, such as fly ash and slag, are by-products of industrial processes, and utilizing them in concrete reduces the demand for primary cement production. This results in lower carbon dioxide (CO_2) emissions associated with cement manufacturing, reducing the carbon footprint (Vargas & Halog, 2015). Chemical admixtures, on the other hand, are substances added to concrete during mixing to modify its fresh or hardened properties (Mehta & Monteiro, 2014). It includes superplasticizers or viscosity modifiers, enhancing concrete cohesion and minimizing segregation and bleeding risk (Khayat & Mikanovic, 2012). Enhanced workability facilitates construction, particularly in complex structures or congested reinforcement areas (ACI Committee 212, 2010). However, adding pozzolanic and chemical admixtures to mixed-design concrete offers various benefits but can also pose challenges in controlling the resulting mixture's properties. While these admixtures can enhance certain aspects of concrete performance, their incorporation requires careful consideration and precise dosing to achieve the desired mechanical properties (Khayat *et al*., 2019; Sikora *et al*., 2020).

Furthermore, it is critical to recognize that attaining the necessary final strength of concrete strongly relies on proper mix design. Conducting several different laboratory experiments, which may be both time-consuming, error-associated, and expensive, is necessary to develop an optimized mix design model to gain proper concrete compressive strength (Shahmansouri *et al*., 2022; Sun *et al*., 2019; Zhang *et al*., 2019). However, the nonlinear solid relationship between the compressive strength and concrete components makes it challenging to derive an accurate regression expression for predicting the concrete compressive strength (Feng *et al*., 2020).

Many researchers focus on soft computing strategies to overcome this complexity today (de-Prado-Gil *et al*., 2022). In recent years, machine-learning techniques have emerged as promising computational approaches for predicting concrete properties and modeling (Deifalla *et al*., 2021; Marani & Nehdi, 2020). For resolving, especially concrete compressive strength prediction problems, several ML algorithms are used; among them, preferred ones are linear regression (LR), artificial neural networks (ANN), support vector machine (SVM), and random forest (RF) (Bassi *et al.*, 2023; Farooq *et al.*, 2021). However, several machine learning algorithms are used in material science, such as recycled aggregate concrete (Khademi *et al.*, 2016), silica fume concrete (A. Nafees *et al.*, 2021), concrete using blast furnace slag (Boğa et al., 2013; Sarıdemir et al., 2009), or concrete using fly ash (Chopra *et al.*, 2018).

Several researchers have explored the application of machine learning for predicting concrete compressive strengths. For instance, Ling *et al.* (2019) used a support vector machine to predict compressive strength based on concrete composition, achieving good results for various input scenarios. Kandiri *et al.* (2021) employed a modified ANN optimized with genetic algorithm (GA), salp swarm algorithm (SSA), and grasshopper optimization algorithm (GOA) techniques to predict the compressive strength of recycled aggregates, with SSA-ANN showing superior accuracy. Behnood & Golafshani (2021) utilized decision trees to predict concrete compressive strength with fly ash and other waste materials, producing reliable predictions for mechanical properties. In another research, Hassan *et al.* (2019) evaluated prediction methods for concrete compressive strength with metakaolin (MK) and silica fume (SF) admixtures. The ANN model, trained on 132 concrete samples, demonstrated high accuracy in predicting compressive strength (correlation coefficients: 0.996, 0.990, and 0.985 for training, validation, and test stages. The multiple linear regression (MLR) model achieved a lower correlation coefficient of 0.794, indicating ANN's superiority in predicting MK and SF admixture concrete strength. In recent years, research on predicting pozzolanic concrete compressive strength using GBR has garnered significant attention. Several studies have investigated the effectiveness of this machine learning technique, showcasing its accuracy and reliability in making predictions (Eyo *et al.*, 2022; Gogineni *et al.*, 2023). Turland *et al.* (2018) explored the application of GBR and conducted a comprehensive comparison with other regression methods. Their findings demonstrated the superiority of GBR in terms of accuracy and predictive power. Similarly, Zhang *et al.* (2021) conducted a study to predict concrete strength using GBR, RF, and SVR. The results consistently favored GBR, outperforming the other two algorithms and providing more accurate predictions. Furthermore, Zhu *et al.* (2021) compared GBR with XGBoost and LightGBM. Their results indicated that GBR attained higher R^2 values, showcasing better explanatory power and overall predictive performance. Collectively, these studies present compelling evidence for the effectiveness of GBR in predicting pozzolanic concrete compressive strength. Its remarkable performance and potential as a valuable tool in the construction industry make it an essential asset for optimizing mix designs and ensuring concrete quality.

This research aims to evaluate and compare the effectiveness of three machine learning algorithms' effectiveness in predicting pozzolanic concrete's compressive strength. Lin & Wu (2021) investigated the ANN algorithm using 85% training and

15% testing data, while Kao *et al.* (2018) utilized ANN with 96% training and 4% testing data from 482 samples. Going beyond previous ANN-centric approaches, this study employs advanced models that offer enhanced predictive capabilities and insights into key factors. This choice is substantiated by their proven applicability in concrete property prediction tasks, as documented in relevant literature. ANNs excel in capturing intricate nonlinear relationships within data, RF demonstrates proficiency in handling mixed data types and elucidating feature importance, while GBR excels in capturing complex interactions. By comparing these algorithms, the study seeks to uncover their respective strengths and weaknesses in the context of pozzolanic concrete's compressive strength prediction, contributing to the optimization of predictive modeling techniques in concrete engineering. Incorporating ANN and two ensemble algorithms with a split of 70% training and 30% testing data contributes to understanding concrete behavior for improved production decisions and sustainability considerations. Performance evaluation metrics, including the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE), were employed to assess the models.

In this study, several novel aspects contribute to the existing knowledge on predicting the compressive strength of pozzolanic concrete. Firstly, we employ three distinct machine learning models—Artificial Neural Networks (ANN), Random Forest (RF), and Gradient Boosting Regressor (GBR)—to comprehensively assess their predictive capabilities. The focus on the ensemble nature of the Random Forest model is a distinctive feature, showcasing its superiority over traditional models like ANN and GBR. Additionally, the study meticulously evaluates the influence of various input parameters, specifically emphasizing the pivotal role of cement and pozzolanic materials in accurate strength predictions. The insights gained from this research provide a nuanced understanding of how these factors impact concrete mix designs. Moreover, the study's approach to addressing biases in existing literature data and exploring a broader range of algorithmic options contribute novel perspectives to the field. This study offers a fresh and comprehensive examination of machine learning applications in predicting pozzolanic concrete strength, presenting valuable insights for academia and the concrete industry.

Furthermore, this study goes beyond its immediate focus and has implications for material science overall. It delves into how algorithms and material properties interact, offering a foundation for precise predictive models. Key takeaways highlight the importance of cement and pozzolanic materials in predicting outcomes, providing valuable insights for improving concrete mixes and construction methods. This unique perspective adds a new dimension to existing research, thoroughly exploring machine learning models in the specific context of predicting pozzolanic concrete strength. Additionally, the proposed machine learning system for designing concrete mixes holds promise for generating solutions accepted in engineering. It caters to user-defined parameters like required strength, pozzolanic admixture replacement rates, and material costs, making it a versatile tool for estimation, prediction, decision-making, and diagnosis.

2. Material and Methods

2.1 Data Collection

In this research, a substantial amount of 482 experimental data on pozzolanic concrete compressive strength was collected to develop prediction models. The data was obtained from the following study by Shen (2013) consisting of 482 concrete compressive strength test results. This study utilized Ordinary Portland Cement (OPC) CEM Type-I, as the binder to formulate 12 concrete mix designs based on the ACI 211.1 code. The dataset is available for download from the NCTU library website (https://ir.nctu.edu.tw/handle/11536/71533). The concrete samples were tested with seven factors mixed in 1m³ concrete, including water, cement, fine aggregate, coarse aggregate, hearthstone, fly ash, and superplasticizer. The compressive strength of the concrete was obtained through standard compressive test procedures on the cylinder specimens. The experimental data comprises eight parameters in total, and Table 1 presents the name, unit, minimum/maximum values, mean value, variance, and standard deviation of these parameters. Furthermore, histograms were generated for each parameter utilizing the distribution fitting function in OriginPro 2018 software. These histograms displayed the parameter distribution and incorporated fitting of corresponding normal distribution curves, as depicted in Figure 1.

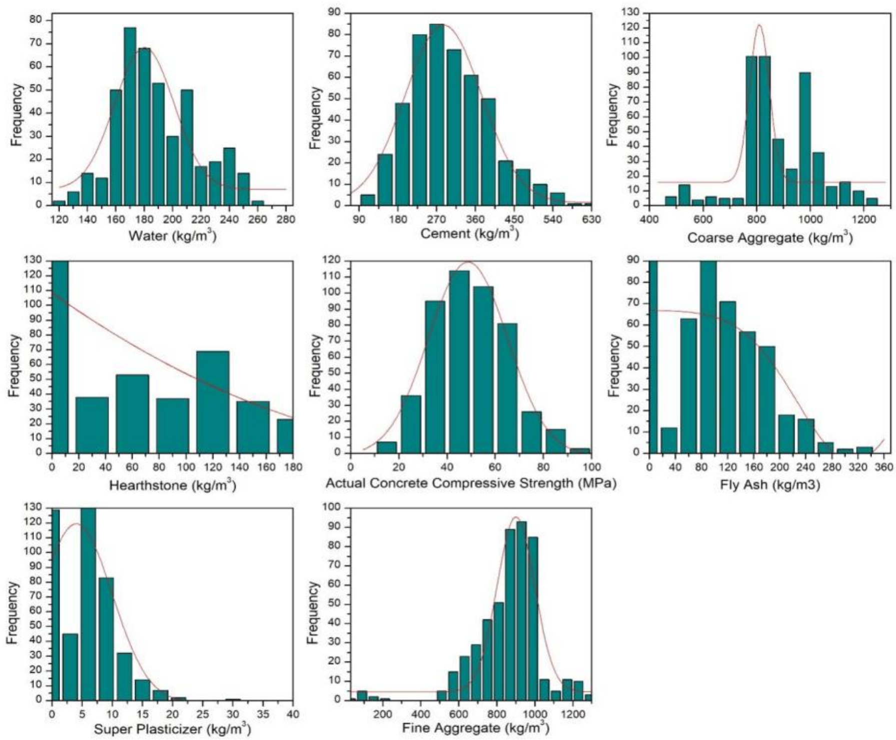


Figure 1: Normal distribution curve of the parameters

In this research, before initiating the learning procedure, it is essential to identify the input and output variables for predicting concrete compressive strength accurately. The ingredients used in the concrete mix and the curing time are recognized as influential factors that impact the final compressive strength of the concrete. Consequently, the study considers seven input variables ($X = X1, X2, ..., X7$) and one output variable (Y).

The input variables ($X1$ to $X7$) represent the ingredients mixed in 1m³ concrete, which include water, cement, fine aggregate, coarse aggregate, hearthstone, fly ash, and superplasticizer. These factors significantly contribute to the concrete's properties and strength. In contrast, the output variable (Y) corresponds to the concrete's compressive strength, which is the target variable for prediction. To provide a comprehensive understanding of the dataset, Table 1 presents the list of input and output variables and their respective ranges of values.

Table 1: Numerical characteristics of the parameters

Parameter	Range	Mean	Variance	Standard Deviation	Type
X_1:Water (kg/m^3)	116.5-255	185.0	851.4	29.18	Input
X_2:Cement (kg/m^3)	74-599	280.8	8412.0	91.72	Input
X_3:Fine Aggregate (kg/m^3)	30-1293	829.7	31014.7	176.11	Input
X_4:Coarse Aggregate (kg/m^3)	436-1226	854.3	20942.0	144.71	Input
X_5:Hearthstone (kg/m^3)	0-375	74.8	6319.4	79.49	Input
X_6:Fly Ash (kg/m^3)	0-330	91.5	4664.3	68.30	Input
X_7:Super Plasticizer (kg/m^3)	0-27.17	4.5	16.8	4.09	Input
Y: Actual Concrete Strength (MPa)	5.66-95.3	45.0	235.1	15.33	Output

2.2 Dataset Pre-processing

Standardizing input and output parameters is essential to ensure meaningful comparisons and prevent errors arising from differing scales (Schielzeth, 2010). This statistical standardization measure enables machine learning estimators to work effectively with features that resemble standard normal distributions (Duan *et al.*, 2020). The sklearn library in Python provides the Standard Scaler function, which calculates the z-score, or standard score, for cluster analysis. By applying this approach, the study achieves standardized variables and reliable results. Equation 1 represents the standard score formula used for the sample data (Saisana, 2014).

$$z = (a - \mu)/s \tag{1}$$

Where, z is the standard score (z-score), a is the sample data, μ is the mean of the sample data, and s is the standard deviation of the sample data. The z-score obtained reflects the extent to which the raw score deviates from the mean in terms of standard deviations. A positive z-score signifies a raw score above the mean, while a negative z-score signifies a raw score below the mean.

2.3 Data Splitting

The classical approach of dividing the database was employed to ensure robustness, using 70% (337 samples) of the entire experimental dataset as the training set and the remaining 30% (145 samples) as the test set. The algorithms were then built on the training datasets and tailored to address the problem. Applying proposed algorithms for concrete prediction empowers one to gain valuable insights into the factors influencing concrete strength and make informed decisions during concrete mix design and optimization.

2.4 Methodology

Figure 2 illustrates the schematic representation of the proposed methodology. It visually depicts the step-by-step process and the interconnected components used in the study.

Initially, the available experimental dataset is divided into five subsets. Four subsets are utilized for constructing the prediction model using a robust learner algorithm, while the fifth subset is reserved exclusively for model validation. This approach ensures that each subset takes a turn as the validation set, with the model being trained and tested five times, each time using a different subset as the validation data. Ultimately, the performance metrics obtained from each validation iteration are aggregated, providing a more robust assessment of the model's generalization capacity and minimizing the risk of overfitting (Li *et al.*, 2023a). This systematic procedure aids in optimizing the model's predictive accuracy and reliability by accounting for variations in dataset composition and enhancing its potential for practical, real-world applications.

For the sensitivity analysis, a methodical approach to gauging the influence of input parameter fluctuations on model outcomes involves several vital steps (Li *et al.*, 2021). First, a representative model, such as the best-fit model in this context, is chosen. Second, the specific input parameters expected to impact the model's predictions substantially are identified. Subsequently, a range of values for each selected parameter is defined. The model is then executed multiple times, varying the parameter values to create a dataset of resultant output predictions. The variations in output predictions across different parameter values are scrutinized, often utilizing statistical measures like correlation coefficients or constructing response surfaces. The outcomes are meticulously interpreted to discern the relative significance of each input parameter on the model's ultimate output. This comprehensive sensitivity analysis process significantly enhances comprehension of parameter sensitivities, aids in optimizing model performance, and facilitates informed decision-making grounded in the varying influences of individual variables. The method of K-fold cross-validation involves several sequential steps to improve prediction model performance while mitigating bias due to random sampling (Chou *et al.*, 2014).

In this study, the process involved conducting a comprehensive hyperparameter tuning or optimization, often referred to as a grid search or randomized search. During this procedure, a predefined range of hyperparameter values was systematically explored, and the combinations that yielded the best performance metrics, such as R^2, RMSE, and MAE, were selected as the optimal configuration for each model. This method ensures the models are fine-tuned to maximize their predictive accuracy and generalizability to unseen data. The specific hyperparameters tuned would depend on the characteristics of each algorithm; for instance, in Random Forest, parameters like the number of trees and maximum depth were likely considered. The transparency and reproducibility of this hyperparameter tuning process contribute to the models' reliability and robustness in predicting pozzolanic concrete's compressive strength.

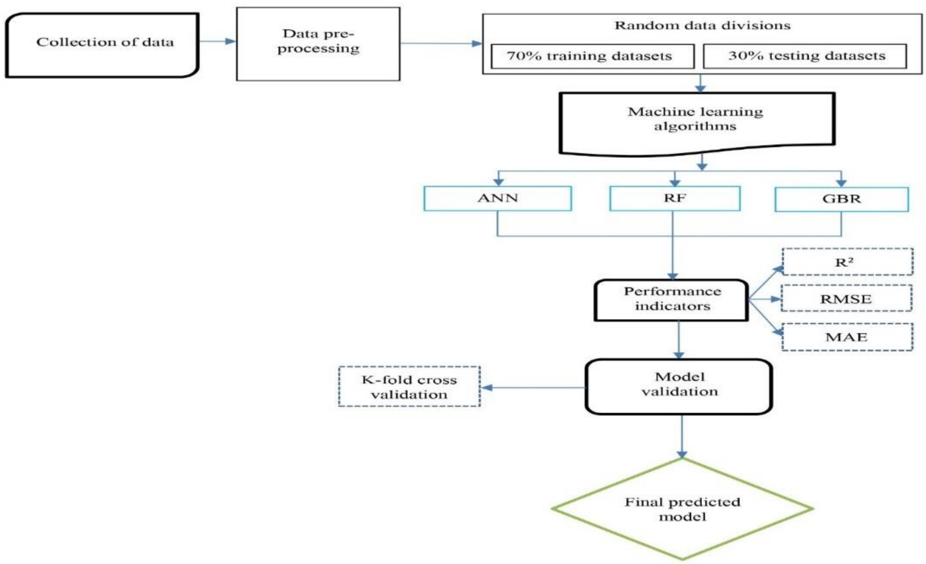


Figure 2: Proposed methodology of the study

2.4.1 Artificial Neural Networks

The Artificial Neural Network (ANN) is a sophisticated analytical tool used to forecast the output variable based on input variables (Dantas *et al*., 2013). Inspired by the biological neural architecture of animal brains, the ANN consists of interconnected neurons, weights, and biases. This intricate structure enables the development of a model that learns from experience to anticipate future results (Thapa, Sharma, & Halder, 2022). The ANN has gained widespread acceptance across various fields, including pattern recognition, time series forecasting, and more (Sezer *et al*., 2020). For successful implementation, the ANN algorithm's effectiveness relies on appropriate learning algorithms, activation functions, and an optimal number of neurons in the hidden layer (Imam, Salami, & Oyehan, 2021).

In this study, the Back Propagation (BP) algorithm, proposed by (Rumelhart, Hinton, & Williams, 1986), is used for the artificial neural network. The BP algorithm adjusts the weights and biases based on the difference between predicted and actual outputs, iteratively minimizing the error (Basheer & Hajmeer, 2000; Kewalramani & Gupta, 2006). The neural network architecture comprises input, hidden, and output layers. Specifically, the concrete mix proportioning database used in this study involves seven neurons in the input layer and one neuron in the output layer. Four hidden layers establish connections between these layers, where each neuron is unidirectionally linked to all neurons in the preceding layer, enabling the signal to propagate from input to output across the hidden layers. Despite its computational intensity, the ANN offers robust generalization capabilities, making it suitable for handling complex, limited, or noisy datasets. The schematic representation of the Back Propagation-ANN utilized in this research is illustrated in Figure 3.

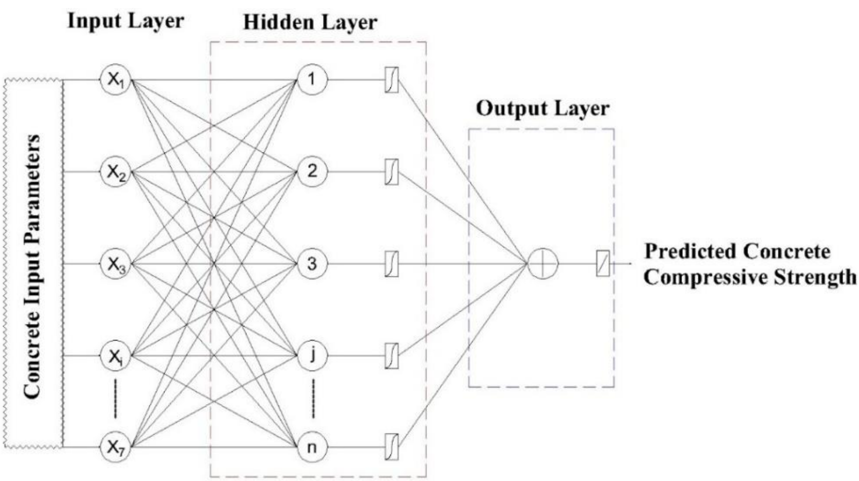


Figure. 3: Illustration of a three-layer Artificial Neural Network (ANN) model

2.4.2 Random Forest Regression

Random forest (RF) is a robust ensemble machine learning algorithm that builds upon the decision tree model within the bagging framework, initially introduced by Breiman (2001). The algorithm constructs multiple decision trees using random subsets of the dataset and combines their predictions to obtain the final result. Each decision tree learns from different features and data points, creating a diverse model set that yields robust predictions. This ensemble learning approach mitigates the risk of overfitting and enhances the model's generalization capability (Breiman, 2001; Liaw & Wiener, 2002).

Therefore, using random forest in this study to evaluate concrete compressive strength brings significant benefits. The random forest can effectively capture complex nonlinear relationships among input variables, such as mix proportions, curing conditions, and aggregate properties often present in concrete mixtures. This enables the model to accurately capture the intricate interdependencies of these variables (Han, Gui, Xu, & Lacidogna, 2019; Pengcheng, Xianguo, Hongyu, & Tiemei, 2020). Furthermore, the random forest does not impose stringent assumptions regarding data distribution, offering flexibility in modeling real-world, concrete scenarios (Cutler et al., 2007; Prasad, Iverson, & Liaw, 2006). Moreover, random forest handles many input variables and automatically selects the most informative features, simplifying the modeling process and enhancing interpretability (Breiman, 2001; Liaw & Wiener, 2002). Python Colab, with its support for decision tree-based algorithms, enables the utilization of libraries like Scikit-learn. Users can import the necessary libraries, pre-process their data, and implement regression tree models directly within Colab notebooks. The interactive nature of Colab facilitates model training, visualization of decision trees, and performance evaluation, providing a comprehensive environment for working with these models. In random forest regression, the algorithm generates results from multiple decision trees and calculates their average value. The regression equation for the random forest algorithm analysis is summarized as follows (Wang *et al.*, 2022):

$$\bar{\mathrm{M}}(\mathrm{x}) = \frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{n}}\left(\mathrm{y_i}(\mathrm{x}, \theta_{\mathrm{n}})\right) \tag{2}$$

Where, $\bar{M}(x)$ is the prediction result, y_i is aggregating the predictions of individual decision tree, θ_n an independent distributed random variable that determines the growth process of a single decision tree, N is the total number of decision trees.

2.4.3 Gradient Boosting Regressor

The Gradient Boosting Regressor (GBR) is a machine learning algorithm belonging to the ensemble learning method family. It is particularly effective for predicting the compressive strength of pozzolanic concrete due to its ability to handle complex relationships and non-linearities in the data (Ikeagwuani, 2021; Phoeuk & Kwon, 2023).

For this study, the first step in using GBR is to gather and pre-process the data using libraries like Scikit. The dataset includes input features or parameters, such as cement, water, fine aggregate, coarse aggregate, pozzolanic material type, and other mixed design characteristics. The target variable is the compressive strength of the pozzolanic concrete samples. The dataset is split into a training set (typically 70% of the data) and a testing set (the remaining 30%) to evaluate the model's performance. The GBR is an ensemble learning technique, combining multiple weak learners (usually decision trees) to form a strong predictive model (Koya *et al.*, 2022). The model is constructed in an iterative manner. Each iteration, or boosting round, fits a decision tree to the residuals (the differences between the predicted and actual compressive strength values) of the previous round (Marani & Nehdi, 2020). Decision trees are used as weak learners in GBR. A decision tree splits the data into smaller subsets based on the input features to create a set of prediction rules (Nyirandayisabye *et al.*, 2022). However, individual decision trees tend to have high variance and may over fit the training data. The boosting technique in GBR addresses this issue by combining the predictions of multiple decision trees to improve accuracy. During each boosting round, the GBR model identifies the samples with high prediction errors and assigns them higher weights. This focuses the subsequent decision trees on the previously poorly predicted samples, allowing the model to learn from its mistakes and reduce errors (Gayathri *et al.*, 2022; Marani *et al.*, 2023).

After training the GBR model, it is evaluated using the testing set. Performance metrics such as R^2, RMSE, and MAE assess the model's accuracy and ability to generalize to unseen data. The strength of the GBR lies in its ability to capture complex relationships between the input parameters and the compressive strength of pozzolanic concrete. It can handle both numerical and categorical features and automatically handle missing data (J.-F. Jia *et al.*). Additionally, GBR is less prone to overfitting than individual decision trees, as the ensemble approach helps improve generalization (Marani *et al.*, 2020). Overall, the GBR is a robust and effective algorithm for predicting the compressive strength of pozzolanic concrete, and its performance can be further enhanced through careful implementation and hyperparameter tuning (Salami *et al.*, 2021).

2.4.4 Performance Assessment

The study evaluates the machine learning model’s accuracy using standard performance measurements, including R^2, RMSE, MAE, and SD. These measurements reflect the level of linear correlation between the predicted and actual data values (Li *et al.*, 2023b). Generally, the predicted accuracy will be the highest value among models when its coefficient of determination R^2 value is near 1 (Badarloo, Kari, & Jafari, 2018). Furthermore, RMSE and MAE demonstrate the deviation between the predicted and actual values (Tran et al., 2021). The RMSE is an efficient measure of data change and remains unaffected by the unit and size of predicted and actual values (D. Yao *et al.*, 2021). On the other hand, the MAE calculates the average error using the absolute difference between actual data and predicted results (Wang *et al.*, 2022).

The highest R^2 is closer to 1, the lowest RMSE, and the MAE values are near zero, which shows the selected model's higher accuracy. The mathematical expression for these three evaluation metrics is shown in Equations (3) to (5) (Rahman *et al.*, 2021).

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(p_y - o)^2}{\sum_{i=1}^{n}(o - \bar{o})^2} \tag{3}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|(p_y - o)\right| \tag{4}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[(p_y - o)\right]^2} \tag{5}$$

Where, n is the number of observations, p_y is the value predicted by the model, o is the observed value, and $\bar{o}$ is the average of the actual values.

Moreover, Taylor diagrams were utilized as a visual representation to compare the predicted target variable with the observed results (Taylor, 2000). These diagrams incorporate statistical measures such as the correlation coefficient, and standard deviation ratio (Chen *et al.*, 2022). The algorithm outputs can be evaluated concerning the actual results by analyzing these statistics. Taylor diagrams offer a quick and intuitive assessment of the agreement between the model predictions and observations, providing insights into the model's potential over or under-prediction tendencies (Shubham *et al.*, 2023). Additionally, the sensitivity analysis of the strength-predicting models was employed to determine the importance of the feature of the input parameters on the output. This analysis allows assessing the influence and significance of the various input parameters on the predicted strength values (Nguyen *et al.*, 2023).

3. Results and Discussions

3.1 Correlation Analysis by Heat Map

The Pearson correlation matrix and statistical analysis are vital in developing predictive models for concrete compressive strength (Gupta & Sihag, 2022). The model's accuracy can be significantly improved by measuring the degree of linear correlation between input and output variables (Kim, Pham, Park, Oh, & Choi, 2020). In Figure 4, two-dimensional heat maps illustrate the correlation analysis between input and output variables. The correlation values are represented in different colors, corresponding to the numerical values within the range of [-1, 1]. A higher absolute coefficient value indicates a stronger correlation, while a value closer to 0 suggests a weaker correlation (Wang, Kang, Liu, Su, & Li, 2022). The correlation analysis reveals that the actual concrete strength shows positive correlations with cement, coarse aggregate, hearthstone, and superplasticizer, while it exhibits negative correlations with water, fine aggregate, and fly ash. Notably, the correlation between actual concrete strength and cement is 0.46, whereas the correlation between fine aggregate and coarse aggregate is the most negative, at -0.61. Based on the provided instruction, the Pearson correlation matrix analysis indicates that no variables show a correlation greater than 0.80, suggesting a lack of multicollinearity (de-Prado-Gil *et al*., 2022). This analysis, facilitated by the standard scaler function in the sklearn library of Python, provides valuable insights into the relationships between input variables and concrete compressive strength in the pozzolanic concrete mix design.

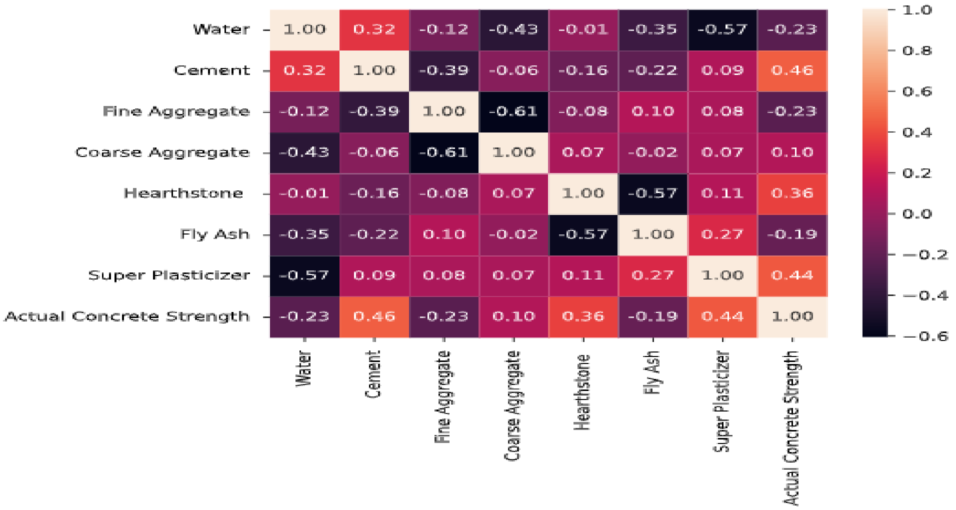


Figure 4: Heat map for Pearson correlation analysis graph of input and output variables

3.2 Model Prediction Results

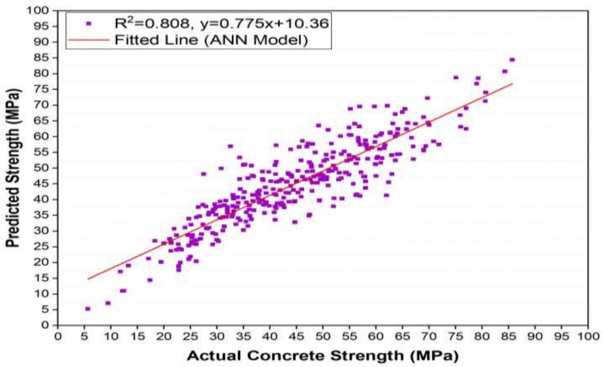
The primary objective of model training is to create a model capable of effectively generalizing and accurately predicting unseen data. In this investigation, regression plots (Figure 5(a), 5(b), and 5(c)) illustrate the relationship between actual concrete compressive strength and model predictions for the three models. During the training phase, all three models exhibited challenges in capturing the intricate patterns within the observation data, leading to a notably high correlation coefficient with the predicted outcomes. Specifically, the RF and GBR models displayed strong correlation values during training, reaching 97.5% and 94.7%, respectively, indicative of robust generalization.

Based on the analysis based on regression Figure 5, the RF model is the most effective and robust approach for predicting the compressive strength of pozzolanic concrete. Overall, the RF outperformed GBR and ANN for predicting the compressive strength of pozzolanic concrete due to several key factors. RF employs an ensemble learning technique that combines multiple decision trees, reducing overfitting and improving generalization on unseen data by capturing complex relationships more effectively. It is robust to overfitting as it randomly selects data subsets and features during tree building, mitigating the risk of memorizing noise in the training data (Sarker, 2021).

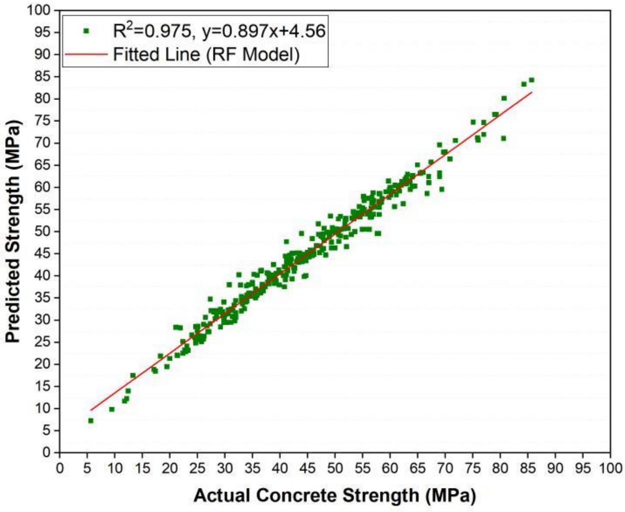
Additionally, the Random Forest (RF) model's superiority lies in its ensemble learning approach, which combines multiple decision trees to achieve robust and accurate predictions. This ensemble nature mitigates overfitting, a common challenge in machine learning, and enhances the model's ability to handle complex, non-linear relationships within the data. Unlike single decision trees, the RF model averages predictions from various trees, resulting in a more stable and reliable outcome. Also, the diversity of trees created by RF's randomness enhances its predictive performance compared to GBR, which builds trees sequentially, potentially leading to correlated trees. RF's simplicity in hyperparameter tuning requires fewer parameters to optimize, leading to quicker convergence to optimal settings. This approach contributes to improved generalization and predictive accuracy, making RF particularly effective for the concrete compressive strength prediction task compared to other models like ANN and GBR.

Furthermore, the decision tree's ability in RF to handle nonlinear relationships in the data contributes to its superior performance in predicting complex characteristics like compressive strength in pozzolanic concrete. Overall, RF's ensemble method, robustness to overfitting, simplicity in tuning, efficient implementation, and handling of nonlinear relationships collectively make it the preferred algorithm for accurate predictions.

(a)



(b)



(c)

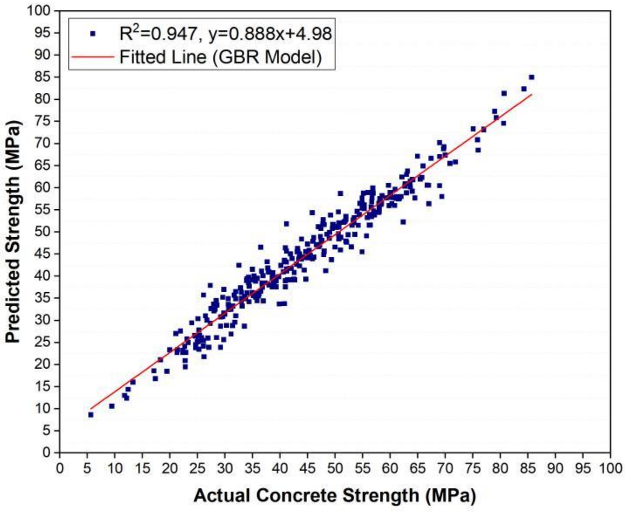


Figure 5: Regression plots of training dataset; (a) ANN model, (b) RF model, and (c) GBR model

3.3 Performance Analysis Between ML Algorithms

Assessing a prediction model's performance involves measuring the disparity between predicted outcomes and actual values. Performance indicators such as R^2, RMSE, and MAE are employed to ensure an objective evaluation. The selected model demonstrated accurate predictions during the training phase. A comparative analysis of three machine learning models (ANN, RF, and GBR) for pozzolanic concrete strength prediction is detailed in Table 2, encompassing evaluation metrics for training, testing, and overall datasets.

The ANN model achieved an R^2 of 0.808 and 0.799 on the training and testing datasets, respectively, indicating moderate predictive performance. However, the RMSE for training and testing is 6.54 and 7.22, respectively, while the MAE is 4.95 for training and 5.74 for testing, demonstrating moderate predictive accuracy. The overall dataset shows an RMSE of 6.76 and an MAE of 5.21, with a standard deviation 13.14. However, the RF demonstrated superior performance with an impressive R^2 of 0.976 on the training dataset and 0.964 on the testing dataset, showcasing its ability to capture complex patterns and relationships. It also achieves the lowest RMSE for training (2.84) and testing (7.81), as well as the lowest MAE for training (2.05) and testing (5.89), showcasing its accuracy. The overall dataset's RMSE is 2.85, and the MAE is 2.03, with a standard deviation 13.42. Moving to GBR, it exhibits an R^2 of 0.947 for training and 0.816 for testing, showing a good correlation with the target variable. However, it had higher RMSE and MAE values compared to RF but lower than ANN, implying better predictive accuracy than ANN but falling slightly behind RF.

Table 2: Summary of performance index of each model

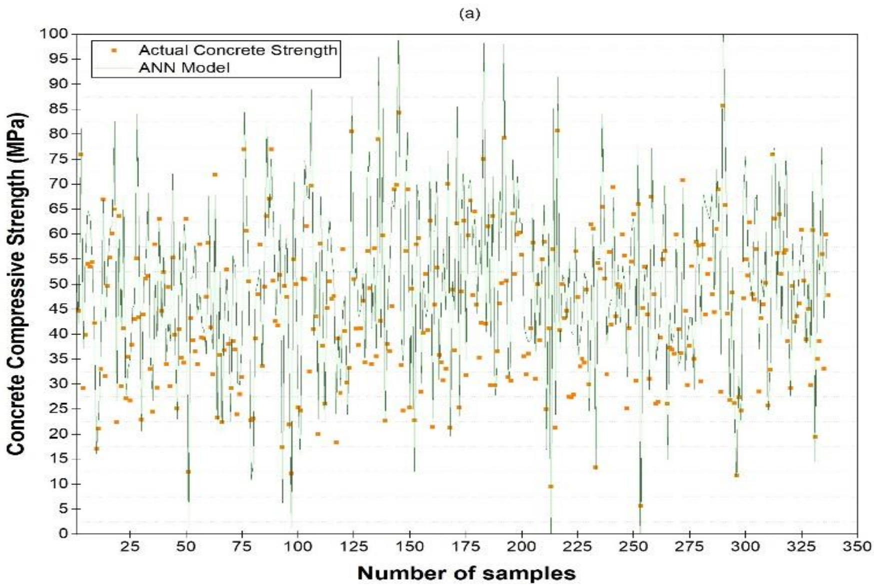
Model Name	R^2			RMSE			MAE			Standard Deviation		
	Training (70%)	Testing (30%)	Overall Dataset	Training (70%)	Testing (30%)	Overall Dataset	Training (70%)	Testing (30%)	Overall Dataset	Training (70%)	Testing (30%)	Overall Dataset
ANN	0.808	0.799	0.805	6.54	7.22	6.76	4.95	5.74	5.21	13.14	14.34	13.47
RF	0.976	0.964	0.965	2.84	7.81	2.85	2.05	5.89	2.03	13.42	12.63	13.95
GBR	0.947	0.816	0.927	3.43	6.89	4.12	2.62	5.28	3.15	13.61	13.69	13.77

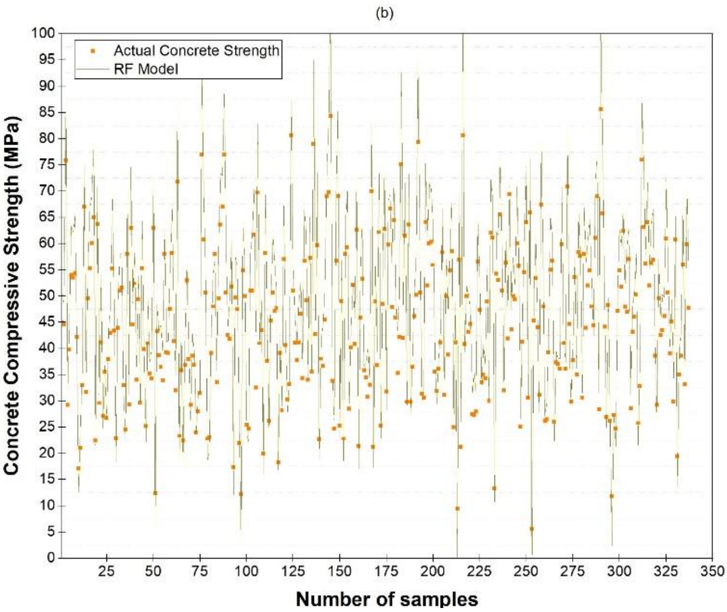
The performance comparison between predicted and actual concrete strength outputs is visualized in Figure 6. The scatter plots in Figure 6(a), 6(b), and 6(c) depict the prediction results of the ANN, RF, and GBR models, respectively. Upon analyzing the post-training performance indices, it's evident that the RF model demonstrates superior performance. The RF model exhibits a higher R^2 than the ANN and GBR models, showing an advantage of 1.20% and 1.03%, respectively.

Similarly, regarding RMSE, the RF model excels with a value of 2.84, showcasing a better performance than the ANN and GBR models by 2.30% and 1.20%, respectively. Additionally, the RF model stands out with the lowest MAE values among all models, measuring at 2.05.

The study evaluated three distinct machine learning models: ANN, RF, and GBR, focusing on their performance in predicting the compressive strength of pozzolanic concrete. RF emerged as the top performer among these models due to its ensemble approach. RF combines multiple decision trees, which helps address overfitting issues often encountered in complex prediction tasks. This attribute enhances the model's robustness and ability to generalize well to new data (Sun *et al.*, 2021). In contrast, ANN can be sensitive to hyperparameter tuning and may become trapped in local minima during training. This makes their performance less consistent, especially in cases where the dataset is limited or noisy (Ouyang *et al.*, 2021).

Additionally, ANN architecture's complex and interconnected nature may not always suit the nuances of pozzolanic concrete strength prediction, which involves intricate relationships between various input parameters. Furthermore, GBR is another popular machine learning technique, yet in this study, it was outperformed by RF. GBR builds an ensemble of weak learners sequentially, and while it can handle non-linearity to some extent, its performance may lag when dealing with intricate interactions among factors influencing pozzolanic concrete strength. For the specific context of predicting pozzolanic concrete compressive strength, the ensemble nature of RF, coupled with its ability to handle complex relationships and mitigate overfitting, makes it the most suitable and accurate choice among the evaluated models.





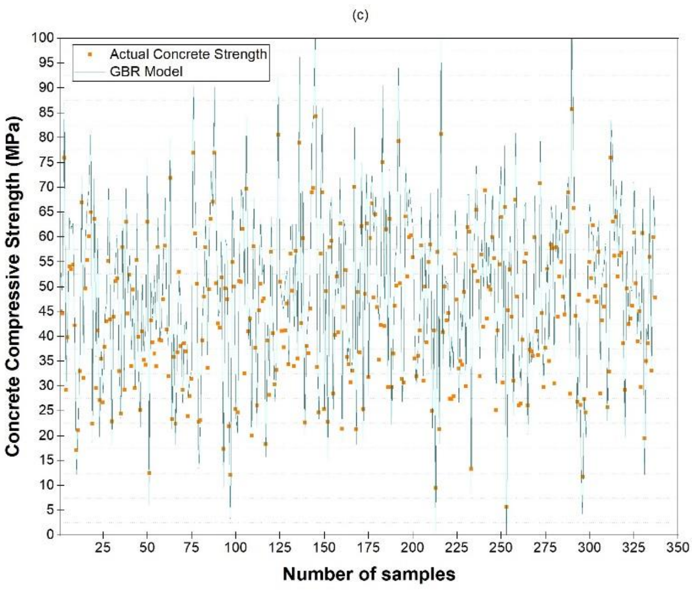


Figure 6: Comparison of measured compressive strength with predictions for training dataset; (a) ANN model, (b) RF model, and (c) GBR model

Figure 7 analyzes the relative error (RE) between the actual and predicted values. The study employed various ML algorithms to identify patterns in the actual data and compared the variation in predicted datasets with the ML models. A higher difference between the actual dataset and ML algorithms indicates higher errors. During the training phase, 337 samples were tested, and each sample's relative error (RE) percentage was calculated. The RE value serves as a measure of prediction model stability and indicates the extent of errors between the predicted and actual values. Analyzing Figure 7 shows that the RF model exhibits the highest stability, with an absolute error percentage of 4.70%.

On the other hand, the ANN and GBR models demonstrate relatively higher absolute errors, with error percentage values of 13.31% and 6.70%, respectively. This analysis confirms that the RF model outperforms the other ML algorithms in terms of prediction stability and accuracy, making it the most reliable choice for this specific regression problem. This analysis confirms that the RF model outperforms the other ML algorithms regarding prediction stability and accuracy, making it the most reliable choice for this specific regression problem.

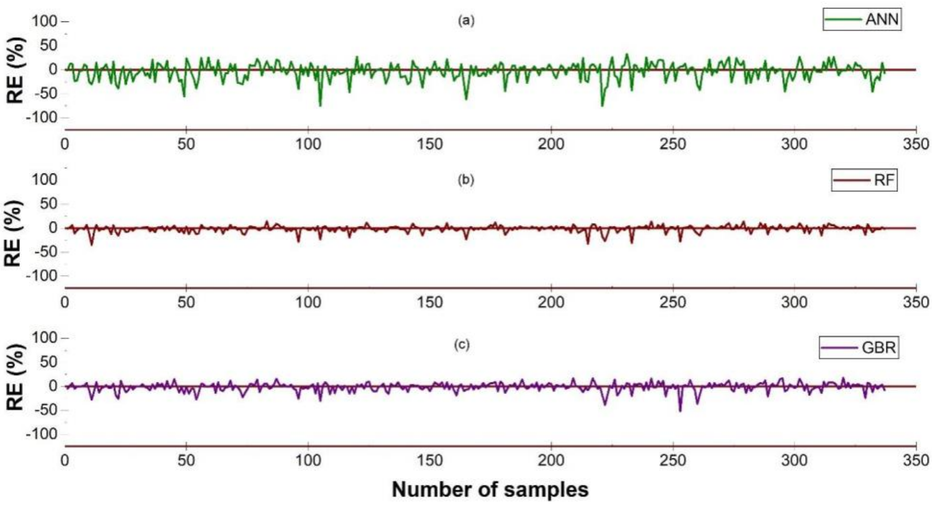


Figure 7: Relative error (RE) plots for the training dataset samples; (a) ANN model, (b) RF model, and (c) GBR model

3.4 K Fold Cross-Validation Analysis for Best-Predicted Model

The results of the five-fold cross-validation demonstrate a strong correlation between the predicted and actual compressive strength values, with a mean R^2 value of 0.959. The high level of accuracy in predicting the mean compressive strength value of 45.0 MPa is evident from the results. Furthermore, the model's predictive accuracy is quantified by the mean RMSE value of 3.04 MPa and the mean MAE value of 2.23 MPa, providing valuable insights into the model's performance. Table 3 presents comprehensive statistical data on the outcomes of the five-fold cross-validation operations, showcasing the model's consistency and overall high accuracy despite occasional fluctuations. Overall, the results suggest that the machine learning model, specifically the one based on RF, performs excellently in predicting compressive strength in pozzolanic concrete. The model demonstrates strong correlation, high accuracy, and reliable generalizability, making it a promising and efficient approach for predicting concrete properties and optimizing its composition in construction applications.

Table 3: Summary of five-fold cross-validation results

Folds	Performance Indicators		
	R^2	RMSE	MAE
Fold 1	0.959	3.05	2.22
Fold 2	0.962	2.90	2.18
Fold 3	0.954	3.17	2.33
Fold 4	0.955	3.18	2.28
Fold 5	0.963	2.89	2.11
Average	0.959	3.04	2.23

3.5 Sensitivity Investigation

The selected RF model, deemed the most proficient for this analysis, underwent a sensitivity assessment illustrated in Figure 8. The results highlight cement as the predominant influencer, commanding 28% of the total input parameters and significantly impacting the RF model's predictive accuracy. Notably, higher concentrations of superplasticizer, reaching up to 25.2%, correlate with increased compressive strength in concrete. Additionally, fine aggregates, coarse aggregates, and hearthstone exhibit comparable contributions of 10.50%, 7.60%, and 13.70%, respectively, in shaping the model's predictive outcomes. Only a small portion of cement can be substituted by fly ash. As a result, fly ash has less impact on concrete's compressive strength than aggregates. Finally, the water content has a favorable effect, which indicates that concrete's compressive strength increases as water content rises (Oner & Akyuz, 2007; J. Shen & Xu, 2019). In general, feature importance evaluations are carried out when the suggested RF model is evaluated. Each input variable's impacts on the compressive strength of concrete, including pozzolanic material, are accurately simulated by the feature importance analysis.

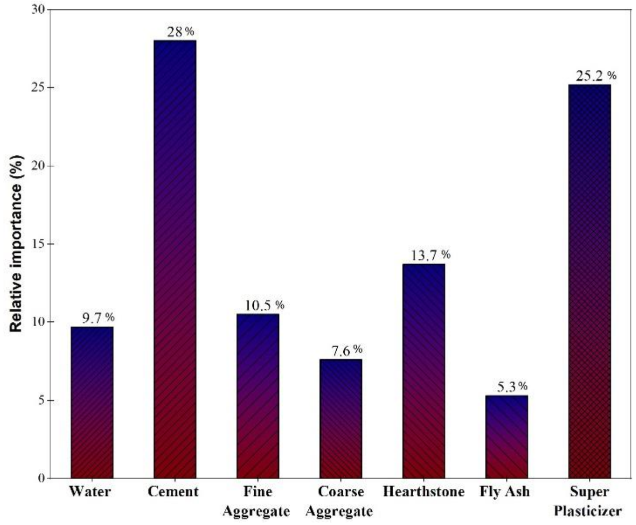


Figure 8: Input parameter's relative importance relevance to pozzolanic concrete strength

3.6 Influence of Input Variable Number

This analysis aims to ascertain the influence on the model's performance when specific data inputs are omitted. Table 4 presents the outcomes of anticipated values compared to actual values and the corresponding performance metrics for seven combinations of input variables. The initial combination, which incorporates all seven inputs (water, cement, fine aggregate, coarse aggregate, hearthstone, fly ash, and superplasticizer), yields the most favorable outcomes as it utilizes the entirety of the accessible data. However, combination six exhibited the lowest performance among all the combinations, as evidenced by an R^2 value of 0.893, an RMSE value of 4.89 MPa, and an MAE value of 3.60 MPa. As evidenced by combinations two through seven, it can be inferred that enhancing model correctness does not necessarily arise solely from including additional input variables. It is noteworthy that combination seven, comprising six input variables (excluding cement), exhibits just a slight improvement in performance compared to combination two, as seen by an R^2 value of 0.958, an RMSE value of 3.04 MPa, and an MAE value of 2.20 MPa.

In contrast, combination three, which incorporates five input variables (excluding fly ash and superplasticizer), performs better than combinations two and four. The key factors that significantly contribute to the attainment of accurate forecasts are the utilization of cement and pozzolanic materials. The above findings underscore the significance of considering these particular inputs within the model.

Table 4: Statistics on performance for analyzing various combinations of input variables

Combinations	Performance Indicators		
	R^2	RMSE	MAE
i. X1,X2,X3,X4,X5,X6,X7	0.961	2.96	2.12
ii. X1,X2,X3,X4,X5,X6	0.958	3.04	2.20
iii. X1,X2,X3,X4,X5	0.960	2.99	2.15
iv. X1,X2,X3,X4	0.940	3.67	2.65
v. X1,X2,X3	0.927	4.03	2.93
vi. X1,X2	0.893	4.89	3.60
vii. X1,X3,X4,X5,X6,X7	0.956	3.13	2.26

3.7 Taylor Diagram for Comparative Analysis

The Taylor diagram is a valuable tool for the comparative analysis of model performance and longitudinal evaluation of a single model's effectiveness (K. Khan *et al.*, 2022). Within the context of this study, prediction models encompass three algorithms: ANN, RF, and GBR. The utilization of the Taylor diagram, depicted in Figure 9, aids in comprehending model performance within a unified scale, consolidating all prediction model outcomes within a singular visualization. Notably, the 'Actual' bold dotted line, representing a standard deviation of 15.33 for actual compressive strength, serves as a reference point. Models (ANN, RF, and GBR) falling within this range are deemed suitable for prediction.

Analysis of the Taylor diagram reveals RF and GBR to be closely aligned with low standard deviation for training datasets depicted in Figure 9(a). In contrast, the ANN model demonstrates comparatively diminished performance in predicting compressive strength. Evaluation of the testing datasets in Figure 9(b) underscores the proximity of the RF model to the REF point, distinguishing it as superior among the two predictive modeling approaches (ANN and GBR).

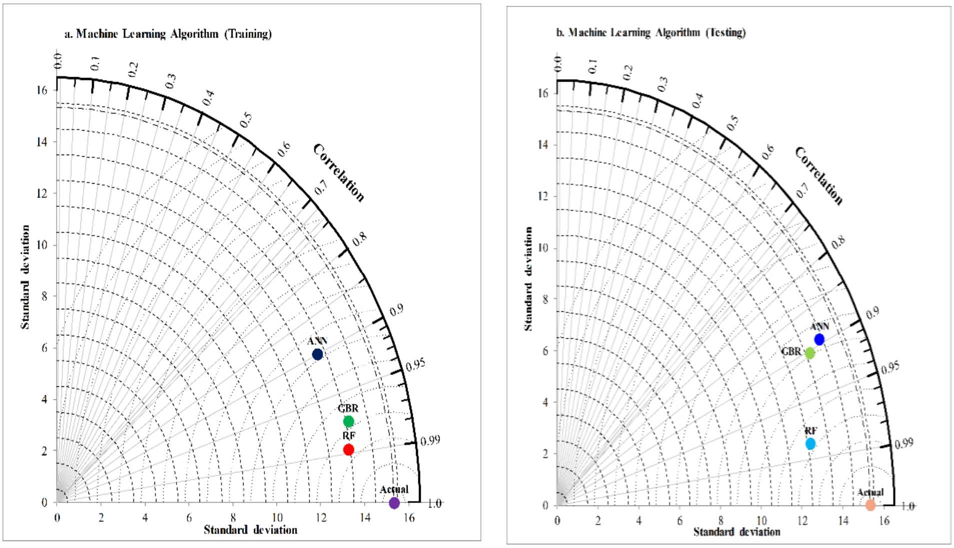


Figure 9: Taylor diagram illustrating the three algorithms utilized in this study

4. Conclusions

This research showcases the potency of machine learning in predicting the compressive strength of pozzolanic concrete, leveraging a dataset of 482 samples. The algorithms were then tailored using the training datasets to address the identified problem. Key findings include the superiority of the RF model over ANN and GBR in concrete strength prediction, attributed to its decision tree ensemble effectively handling overfitting and nonlinear relationships. The RF model achieved the highest R^2 values (0.976 in training, 0.964 in testing) with the lowest RMSE and MAE values, signifying exceptional predictive accuracy. In comparison to ANN and GBR, the RF model demonstrated higher R^2 and lower RMSE and MAE, affirming its reliability in predicting concrete strength. The RF model's stability, assessed through K-fold cross-validation, consistently exhibited high performance. Cement emerged as the most influential input parameter (28%) for accurate strength prediction, followed by superplasticizer concentration (25.2%). In conclusion, this study advocates for the RF model as the optimal method for predicting pozzolanic concrete's compressive strength in regression analysis, underscoring the pivotal roles of cement and pozzolanic materials. The findings offer practical insights for improving concrete mix designs and construction procedures, urging future research to address biases and explore diverse algorithmic options for broader applications in the concrete industry.

Availability of data, material, and code Some or all data, models, or codes generated or used during the study are available from the corresponding author by request.

Dataset link https://github.com/Sirfowahid/Dataset/blob/main/CCS.xlsx

Conflict of interest

The authors declare no potential conflict of interest regarding the publication of this work. In addition, the ethical issues including plagiarism, informed consent, misconduct, data fabrication and, or falsification, double publication and, or submission, and redundancy have been completely witnessed by the authors.

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