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Ensemble machine learning approach for evaluating the material characterization of carbon nanotube-reinforced cementitious composites

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Abstract

Time and cost-efficient techniques are essential to avoid extra conventional experimental studies with large date-set to characterize the mechanical properties of composite materials. Correlation between the structural performance and mechanical properties could be captured through the efficient predictive models. Several ensembled Machine Learning (ML) methods were implemented in this study, to materially characterize carbon nanotube (CNT)-reinforced cement-based composites. Proposed models were compared with each other to represent the accuracy of each method. The Flexural and Compressive Strength (target values) of CNT reinforced composites were predicted based on the data-rich framework provided in previous experimental investigations. These data were utilized for training of the proposed models through employing SciKit-Learn library in Python, followed by hyper-parameter tuning and k-fold cross-validation method for obtaining an efficient model to predict the target values. Random Forest (RF) and Gradient Boosting Machine (GBM) were developed for this purpose. The findings of this study would be useful for prospective composite designers in case of sufficient experimental data availability for ML model training.

Keywords: Machine Learning, CNT-reinforced Cement-based Composites, Mechanical Attributes, Predictive Models

1. Introduction

Cement-based materials have shown their capacity in various engineering applications due to their durability, low cost, and high compressive strength. However, low tensile strength hinders them from reaching their full potential. Thus, during the past decades fibers in different scales have become popular since they improve the structural performance of the cementitious materials [1, 2, 3] thanks to their specific mechanical attributes. Among those fibers, nano-fibers/tubes, higher amendment of crack initiation and propagation with respect to fibers in other scales, have been integrated into the cementitious materials for reinforcement purposes to obtain better structural integrity [4].

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Various researches have been conducted to characterize the CNT-reinforced cement-based structures mechanically and materially. Series of experimental tests have been implemented in order to specifically obtain the mechanical properties of those materials. Compressive strength of the carbon nanotubes cement-based composites were investigated under different conditions [5, 6, 7, 8, 9]. Flexural strength has been another important mechanical property, which was studied experimentally as well [10, 11, 12]. Other properties, e.g., tensile [13], thermal [14], electrical [15], and etc., even though less, but have been studied.

Employing the CNT reinforced cementitious materials have been intensified recently in different infrastructures such as bridges, buildings, and fuselages [16] over the conventional materials due to their outstanding properties. In order to take full advantage of these materials, experimental tests are required to understand their mechanical attributes in different loading conditions. However, dealing with lots of experimental tests and data acquisitions of CNT reinforced cementitious structures have been a challenging task for researchers due to the time required for preparing and conducting the tests as well as the labor expenses. Hence, some novel techniques due to the evolution of computing power and available prevalent data-sets, have attracted the attentions during the recent years for improving the time and cost efficiency of obtaining the targeted mechanical properties. Machine Learning (ML) method is one of those techniques which expedites the whole process through predicting the target values via training approaches utilizing gathered input values from previous experimental tests. It should be mentioned that making correlations between design parameters paves the way for application of ML methods for the intelligent product design. Thus, the designing phase is hastened while the investigation of intact intelligent design concepts through various advanced level predictive models will become possible. In this context, CNT reinforced cement-based materials could be considered as a potential candidate for application of ML techniques.

Various ML models have been utilized for anticipation of mechanical properties of composite materials as mentioned in a recent review article [17]. Several works specifically reported the application of ML techniques for predicting the physical properties of carbon nanotube and mechanical properties of CNT reinforced cementitious composites. Lyngdoh et al. employed Neural network technique for predicting the strain sensing properties of nano-engineered smart cementitious composites [18]. Jalal et al. applied Optimized neural network for data mining purpose in the functionally graded carbon nanotube reinforced composite structures [19]. Huang et al. integrated the Artificial neural network (ANN) with the Support vector machine (SVM) in order to predict the mechanical properties of CNT-reinforced cement composites [20]. Convolutional neural network technique was used for material characterization of carbon nanotube-polymer structures [21].

An ensembled ML technique was proposed in this article in order to predict the Compressive and Flexural strength (CS and FS), target values, of the CNT reinforced cementitious composite structures. In this study, the ML model, including the Random Forest (RF) and Gradient Boosting Machine (GBM) models were developed to predict the target values of those materials for the first time. Different applications could be supported by the proposed approach here. Not only the experimental tests for mechanical and material characterization purpose are reduced while applying the developed method in this study, but also it could be extended for different types of composite materials in any application.

2. Material and methods

2.1. Data collection and preprocessing

Extensive data-set framework including various parameters, which alters the structural performance of CNT-reinforced cement-based composites should be constructed for training purpose. Here, numerous mechanical attributes were collected via experimental tests conducted in previous literature [22, 23, 24, 25, 26, 27, 28, 29, 30]. The properties which influence the mechanical behavior of NCT-reinforced materials were Cement type, Water-to-cement ratio (WC), Content of carbon nanotubes, External Diameter, Length, Functionalization method, Curing days, Curing temperature, and Dispersion method with the minimum and maximum value of 1, 2, 0.2, 0.5, 0.2, 0.5, 4, 250.250, 1, 250.250, 1, 4, 3, 28, 20, 30, 1, 5 respectively [20]. It should be mentioned that the target values (FS & CS) have a non linear relationship with each other that makes the problem challenging.

2.2. Machine Learning Methods

2.2.1. Feature Selection Methods

Training an ML model including all the available data generally leads to the decline in model accuracy and overfitting issues. In order to train ML algorithms efficiently, the redundant and unnecessary features of the data-set should be eliminated. Therefore, feature selection (FS) methods were utilized to omit the redundant dimensions of the data-set while only keeping the most relevant features. The relevancy is associated with the contribution of the feature to increase the ML model accuracy. The linear correlation of variables could be investigated by Pearson correlation (Eq.1) [31].

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 (y_i - \bar{y})^2}} \tag{1}$$

wherein the r, x_i, $\bar{x}$, y_i, $\bar{y}$ are correlation coefficient, values of the x-variable in a sample, mean of the values of x-variable, values of the y-variable in a sample, and mean of the values of y-variable, respectively.

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2.2.2. Random Forest (RF)

Ensemble learning is a method that mixes the prediction effects of more than one algorithms to gain a high-quality final output. Random Forest (RF) is an ensemble method that implements a bootstrap aggregation to generate decision trees. The very last output of this algorithm is an aggregation of the prediction of all developed decision trees. This technique enables to consider all data dimensions almost equally and forestalls trees to come to be extremely correlated [32]. In this study, four random forest models were developed with different hyper parameters (Table. 1). Higher n_estimators were assigned for the RF _ IV case than three other methods in order to evaluate the effect of computational time on the accuracy of the target value.

Table 1: Parameters utilized for RF models

Random Forest	n_estimators	min_samples_leaf	max_depth	Computational Time
RF_ I	3	3	2	9.9
RF_ II	3	10	2	10.3
RF_ III	3	10	10	12.4
RF_ IV	500	2	2	455.33

2.2.3. Gradient Boosting Machine (GBM)

GBM is a tree based machine learning model which could be considered as an upgraded version of RF. The main difference between GBM and RF is the construction tree method in the ensemble formation. In the boosting technique, new trees are added in order to shrink the error of prediction of depended dimensions. By adding new tree to the GBM structure with a constant learning factor, the estimation error reduces till achieving the maximum possible accuracy of the model [33].
Hyper-parameters are extremely important for developing GBM models, and they can really affect the model precision. After many trial and errors in this study, the following four models were chosen to provide comparison of different factors (Table. 2).

Table 2: Parameters utilized for GBM models

Gradient Boosting Machine	n_estimators	Learning rate	min_samples_split	Computational Time
GB_ I	5	0.1	4	6.94
GB_ II	30	0.01	5	12.29
GB_ III	50	0.01	5	14.2
GB_ IV	500	0.01	7	100.2

Material inputs, as well as the target values and ML techniques employed in this study, were represented in Fig. 1. It should be highlighted that for this study, as also highlighted in [20], some parameters that could affect the target values were not collected due to the Scattered inconsistent previous studies.

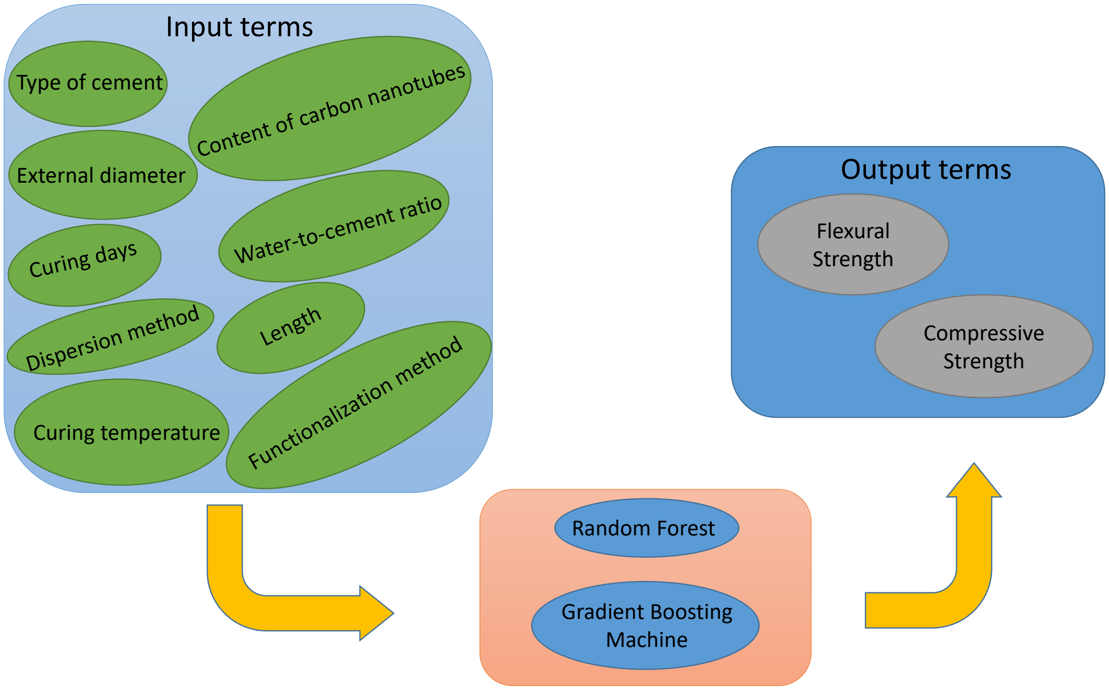

Figure 1: An overview of the ML methods application process

2.2.4. Model Metrics

Several common methods have been implemented to measure the quality of the machine learning models. These methods (model metrics) show how accurate the model prediction is in different conditions, i.e. on test data set. Among those, the Mean Squared Error (MSE), Mean Absolute Error (MAE), and Coefficient of Determination (R^2) were considered for this study.

$$\mathrm{R}^2 = 1 - \frac{\sum(a_i - P_i)^2}{(a_i - \mu_a)^2} \tag{2}$$

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(a_i - p_i)^2 \tag{3}$$

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n} \mid a_i - p_i \mid \tag{4}$$

Where i = 1, 2, ..n is the number of observations and n is the total number of records. Also, a_i, p_i, and μ_a are output, as real values, and mean value, respectively.

3. Results and discussions

The Distribution of the data (target variables) has an important role in the accuracy of the ML models while encountering new unseen test data. If the train and validation data set shape a natural distribution, then the ML model could generalize the patterns within the data more accurately. The collected data thereafter was utilized to predict the target values (CS and FS). Data distribution of CS and FS of CNT-reinforced cementitious materials was represented in Fig. 2. As it is evident, the distribution of FS was similar to natural distribution, while the CS values were distorted with positively-skewed distribution (right-skewed, representation of the extent to which a given distribution varies from a normal distribution), which possibly led to decrease in ML model accuracy on this feature.

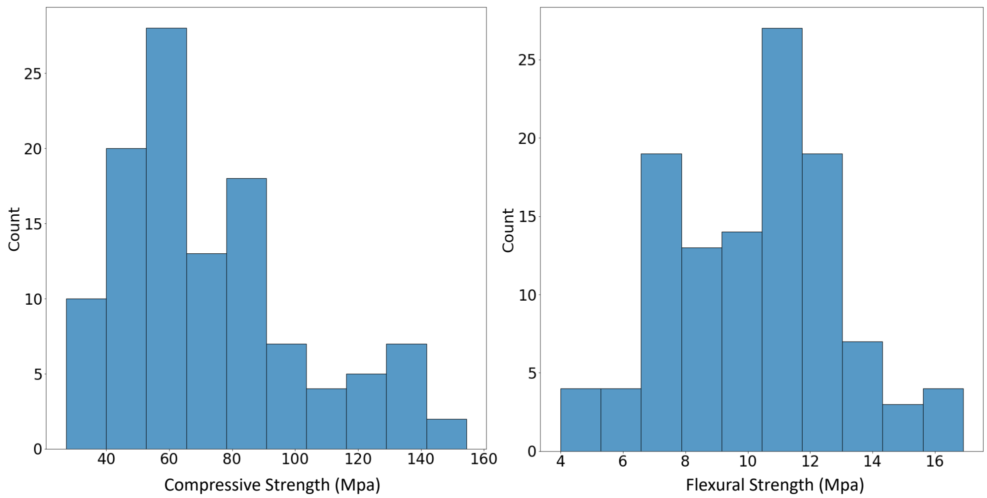

Figure 2: Data distribution of the ML model

Pearson correlation heat-map investigates the relationship between features of the data-set. Each feature was illustrated with the numbers between -1 & 1 in which -1 refers to the highly negative and 1 refers to highly positive correlation. Two features were considered as highly correlated in case the correlation is more than 0.75 or less than 0.75 [34]. Heat-map of the data-set framework was represented in Fig. 3. Overall, the length of Nano-tubes can be identified as a redundant feature as it had almost zero correlation with the target variables. It was observed that CS values were highly correlated with water to cement ratio (WC) with a negative slope, followed by curing days and curing temperature of CNT. In contrast, FS had lower correlation with WC and content of CNT, while demonstrating higher relations with the curing days. Also, as it was expected, type of cement had more impact on FS than the remaining factors. It is worth noting that none of the independent variables (input features) had more than 0.75 correlation with each others. Thus, the data-set framework did not have any multicollinearity issue.

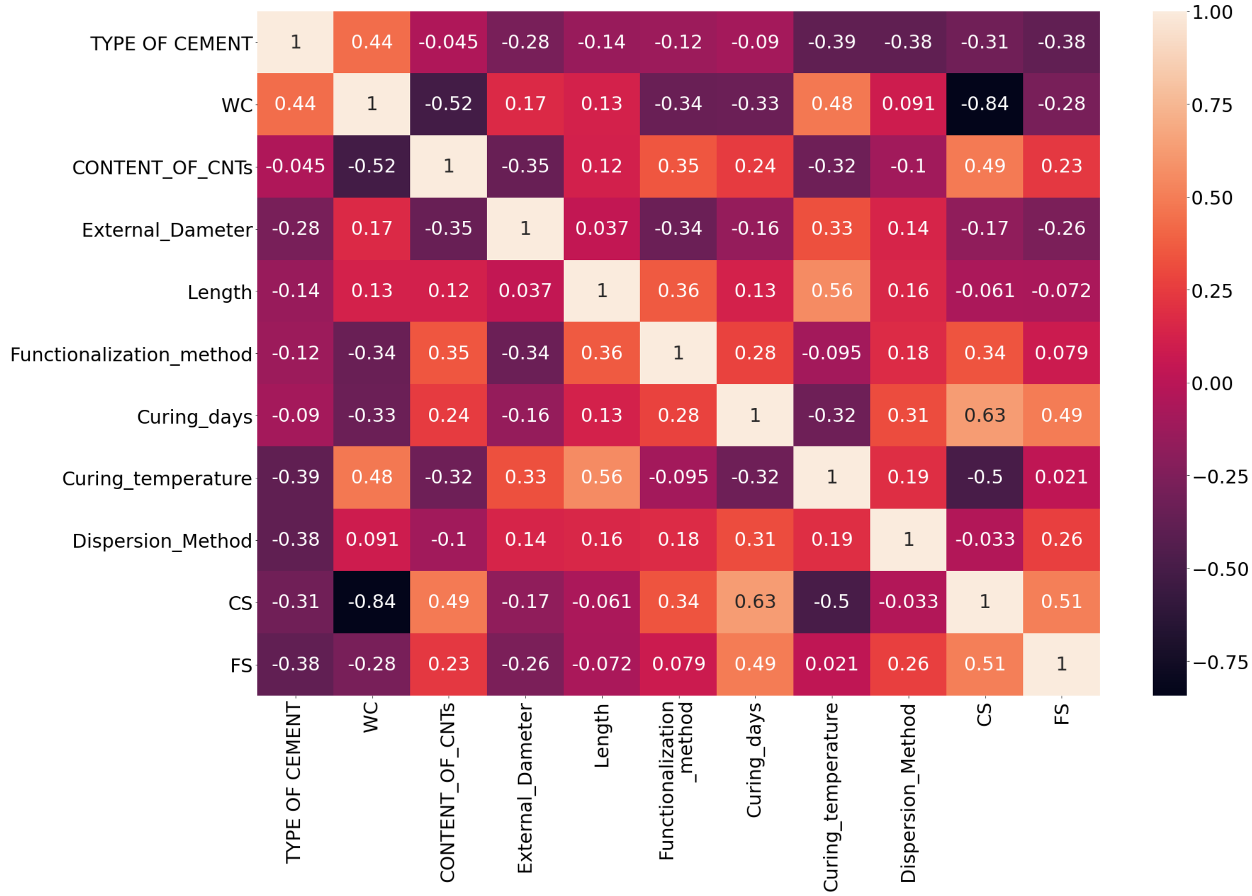

Figure 3: Pearson correlation heat map

Exhausting trial and errors are required to select a proper model and tuning hyper-parameters. According to the literature, cross validation is the most common way to capture model accuracy [35]. The proposed models from Table 1 and Table 2 have been given to the 5-fold cross validation with a variation of train-test size. In this algorithm the training data set size varies from 5 to 90 percent, and more than 420 train-test are performed for each model to find the best hyper-parameters (Fig. 4, Fig. 5).

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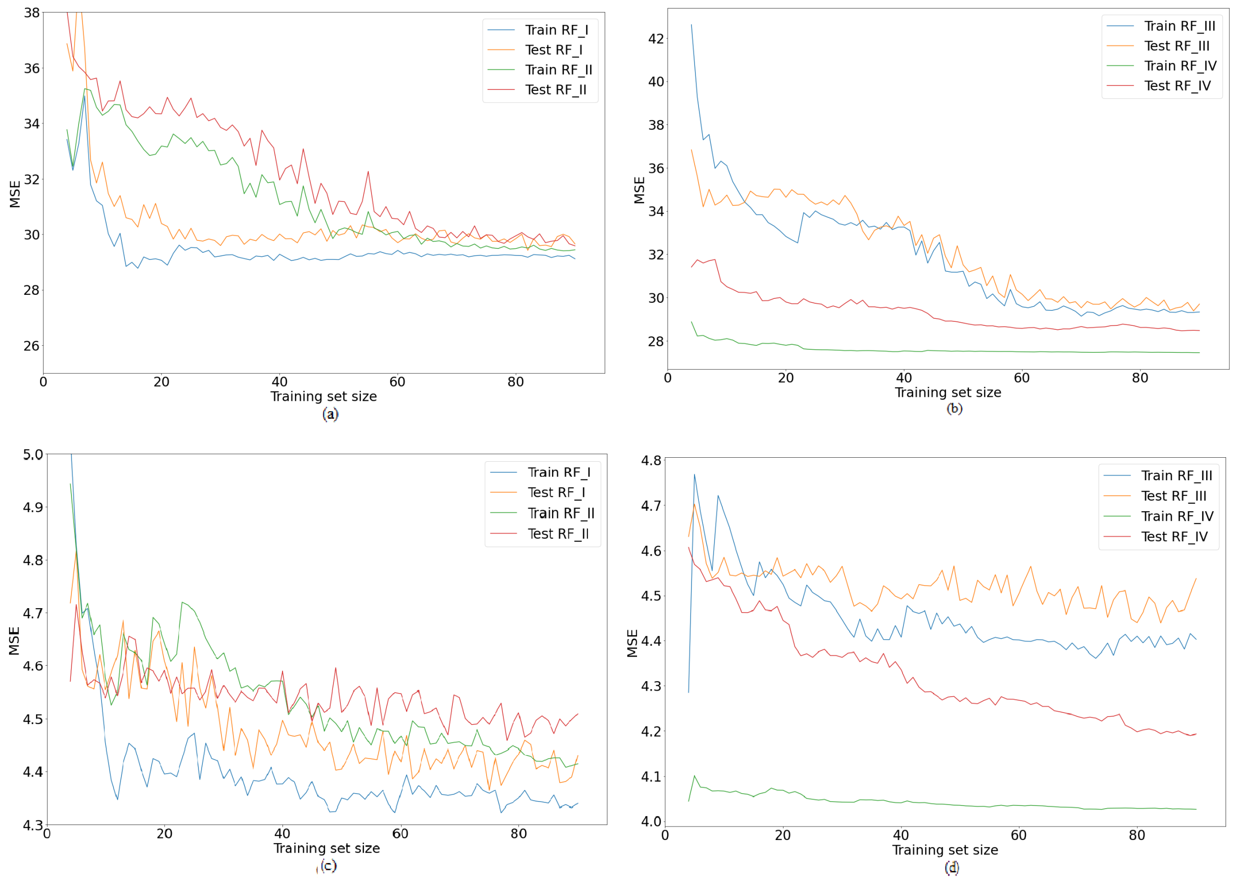

Figure 4: Mean squared error vs training set size values (a) RF-CS (b)RF-CS (c) RF-FS (d) RF-FS

During the mentioned 5 fold cross validation, it was observed that the MSE on training set was converged to minimum faster than the testing data set. Although (RF _ IV, GBM _ IV) having higher number of estimators (tree) led to lower MSE, the gap between training curve and testing curve indicates that the proposed model was more vulnerable to over-fitting issues than others.

The graphs in Fig. 4 and Fig. 5 indicate that the training models on CS data was more effective and caused reduction on MSE with increasing the training size, while the FS prediction error decreased slightly. Hence, the FS prediction was more difficult than prediction of the CS values prediction with the given data-set. This was possibly due to other parameters which can be effective in FS estimation and was not considered in this study.

Considering the number of estimators (tree), the models which were more dense (RF _ IV and GBM _ IV) were reaching the minimum amount of error after giving around 85 records of data as a training set while other models reached their maximum capacity within 55 records of data. In the case of the prospective studies with more data availability, a large number of estimators will be proposed to perform better estimations.

On the other hand, a high level of fluctuation was observed in the training curve of the RF, while GBM looked

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more robust in this term. The RF algorithm was more sensitive to selection of data (train-test splitting) than the GBM developed model, and it more depends on luck as it was shuffled randomly. Therefore, for the cases with harder records (more difficult to predict), the proposed GBM model was more likely to have a better prediction of target values.

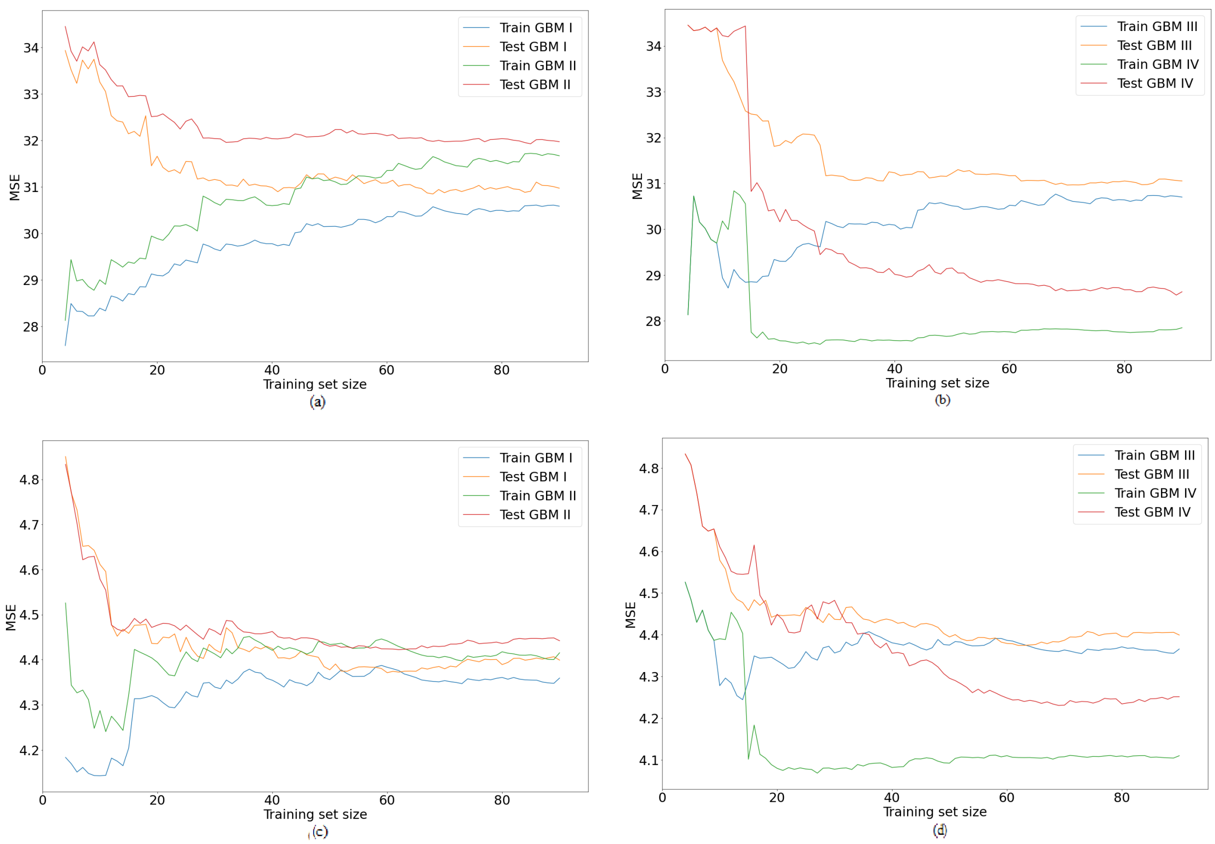

Figure 5: Mean squared error vs training set size values (a) GBM-CS (b) GBM-CS (c) GBM-FS (d) GBM-FS

Considering 25 percent of data as testing and 75 percent for training, the detailed model metrics (R^2, MAE, MSE and training time) for CS and FS were given as below (Table. 3 and Table. 4), respectively. It was observed that models with high number of estimators (trees) are more computationally expensive, but they provide a better accuracy. Concerning the CS as the target value, the best accuracy was obtained via Gradient Boosting Machine (GBM _ IV) with 0.86 for coefficient of determination followed by Random Forest (RF _ IV) with 0.82. It should also be highlighted that, the RF models were computationally more expensive than the GBM proposed models as illustrated in training time, such that the training time for GBM _ IV was approximately 20% of RF _ IV.

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Table 3: Model metrics for CS of CNT-reinforced cementitious material

	Test Data-Set			Train Data-Set			
Model	R^2	MSE	MAE	R^2	MSE	MAE	Training Time (s)
RF_ I	0.69	334	14	0.74	211	11	0.04
RF_ II	0.66	368	14	0.66	273	13	0.02
RF_ III	0.65	376	15	0.7	243	12	0.04
RF_ IV	**0.82**	**95**	**6.8**	**0.99**	**14.57**	**2.54**	**0.36**
GBM_ I	0.4	646	18	0.52	387	16	0.01
GBM_ II	0.27	778	20	0.36	520	18	0.02
GBM_ III	0.38	665	19	0.51	399	16	0.02
GBM_ IV	**0.86**	**71.89**	**6.16**	**0.94**	**59.81**	**5.07**	**0.07**

Similarly by investigating the data provided in Table. 4, Rf IV, and GBM IV were the best models for FS prediction with 0.62 and 0.54 as model accuracy, as illustrated in test data-set.

Table 4: Model metrics for FS of CNT-reinforced cementitious material

	Test Data-Set			Train Data-Set			
Model	R^2	MSE	MAE	R^2	MSE	MAE	Training Time (s)
RF_ I	0.17	7.4	2	0.32	4.2	1.6	0.03
RF_ II	0.13	7.8	2.1	0.21	4.8	1.7	0.01
RF_ III	0.17	7.4	1.9	0.35	3.9	1.5	0.01
RF_ IV	**0.68**	**3.09**	**1.35**	**0.94**	**0.34**	**0.42**	**0.35**
GBM_ I	0.27	6.5	1.9	0.33	4.1	1.6	0.01
GBM_ II	0.2	7.2	2.1	0.22	4.7	1.7	0.02
GBM_ III	0.27	6.5	1.9	0.31	4.2	1.6	0.02
GBM_ IV	**0.69**	**2.95**	**1.18**	**0.82**	**1.06**	**0.72**	**0.07**

As shown in Fig. 6, overall, CS prediction was carried out more accurate than the predictions for FS which was also expected from Pearson correlation heat-map. This figure shows the best proposed models (GBM IV and RF IV) prediction versus real values. It was found that the higher CS (more than 100 MPa) values reached, the more cumbersome task it was required to be done to predict them via proposed models. However, this is not the case for predicting the FS values through the developed models as can be seen in Fig. 6 ((c) , (d)).

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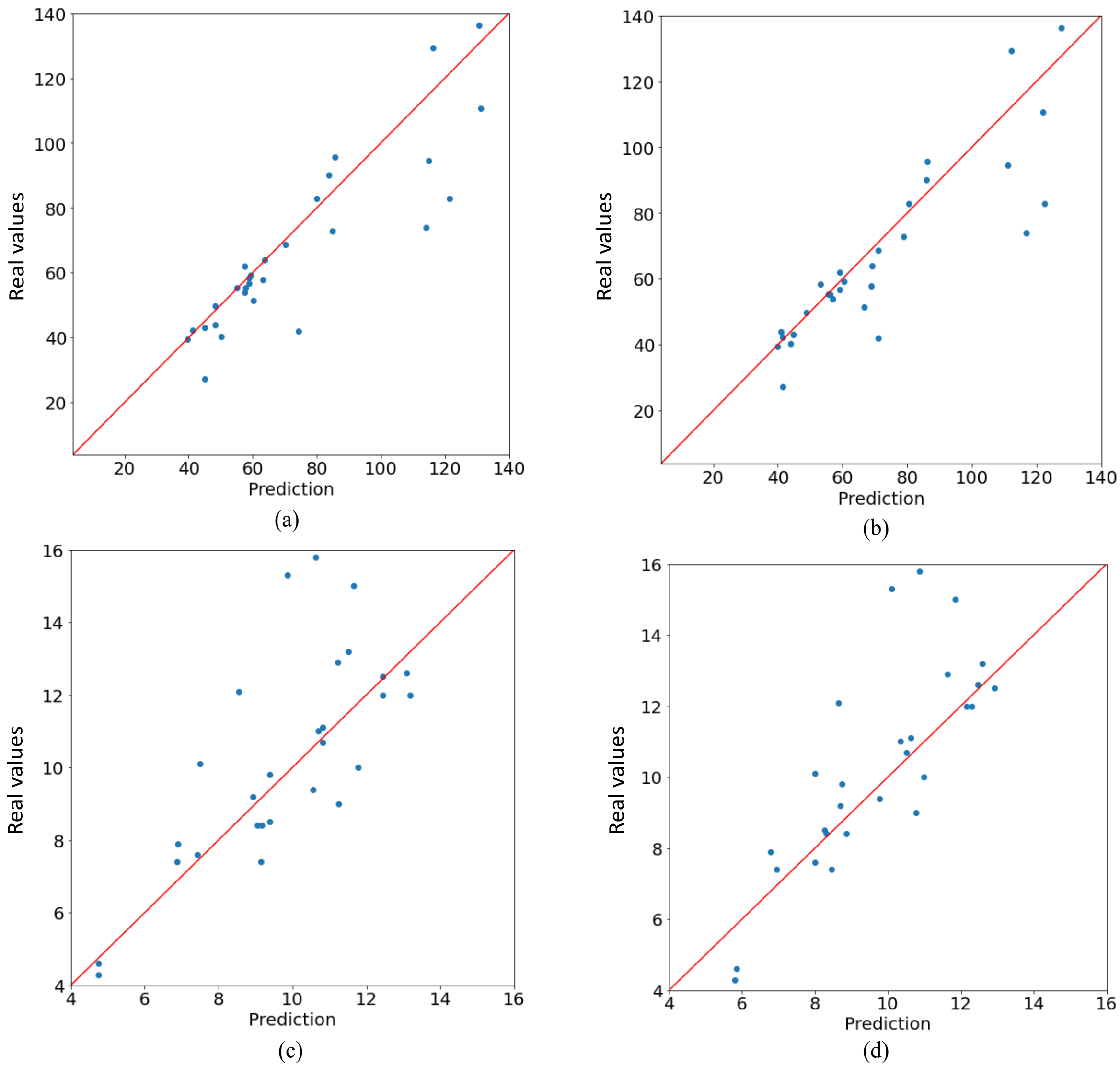

Figure 6: Real versus Prediction values on test data-set (a) GBM-CS (b) RF-CS (c) GBM-FS (d) RF-FS

Testing results of each ML technique applied on the FS and CS was shown in Fig. 7. The target values anticipated via the ML models for the remaining data-sets match well with the real values. It is worth mentioning that there is a few differences between the real and predicted values for both FS and CS which is associated with the parameters that are not defined here. The accuracy of prediction was affected by those parameters which can be improved by increasing the data-set records. Thus, RF and GBM models can be employed to predict the FS and CS of CNT-reinforced cement-based composites.

As it is shown (Fig. 7), the point by point prediction of RF and GBM was very similar, but as mentioned before, GBM could generalize the patterns more comprehensively than RF model, and it had less dependency to the selection of the validation set (luck). Also, both of the algorithms predicted the CS feature with higher accuracy with respect to the FS. It was observed, FS high values (more than 12) were more likely to be underestimated whereas, the majority of the errors regarding this feature fell in overestimation area.

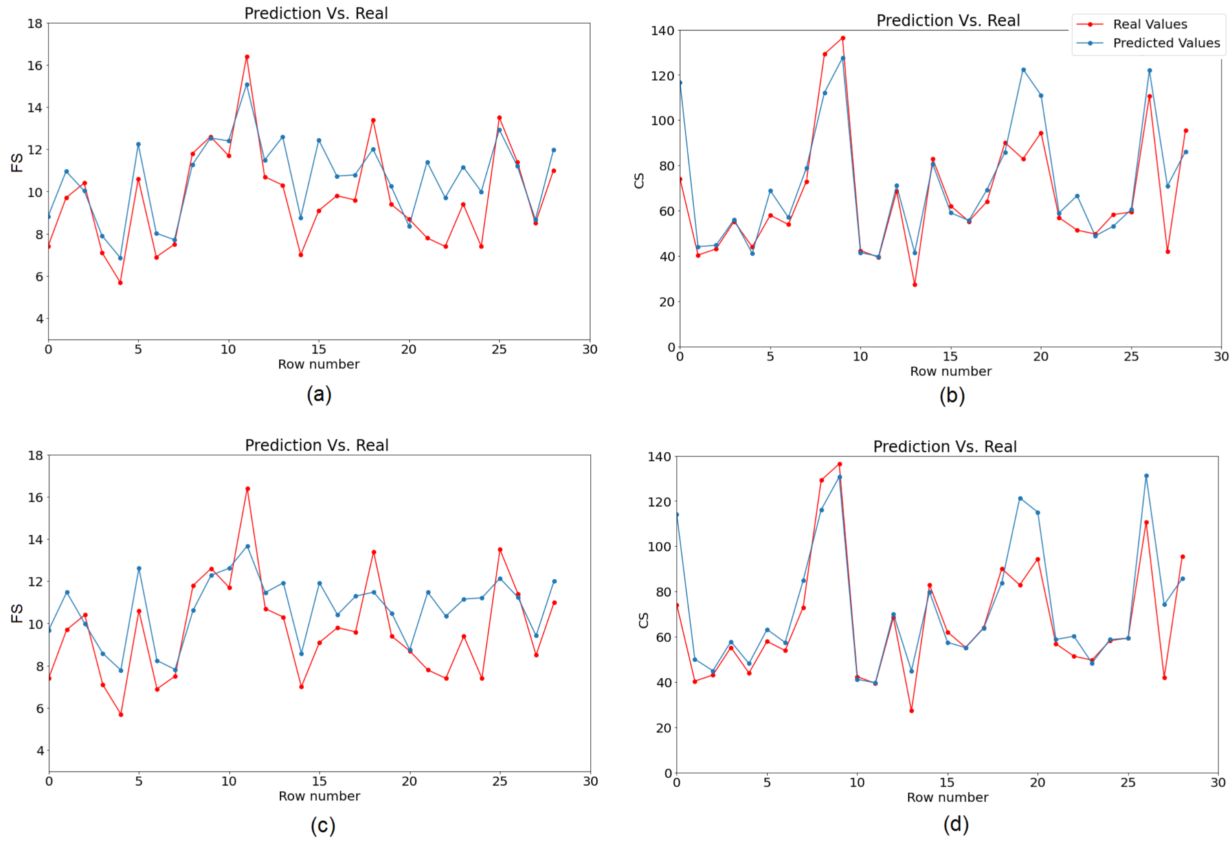

Figure 7: Testing results for each ML model (a) RF-FS (b) GBM-FS (c) RF-CS (d) GBM-CS

4. Conclusions

In this study, the state-of-the-art ensembled ML algorithms including RF and GBM were developed via SciKit-Learn library in Python integrated with the hyper-parameter tuning and k-fold cross-validation method in order to predict the target mechanical attributes, CS and FS, of CNT-reinforced cementitious composite structures. 114 samples were gathered from the literature [20] to train the models.

It was found that the CS values were predicted by the proposed models more accurate than the FS counterparts. 500 estimators (tree) were essential to construct relationship between the nine independent inputs, i.e., cement type, Water-to-cement ratio, Content of carbon nanotubes, external diameter, Length, functionalization method, Curing days, curing temperature, and dispersion method to two different types of strength containing CS and FS. The developed model of GBM has less sensitivity to the alteration of test data than the RF proposed model.

Among all the considered parameters, the effect of the length of CNT on both the target values was negligible, while WC and curing days presented highest influence on the CS and FS, respectively.
The provided data was more suitable for the CS prediction. It was shown that the data-set had skewness for the FS of CNT-reinforced cement-based composite structure which led to reduction in the accuracy of the ML models. Also, it was shown that a few errors included in the predicted models were negligible enough to utilize them for the future studies. These errors could be attributed to undefined parameters such as sonication time and energy. A few parameters that could affect the CS and FS of CNTs were not collected due to the scattered inconsistent previous studies. The results of this study could pave the way for predicting the strength of other composite materials provide that enough, though not large numbers of experimental data are available.

CRediT authorship contribution statement

Faramarz Bagherzadeh Methodology, Investigation, Writing - review & editing, conceptualization **Torkan Shafighfard** Writing-original draft, Conceptualization, Software.

Declaration of competing interest

The authors assert that no potential competing financial interests or personal relationships were appeared to affect this study.

Data Availability

The raw data required to reproduce these findings are available to download from [20]. The processed data required to reproduce these findings are available to download from Mendeley Data:
https://data.mendeley.com/datasets/p9k93zkcns/1 [36],
and the codes for developing mentioned algorithms and graphs are available at the author's GitHub address as follow:
https://github.com/Faramarz-bagherzadeh/MLCompositNanoTube.

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