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Predict the Mechanical Properties of Cementitious Materials Containing Carbon Nanotubes Using Machine Learning Algorithms

Niranjana A. R.

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Abstract: In this work, the use of machine learning algorithms to predict the mechanical properties of cementitious materials boosted with carbon nanotubes (CNTs) is investigated. The main goal is to estimate the flexural strength and elastic modulus of these novel composite materials, which have the potential to have a big influence on the building industry. The water-to-cement ratio, sand-to-cement ratio, curing age, CNT aspect ratio, CNT content, surfactant-to-CNT ratio, and sonication duration were among the seven crucial factors that were investigated. Support vector regression, histogram gradient boosting, and artificial neural networks were among the prediction techniques used. The neural network model was also used to develop an easy-to-use formula. Each model's performance was evaluated, and the results showed that the neural network was the best at predicting the elastic modulus and the histogram gradient boosting model was the best at doing so for flexural strength. These findings demonstrate how well the methods used may predict the characteristics of cementitious materials boosted by carbon nanotubes. Furthermore, the formulas that are extracted from the neural network provide important information on how input parameters and mechanical qualities relate to one another.

Keywords*: Carbon nanotubes, Composite materials, Computational intelligence, Elastic modulus, Flexural strength.*

1. Introduction

In modern construction, concrete is the foundation. However, researchers are constantly looking for new ways to improve this essential material as the need for stronger, more durable, and sustainable constructions grow. Nanotechnology has revolutionized many industries in recent years, and the construction industry is no exception. Carbon Nano-Tubes (CNTs), one of the major developments driving this change, have shown tremendous promise in structural engineering and are among the most exciting opportunities in this developing field [1]. Compared to their bulk counterparts, engineered materials have unique properties that stand out. Their exceptional adaptability to different design and structural requirements supports their widespread use in the building industry [2]. A novel approach to the development of composites is the cooperative integration of carbon nanotubes (CNTs) with cement-based materials. In this regard, CNTs have a major impact on the material's mechanical characteristics. This innovative method has spurred a great deal of research to fully evaluate these composites' performance under various circumstances [3]. [4] investigated the impact of carbon nanotube configurations on cement composites' mechanical characteristics. In the cement paste, different kinds of carbon nanotubes and dispersion methods were used. The findings showed that the mechanical properties of the composites were greatly impacted by the structural features, dispersion techniques, and interactions with the cement matrix. [5] Examined the use of solutions of highly concentrated carbon nanotubes as additives for cementitious composites reinforced with nanofibers. Their creative study developed a method for using a centrifugal process to reduce the water content of CNT suspensions. These concentrated suspensions successfully preserved their reinforcing qualities while keeping their solubility and dispersion when incorporated into cement paste. Numerous aspects of the inclusion of carbon nanotubes in cementitious materials have been investigated by researchers, including synthesis methods, microstructural study, and mechanical property investigation. These studies have produced important new information that helps to improve cement-based composites. Many studies have looked into how CNTs affect mechanical characteristics. Even at higher temperatures, studies by [6] showed gains in characteristics like compressive and flexural strength. [7,8] underlined once more how crucial CNT diameter is in affecting these characteristics. Various CNT kinds and surface treatments have been investigated to increase dynamic strength and adhesion. [9] shown through experiments and simulations how sodium dodecyl sulfate surface treatments improved CNT-cement matrix adhesion. [10] examined how different CNT kinds affected dynamic compressive strength, emphasizing how type and dosage depend on one other. [11] It has also been demonstrated that surface treatments improve interfacial bonding and dispersion. By utilizing the power of data analysis, machine learning (ML) makes

Assistant Professor of Physics, GFGC Koppa - 577 126, Chikkamagaluru District, Karnataka State, INDIA.

significant progress and predictions possible in a variety of fields. [11], [12], and [13]. By using data to make well-informed decisions, this methodology helps civil engineers choose better building materials and designs that will be stronger and more durable [14]. Machine learning algorithms are used to predict the key factor that determines concrete strength [15] and to improve corrosion inhibitor formulation, which extends the life of structures [16]. This method improves recycled concrete's resistance to temperature changes [17] and improves the mechanical and electrical properties of new concrete formulations [18]. Apart from material enhancements, machine learning is having a substantial impact on structural analysis and health monitoring, including the assessment of reinforced concrete elements and the estimation of recycled concrete composites' tensile strength [19]. The goal of this study is to assess the flexural strength and elastic modulus of cementitious composites reinforced with carbon nanotubes (CNTs) using machine learning algorithms. Through the combination of computer modeling and experimental data analysis, the study seeks to produce reliable forecasts of these crucial mechanical properties. The anticipated outcomes may have a significant influence on the development and use of cutting-edge, high-performance materials in the building industry. Furthermore, the carefully examined results from the Artificial Neural Network (ANN) model will be converted into a formula that is easy to understand. The results are more practically relevant as a result of this effort to elucidate the basic relationships between input variables and mechanical behaviors.

1.1 Research significance

The intricate interactions between carbon nanotubes (CNTs) and the surrounding matrix make it difficult to anticipate the mechanical behavior of cementitious composites reinforced with CNTs. A reliable method that makes it possible to forecast these characteristics without the need for time-consuming and expensive testing processes is machine learning. This study investigated the use of three sophisticated models: Histogram Gradient Boosting (HGB), Support Vector Regression (SVR), and artificial neural networks (ANN). The ANN model provided a significant advantage in terms of interpretability in addition to its excellent accuracy. Researchers discovered significant insights into the relationships between input parameters and the final mechanical properties by deriving formulas from the ANN. This knowledge can be applied to improve the creation and design of CNT-reinforced composites that meet particular needs. The investigation's findings are especially encouraging for the building industry. Machine learning-driven predictions of mechanical characteristics can speed up the development of cutting-edge materials by permitting the synthesis of novel composite materials with improved performance, thereby improving the caliber and reliability of building projects. For broader acceptability among practitioners and academics, interpretable models—such as artificial neural networks (ANNs) with their derived formulas and statistical evaluations—must be developed. This method greatly increases the research's impact and accessibility.

2. Literature review

One important area of attention has been predictive modeling. [26] suggested a model based on CNT dispersion and volume fraction for flexural strength and elastic modulus. Many studies have looked into how CNTs affect mechanical characteristics. Even at higher temperatures, studies by [27] showed gains in characteristics like compressive and flexural strength. [28] underlined once more how crucial CNT diameter is in affecting these characteristics. Various CNT kinds and surface treatments have been investigated to increase dynamic strength and adhesion. [29] demonstrated through tests and simulations how sodium dodecyl sulfate surface treatments improved CNT-cement matrix adhesion. [30] examined the effects of several CNT types on dynamic compressive strength, emphasizing the dosage and type dependence. [31] Surface treatments have also been shown to enhance interfacial bonding and dispersion. In addition to mechanical qualities, research has tackled issues including rheology and dispersion. [32] investigated the best additive concentrations for dispersion and how they affected mechanics and hydration. Organosilanes were studied as coupling agents to enhance bonding and dispersion [33]. [34] created a model to forecast viscosity by examining the rheological behavior of CNT-cement composites. The emphasis on high-performance nanocomposites goes beyond modeling to include predictive methods. [35] Investigated deep neural networks for elastic modulus and flexural strength prediction. This method promotes the design of these materials and supports modeling efforts. Incorporating CNT has also improved fire resistance and other qualities. [36] looked at how the composition of the cement matrix affected the strength of the adhesion between CNTs and the matrix. [37] Investigated the application of hybrid aqueous solutions to promote interfacial bonding and dispersion, which will improve mechanical properties. Last but not least, [38] demonstrated that CNTs, even when derived from mining tailings, can improve mechanical qualities and decrease porosity. The vast amount of research highlights the complex ways in which carbon nanotubes affect cementitious materials' mechanical characteristics. The CNTs have a profound effect on the overall strength and structural integrity of concrete by greatly enhancing the crucial building engineering characteristics of flexural strength and elastic modulus.

The structure of the proposed work is as follows: section 1 explains the introduction, section 2 explains the literature review, section 3 explains the proposed methodology, section 4 explains the discussion of the proposed work, and the conclusion part in section 5.

3. Proposed methodology

As a subfield of artificial intelligence, machine learning (ML) has become a powerful tool in the engineering field, especially in structural engineering. It increases the accuracy of structural performance forecasts, simplifies design processes, and makes it easier to analyze complex data. Despite the fact that machine learning techniques have shown effective in predicting the behavior of various reinforced concrete components, a careful review of the existing literature reveals that precise methodologies are often not presented. In order to predict the elastic modulus and flexural strength of cementitious composites enhanced with carbon nanotubes (CNTs), this study employs three main machine learning techniques, acknowledging the importance and efficacy of these approaches in addressing complex and non-linear behaviors in structural engineering. The next subsections provide a thorough description and explanation of the methods used. Additionally, a model of a single-layer artificial neural network is created to do complex statistical studies, with the aim of determining mathematical relationships and providing easily understandable insights for determining the goal parameters.

3.1 Support Vector Regression (SVR)

One of the most efficient techniques for simulating nonlinear connections is Support Vector Regression (SVR). This method converts complicated nonlinear qualities into controllable linear ones by using kernel functions. It is a simple yet effective variation of SVMs and has been successfully used in a number of domains outside of structural engineering, [20] demonstrating its strength as a prediction method.

3.2 Histogram gradient boosting regressor (HGB)

HGB is a tree-based machine learning technique that efficiently handles numerical information by utilizing the benefits of histograms and gradient boosting. This sophisticated technique entails building an ensemble of decision trees one after the other, with each new tree being taught to fix the mistakes of its predecessors. By using gradient descent to optimize a loss function during the training phase, HGB enables [21] the algorithm to iteratively improve its model in order to lower prediction errors and increase accuracy. Data scientists and machine learning experts appreciate HGB because of its exceptional efficiency, which is particularly noticeable when working with datasets that have more than 10,000 samples. In these cases, it outperforms conventional gradient-boosting regressors greatly.

3.3 Artificial neural network (Multi-layer perception)

The multilayer perceptron (MLP) is one of the most basic forms of artificial neural networks (ANN). An input layer, one or more hidden layers, and an output layer make up this design. While the number of intended outputs defines the output layer, the number of input features determines the input layer. User [22] requirements are used to establish the hidden layer configuration. Depending on the type of data being processed, the weights assigned to each layer might form simple or complex networks. Beyond structural engineering, MLP-ANN has shown promise in a number of other domains. Equations (1) and (2) determine the number of neurons in each of the m hidden layers that make up the internal structure.

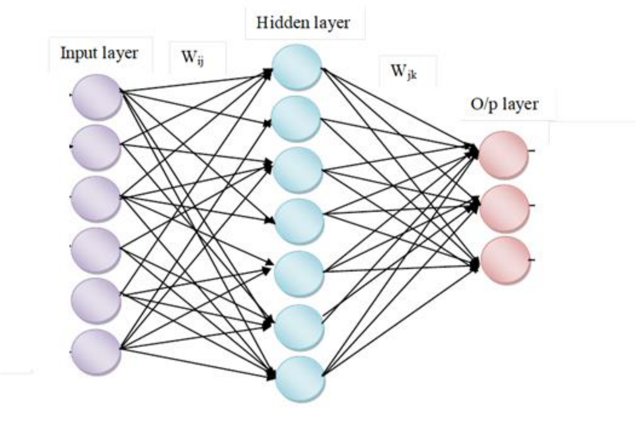

Fig 1: ANN architecture

$$I=\sum_{j=1}^{no} W_{jn} go(x_j)+a_n \text{ ……………………} (1)$$

$$O=g_1(I_n)=(1+e^{-in})^{-1} \text{ ……………………………} (2)$$

Where I is the input, o is the output, a_n is the threshold of n^{th} neuron, w_{jn} is the weight value of j^{th} input neuron and g_k is the activation function of k^{th} layer.

Consequently, the input and output of the neurons in the output layer are represented by Equations (3) and (4), respectively.

$$I_1=\sum_{j=1}^{n_m} W_{j1} o_j + a_1 \text{ ………………………….. } (3)$$

$$o_1 = i_1 \text{ ……………………….. } (4)$$

Here, o1 stands for the output, i1 for the input, and a1 for the output layer's neuronal threshold. A key component of model training is backpropagation. The algorithm creates predictions and then adjusts the weights to improve on them based on the inaccuracy found. The seven input variables is calculated by using eqn (5)

The MLP model's architecture, shown in Figure was painstakingly created with a clear framework. It had a first input layer with five different input features. This layer was linked to two hidden layers, each of which had 40 neurons and 50 neurons in the first layer. With the use of the 'ReLU' (Rectified Linear Unit) activation function, these hidden layers played a crucial role in spotting intricate patterns in the dataset. [23] The 'ReLU' function is well known for its efficiency and ability to improve gradient propagation across the network, which helps to speed up convergence during training. The 'adam' solver was used to improve the performance of the MLP model even more. The model's effective convergence towards an ideal solution is made possible by this solver's use of adaptive learning rates and momentum. By setting the training schedule to a maximum of 1000 iterations, the model was able to understand complex correlations in the data while reducing the possibility of overfitting, a common problem in machine learning applications.

3.4 For elastic modulus strength

Three extremely precise machine learning-based computational frameworks for calculating the elastic modulus were shown in the section before this one. Another method using a trained single-layer neural network is introduced in this section. A neural network with a single hidden layer is first trained using this method. A number of sophisticated statistical analyses are then performed using the weight values that were acquired throughout the model training procedure. In the end, a simpler and well-organized formulation is produced for engineering applications [24], guaranteeing a trustworthy target parameter prediction. A single-layer perceptron neural network with the architecture shown in Figure is first trained to determine the elastic modulus in order to demonstrate this procedure. Six neurons, chosen by a trial-and-error method, make up this network's hidden layer.

$$Q_{ik}=\frac{\sum_{j=1}^{nhidden}\frac{W_{ji}}{\sum_{l=1}^{ninput}\left|W_{ji}\right|}W_{oj}}{\sum_{k=1}^{ninput}\left(\sum_{j=1}^{nhidden}\left|\frac{w_{jk}}{\sum_{l=1}^{ninput}\left|w_{jl}\right|}W_{oj}\right|\right)} \text{ …………………………. } (5)$$

where W is the weight, j is the number of nodes in the middle layer, i is the number of input nodes, k is the number of output nodes, nhidden is the number of nodes in [25] the middle layer, and Qik is the percentage influence of each parameter. Ninput is the number of inputs, and Woj is the connection weight between the output node and the middle layer nodes. Finally, Eq. (6) is obtained using regression analysis. In the context of sensitivity analysis, E1 stands for the elastic modulus (Target) that was obtained from the network.

E1 = 0.245 X1, 3 + 18.29………………………….. (6)

Table 1: Hyperparameters for elastic modulus estimation models

Model	Hyperparameter	Hyperparameter value
HGB regressor	max_iteration	50
SVR Regressor	C_parameter	2
	epsilon	0.5
MLP Regressor	Number of hidden layers	2
	hidden_layer_sizes (neurons)	(50, 40)
	activation	'relu'
	solver	adam

	max_iteration	1000
	random_state	43

3.5 For flexural strength

The specifics of the models used to determine the flexural strength are described in this section. Every model is characterized by its hyperparameters, which are crucial elements impacting its capacity for prediction. A detailed overview of the hyperparameters used for each model is provided in Table 5. As illustrated in Fig. 15, our MLP model's design included an input layer, a single hidden layer with 30 neurons, and an output layer. There are seven inputs in the input layer. Finally, each mean graph's regression equations are calculated and shown in Eqs. (13)–(18). Eq. (19) can be used to find the flexural strength in the end. The results of this section for the neural network and the formula produced from it are shown in Fig. 2. It is important to note that Table 3 introduced the variables X2,1 through X2,7 for the flexural strength problem before.

$C(X_{2,1}) = 0.96X_{2,1}^2 - 3.06X_{2,1} + 3.11$ ……………………….. (7)

$C(X_{2,2}) = 0.09X_{2,2}^2 - 0.12X_{2,2} + 1.02$ ………………………. (8)

$C(X_{2,3}) = 0.07X_{2,3}^2 + 0.04X_{2,3} + 0.89$…………………… (9)

$C(X5) = -0.01X_{2,5}^4 + 0.07X_{2,5}^3 - 0.26X_{2,5}^2 + 0.10X_{2,5} + 1.09$ …………… (10)

$C(X_{2,6}) = -0.04X_{2,6}^2 + 0.21X_{2,6} + 0.83$ ……………….. (11)

$C(X_{2,7}) = 0.23X_{2,7}^2 + 0.02X_{2,7} + 0.76$ ………………….(12)

$1.92 \leq (Y2(MPa) = M1\, C(X_{2,1})\, C(X_{2,2})\, C(X_{2,3})\, C(X_{2,5})\, C(X_{2,6})\, C(X_{2,7})) \leq 12.9$……….(13)

Table 5: Hyperparameters for flexural strength estimation models

Model	Hyperparameter	Hyperparameter value
HGB regressor	max_depth	2
	max_iteration	100
SVR Regressor	C_parameter	4
	epsilon	0.7
MLP Regressor	Number of hidden layers	1
	hidden_layer_sizes (neurons)	30
	activation	‘relu’
	solver	adam
	max_iteration	1000
	random_state	43

4. Discussion

The inability of machine learning models to effectively generalize outside of the data they were trained on is a significant drawback. This implies that only inputs falling within the range of values the model has experienced during training can yield accurate predictions. The model's predictions could become erroneous or unreliable if an input is provided that is outside of this range, which could produce misleading results. This restriction highlights how crucial it is to carefully choose and assess models, taking testing and training performance into account. For each model, performance indicators such as the correlation coefficient (R), mean absolute error (MAE), and root mean square error (RMSE) are presented with respect to Training Data, Test Data, and the combined dataset, known as All Data.

4.1 Database

This research makes use of a large database that has 165 datasets on cementitious materials that have been improved using carbon nanotubes. Elastic modulus and flexural strength are two important mechanical qualities that can be predicted using machine learning models built on top of the database. By combining data from multiple experimental sources, data curation guarantees robustness. When creating a machine learning model, the data is carefully divided into training (60%) and sets for testing (20%) and validation (20%). Normalization and randomization are crucial steps in data preprocessing for these sets. The database is carefully analyzed to guarantee model efficacy for each goal property (flexural strength and elastic modulus). For the particular target attribute for which they lack data, datasets with missing values for input variables are not included in the analysis.

Table 3: Summary of results for predictive models of Elastic Modulus

Model	Training data			Validation data			Test data
	RMSE	MAE	R^2	RMSE	MAE	R^2	RMSE
MLP	2.18	1.86	0.92	3.00	1.68	0.85	2.93
HGB	2.95	2.42	0.87	2.06	1.86	0.84	3.16
SVR	0.65	1.83	0.90	2.52	1.96	0.88	3.57
Formula	3.29	2.65	0.82	4.30	3.54	0.75	2.95
ANN	1.94	1.48	0.94	2.70	2.78	0.99	2.90

Table 4: Summary of results for predictive models of flexural strength

Model	Training data			Validation data			Test data
	RMSE	MAE	R^2	RMSE	MAE	R^2	RMSE
MLP	2	0.74	0.81	1.44	1.13	0.83	1.27
HGB	0.92	0.69	0.85	1.32	200	0.85	1.32
SVR	0.93	0.68	85	1.32	1.06	0.87	1.32
Formula	1.95	1.6	0.57	1.68	1.32	0.73	1.75
ANN	0.96	0.72	0.84	0.82	0.65	0.88	1.32

The thorough examination of the flexural strength and elastic modulus prediction models, as shown in Tables 3 and 4 and the accompanying figures, enhances knowledge of their application. These observations not only help choose the right model for precise forecasts, but they also add to the larger discussion on the developments and difficulties in material property prediction. The results offered here is a useful guide for directing future research paths and easing the incorporation of predictive models into practical applications as the area develops.

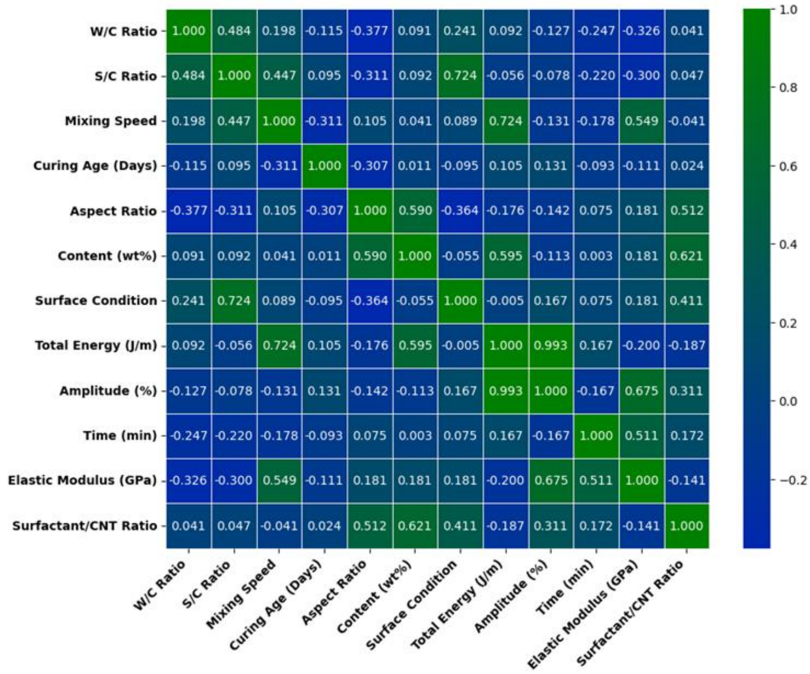

Fig 2: Correlation analysis of elastic modulus estimation parameters

Curing age and the sand-to-cement (S/C) ratio have the strongest positive correlations with the output, whereas the water-to-cement (W/C) ratio has the strongest negative association, as shown in Figure 2. The W/C ratio, S/C ratio, curing age, CNT content, and surface condition were specifically chosen as X factors. The Elastic Modulus, one of the two mechanical characteristics examined in this article, is the Y parameter of importance in this research. A crucial component of the database is the connection between the elastic modulus and the X parameters. Furthermore, the correlation matrix that is displayed (see Figure 2) is customized for this specific database and offers important information about the relationships between the variables. This matrix is a tool for understanding the connections and possible correlations between the elastic modulus and the X parameters. For a more thorough rundown of the database.

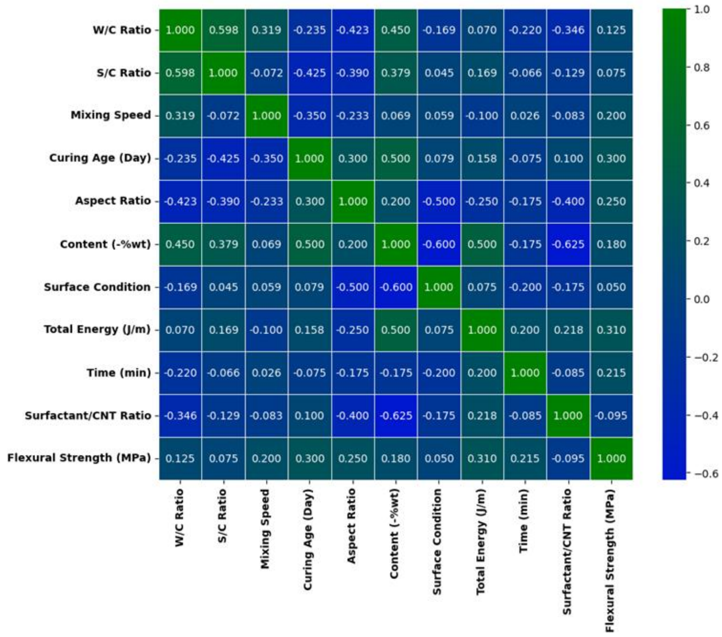

Fig 3: Correlation analysis of flexural strength estimation parameters

Time (min) showed the strongest positive link with flexural strength, whereas the W/C ratio showed the strongest negative correlation, according to an examination of the correlation matrix (Figure 3). The W/C ratio, S/C ratio, aspect ratio, curing age, CNT content, surfactant/CNTs ratio, and time were among the X factors used for the model. These characteristics were selected because to their initial correlation, influence on model complexity, and applicability to flexural strength estimate.

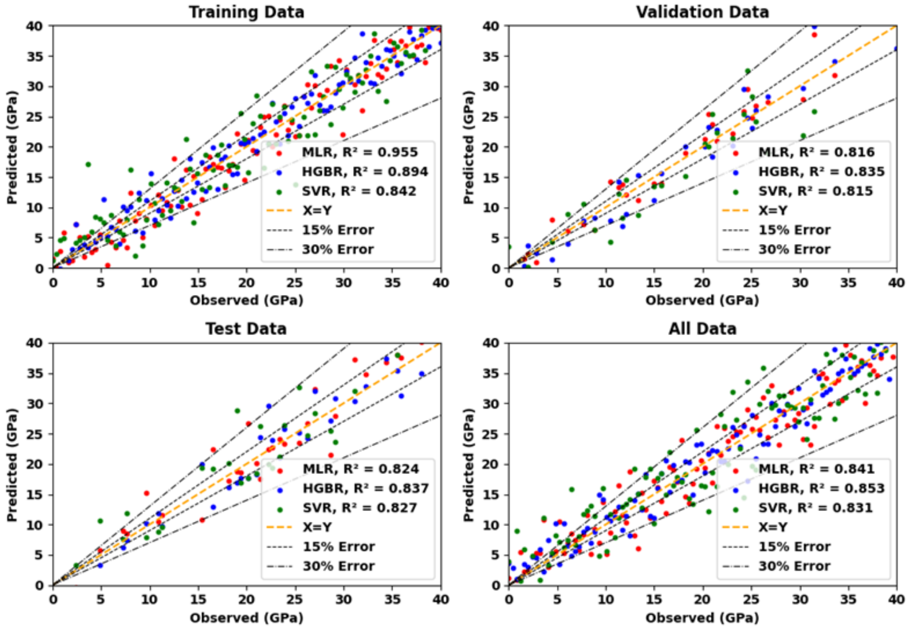

Fig 4: Comparison of observed and predicted elastic modulus

Each model's observed and anticipated elastic modulus, including training and test data, are displayed in Figure 4. The best performance is shown by ANN, which makes correct predictions on both datasets. The excellent predictive skills of ANN are demonstrated by the close correspondence between observed and forecasted values. Moreover, HGB and SVR exhibit excellent performance. These results highlight how well ML, and particularly ANN, capture intricate relationships for the calculation of elastic modulus in cementitious materials reinforced with carbon nanotubes.

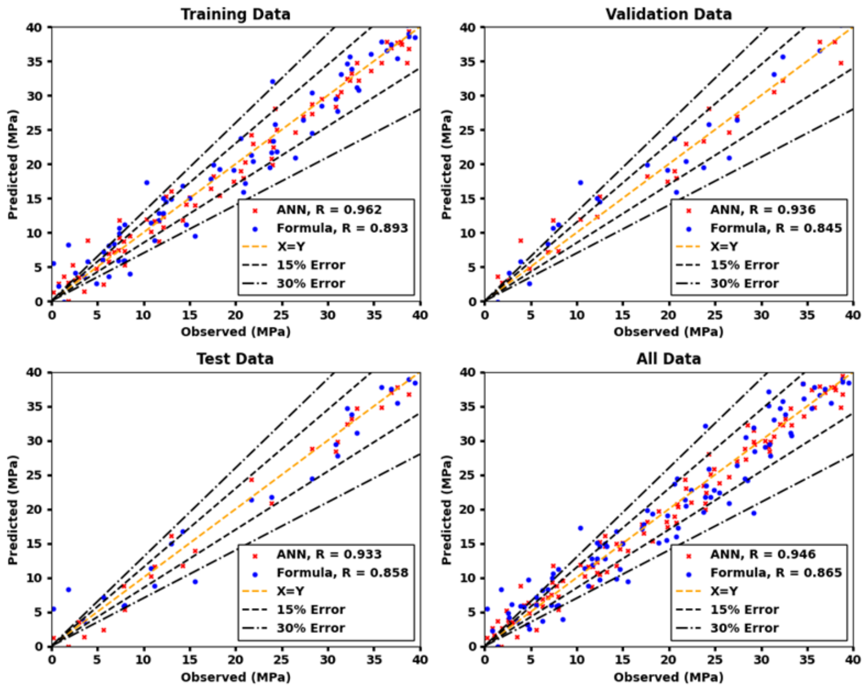

Fig 5: Elastic modulus comparison between observed and predicted values using the formula and its reference ANN.

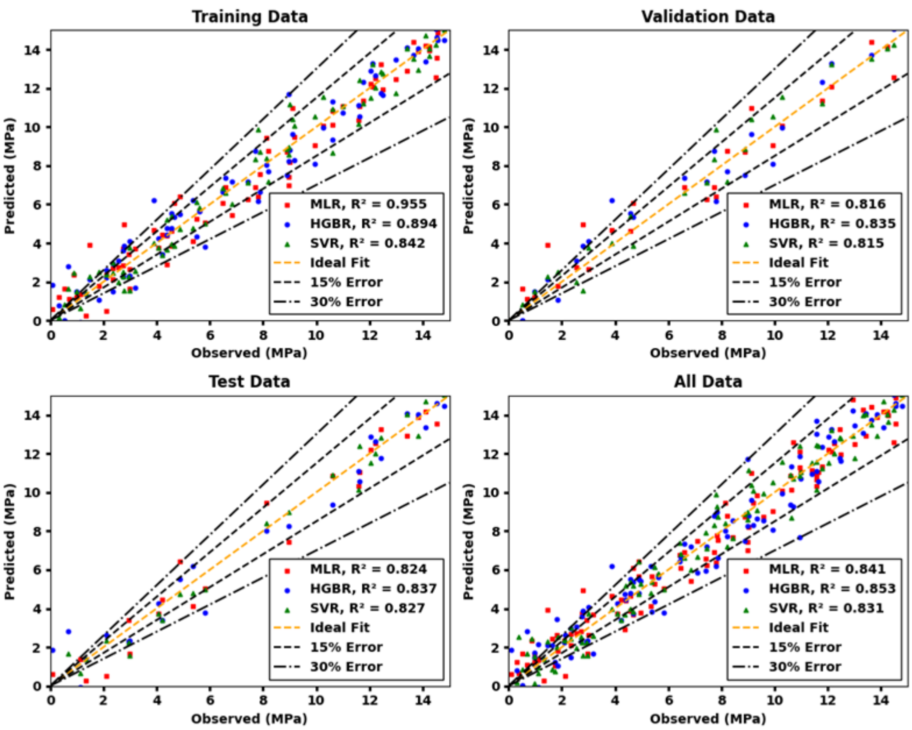

Fig 6: Comparison of Observed and Predicted Flexural Strength values

ANN for the complete database, which is used to calculate the elastic modulus, is shown in Figure 5. A visual comparison of each model's predicted and actual flexural strengths for the training and testing datasets is presented in Figure 6. According to the figure, the SVR model predicts the most accurately, with the HGB model coming in second. Similar to the HGB and SVR models, the ANN model performs well, albeit with a little less accuracy.

5. Conclusion

A paradigm change in the creation and design of cementitious materials is made possible by this research, which represents a major advancement in the field of material property prediction. The study's main conclusions highlight the unique advantages of particular machine learning algorithms for forecasting important mechanical characteristics. With low mean absolute error and root mean squared error values, the artificial neural network was found to be the best accurate predictor of elastic modulus. Remarkably, by extracting interpretable formulas, the ANN also offered important insights into the complex interactions between the input parameters and the final mechanical properties. Additionally, the histogram gradient boosting model performed consistently and competitively across all datasets, exhibiting exceptional flexural strength estimation capabilities. High correlation coefficients demonstrated the ANN and HGB models' resilience in encapsulating the complex interactions seen in the corresponding datasets. Beyond the immediate advantages of correct predictions, the ANN model's interpretable formulas provide a significant advantage. With this information, engineers and researchers may better formulate and build CNT-reinforced composites for particular applications. The ANN offers important insights that can be used to customize the material properties for particular applications by revealing the intricate relationship between input parameters and mechanical qualities. In addition to advancing knowledge of cementitious materials reinforced with carbon nanotubes, the results given here provide a more comprehensive view of how machine learning could transform the design and optimization of a wide range of materials in numerous industries.

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