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Technical Paper

Comparative study of advanced computational techniques for estimating the compressive strength of UHPC

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Abstract: The effect of raw materials on the compressive strength of concrete is a complex process, especially in the case of ultra-high-performance concrete (UHPC), where a higher number of inter-dependent parameters are involved in the strength development. In this era of digitalization, advanced machine learning methods are used to predict the material's mechanical characteristics because of their superior performance compared to conventional and nonlinear statistical regression models. Thus, the goal of the current study is to estimate the compressive strength of UHPC from the designed raw materials using advanced machine learning techniques. The compressive strength of UHPC is predicted from the 14 input parameters, i.e., cement, fly ash, slag, silica fume, nano-silica, limestone powder, sand, coarse aggregate, quartz powder, water, superplasticizer, PE fiber, steel fiber, and curing time. A total of eight machine learning models were compared that include multi-layer perceptron neural network (MLPNN), MLPNN Bootstrap aggregating (MLPNN-BA), MLPNN adaptive boosting (MLPNN-AB), Gradient boosting (GB), Decision tree (DT), DT Bootstrap aggregating (DT-BA), DT adaptive boosting (DT-AB) and Random Forest (RNF). The validation and performance evaluation of the above models were checked by using K-fold cross-validation, mean absolute error (MAE), root mean square error (RSME), coefficient of determination (R2), relative root mean square error (RRMSE), performance index (PI), and Nash Sutcliffe efficiency (NSE). The optimal model was selected based on the results of all statistical checks. It was found the ensembled machine learning models especially decision tree-based models outperform the neural network-based models with higher accuracy and low error. Thus, the recommended machine learning model is random forest having superior prediction capacity followed by DT Bootstrap aggregating and DT adaptive boosting.

Keywords: Compressive strength; UHPC; machine learning; validation; optimal model.

1. Introduction

Ultra-high-performance concrete (UHPC), as a major development in concrete technology in the past two decades, has been used for various civil engineering applications [1-9]. UHPC usually has a 28d compressive strength of UHPC greater than 120 MPa and a dense microstructure. Nowadays, different chemical admixtures and minerals are usually incorporated in concrete depending on strength and durability requirements [10]. Based on the heterogeneous nature of concrete, it is quite complex to predict its accurate compressive strength along with its prevailing factors. The mechanical properties of UHPC rely on different parameters like *w*/*c* ratio, the content of cement, filler, fibers properties, type of pozzolana and superplasticizers, etc. The basic ingredients of UHPC are shown in Figure 1. When the UHPC is reinforced with fibres, the formed ultra-high-performance fiber-reinforced concrete (UHPFRC) has even more complex material properties, which are affected by dosages of cement, supplementary cementitious materials (SCMs), and fibers (single or hybrid type). It is worth mentioning that laboratory testing consumes extensive time and cost. Probabilistic models can be implemented to predict the concrete mechanical properties to avoid time and cost consumed in labor-intensive laboratory processes [11]. However, the applicability of such models for UHPC is still questionable because of UHPC is involved with the use of various material components that can have complex inter-relations [11-13]. For instance, in the case of UHPFRC having various SCMs and fibers, accurate prediction cannot be achieved by using traditional techniques due to the multiple

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numbers of parameters [13]. Exploring an effective computational approach for predicting the hardened properties of UHPC is becoming a critical consideration of engineers and designers recently.

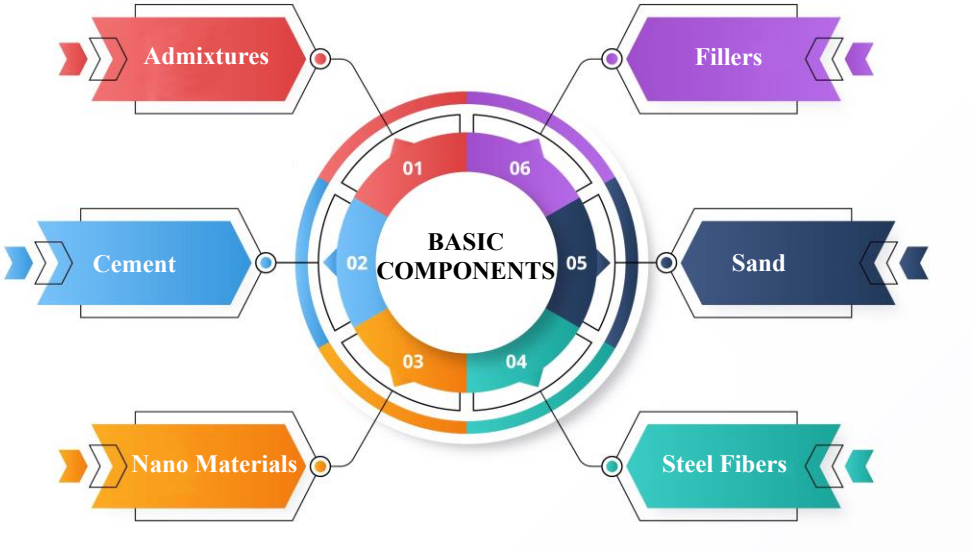


Fig. 1 – Basic ingredients of UHPC

Multiple statistical techniques have been implemented to forecast concrete mechanical characteristics in past decades. Among these, the more prominent are linear, multilinear, and nonlinear regression methods [14-17]. Machine Learning (ML) based on data analysis techniques are also gaining popularity in different study areas [18-22], by which a robust and precise prediction model for the compressive strength of concrete could be developed upon analyzing crucial data [23-26]. In recent studies, artificial neural network (ANN) and Decision trees (DT) have come out with more potential for predicting the more accurate compressive strength [27-29]. Previously, the individual artificial learning model-based prediction systems were used for prediction. Nowadays, several studies resulted in more accurate predictions of ensemble ML techniques than individual ML techniques, which is why ensemble machine learning methods have more popularity for cementitious materials [30]. In the ensemble ML, multiple learning algorithms are used which may achieve a more accurate prediction performance than any constituent learning algorithm alone. The ensemble ML techniques operate differently; such approaches usually train various weak learners initially by deploying training data and then converting the weak learners into stronger ones. These weak learners are individual approaches like a decision tree. Consequently, the exploration of ML techniques needs to be investigated for assisting researchers and engineers in developing the prediction models to optimize UHPC mixes. Therefore, ensemble and individual ML methods are compared in the present study to identify a superlative model to estimate the compressive strength of UHPC.

Nowadays, predicting results with minimum variation in experimental outcomes has been widely evaluated using machine learning (ML) techniques. In experimental procedures, there is a detailed casting and testing procedure having multiple parameters that take a lot of time, effort, and cost. This raises the need for the development of algorithms that are based on modeling through data, accorded with the identification of closely related independent variables and swiftly decreasing the input matrix dimensionality. In an alternative manner, the compressive strength of UHPC can also be proposed for prediction by using machine learning algorithms. Therefore, in this study, different individual and ensembled ML techniques are used for estimating the compressive strength of UHPC. Two different types of analysis approaches are used individual and ensembled ML techniques, i.e., neural network-based approach for multi-layer perceptron neural network models and tree-based approach for decision tree models. Furthermore, an optimal model from both network-based and tree-based models is established. In a nutshell, suitable ensemble learning techniques are recommended in this study for estimating UHPC compressive strength accurately.

2. Machine learning models

2.1 Multi-layer perceptron neural network (MLPNN)

For MLPNN, the nodes are often organized sequentially to form a chain of layers, with one or more hidden units between each layer, as shown in Figure 2. The first stage of the input function is the input data. After that, the hidden layer(s) receives inputs with varied weights dependent on the architectures. The network's updated outputs are almost identical to the observed result after the included bias term. Several ANN architectures employ MLPNN; however, they are usually trained using a backward propagation of errors technique [31]. But all nodes other than the input nodes are subject to nonlinear activation functions, most often sigmoid functions. MLPNN is unique in that each neuron in a layer is linked by weights to all of the neurons in the following layer, allowing for independent computations on input data. The procedure is reversed after the feed-forward iteration is complete. During this cycle, a backward propagation of errors technique would be used to change the weights in the network until the desired fitness level is achieved [32].

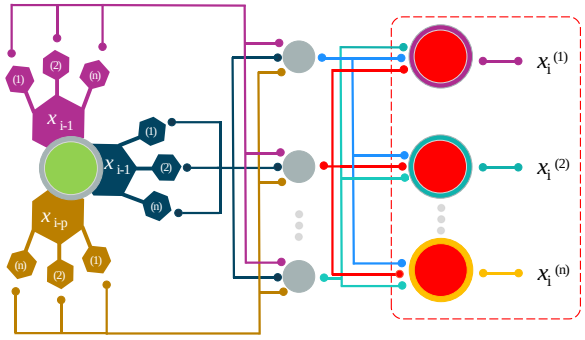


Fig. 2 – Multi-layer perceptron neural network [32]

2.2. Decision tree (DT)

A subclass of machine learning known as a "decision tree" has a tree-like shape with nodes and branches (refer to Figure. 3). A leaf is a node that does not have any outer corners, while an inner node has these features. The classification and regression problems case are divided into several classes via internal conscious planning to a particular function. The training process can observe a decision-making forest from a set of examples. The most influential decision tree may be found by decreasing the fitness function. The dataset is divided many times for every variable. The gap between the predicted and experimental values of the pre-specified optimization process at each division point. Each parameter has an identical number of errors, and a difference between the two terms has been determined based on the worst fitness function values. For the benefit of the model, this process is continuously performed until optimal performance is achieved [33].

2.3. Bootstrap aggregating and adaptive boosting

The optimization of machine learning activities is accomplished via ensemble techniques by combining and combining a large number of inferior forecasts (i.e., sub-models of components). The methodologies of these ensemble techniques support alleviating the issues associated with excessive training data. It is feasible to build a massive number of sub-models/classifier parts (1, 2, 3,…., n-1, n) because of the careful manipulation of the dataset. This might result in a more efficient learner. On the other side, the ideal classification method may be constructed by aggregating combined operations on sub-models that have been independently confirmed. Bagging, along with the bootstrap interpolation approach and advantage collation, is widely regarded as one of the industry's most commonly used ensemble modeling techniques. The quality model is substituted with the first training set (bootstrap trials up to the training set size), which is then changed by the second training set. Many data sets may present many instances in models, while others may not show. Finally, the final result is generated by averaging the outcomes of the component models. As a result of its widespread application, bagging and other ensemble modeling approaches such as the bootstrap interpolation strategy and benefit collation is often recognized as one of the most commonly utilized approaches. After the first training set (bootstrap trials up to the training set size) has been replaced for the quality model, the second training set alters the quality model, and so on. It is feasible that many data groups will produce repeated examples in models, and some may not produce any cases in any model. Eventually, the overall result is obtained by taking the average of the results of the component models and adding them together.

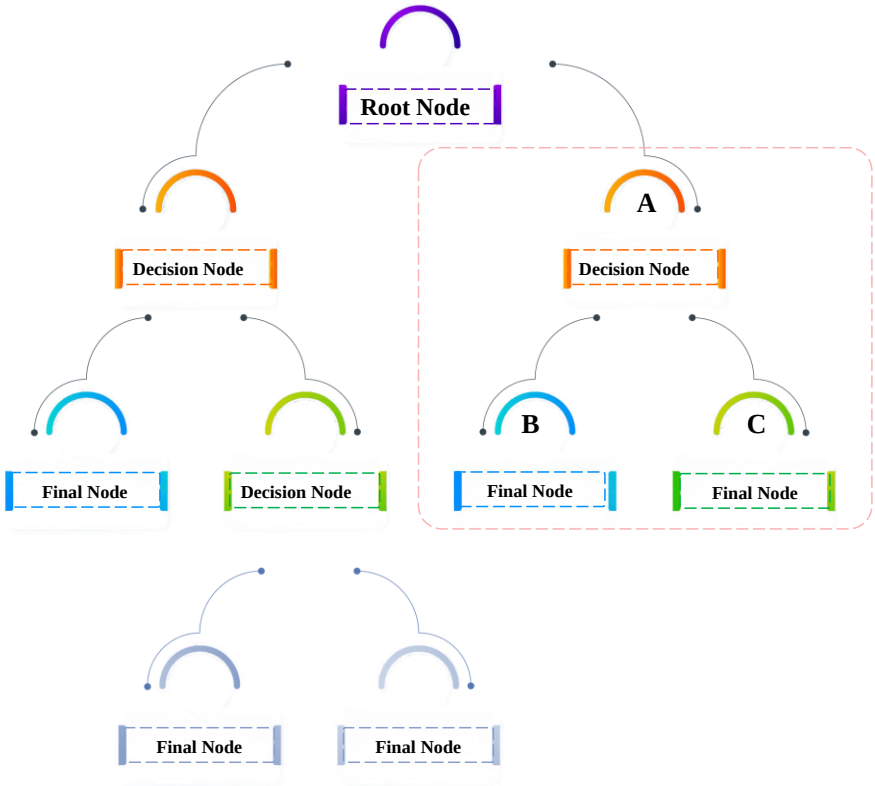


Fig. 3 – Decision tree [34]

2.4. Gradient boosting (GB)

When a series of simple base classifiers are combined, a panel outperforms any single base classification. Boosting is based on the idea of adding new models to an ensemble classifier one at a time. The failure of the whole ensemble is taught to a new model for worse basic learner model with each repetition. The optimization issue is addressed in an ensemble of weak forecasts and is constructed using the gradient descent technique. So, it may be utilized for classification and regression-based tasks. The GB has three parts: the gradient booster, the additive model, a weak learner, and the loss function. In order to maximize the connection between new basic instructors and the negative Gradient of loss factor associated with the whole ensemble, this method employs a number of different techniques. When the functional form is the conventional square-error loss, then error-fitting might occur. In general, it is up to the researchers to choose the loss function, where they have access to a wide variety of loss functions and may apply their own undertaking losses if they choose so [35]. Gradient descent is used by GB to attempt a numerical solution to the error function issue. Any variational loss function may be used to calculate the GB gradient, which is the reverse Gradient of the loss function assessed (see Figure 4).

2.5. Random Forest

The Random Forest Regression (RF) approach has been widely employed for decision tree algorithms by combining a high number of points from a decision tree with bootstrap and aggregation ideas. The development of each tree is controlled by a randomized set of predictor variables in this model, which is also termed as random forest. All current decision trees are converged using bagging (i.e., bootstrap aggregation) [37]. Random forests build each tree using a replacement sample, as demonstrated in Figure 5. Members of the ensemble will use a bootstrap set of pre-prints drawn from the training data set. Separation through tree development no longer allows for the classification split task that was previously recommended. The best possible split over a random subset of characteristics is the one that is not chosen. As a result of this inherent unpredictability, forest bias tends to grow with time (as regards the bias of a single non-random tree) [31]. Its standard deviation is also lowered, which generally more than balances the increase in bias, resulting in a technically better forecast because of the average. All decision trees averaged goal values are used to create an output data point in the regression framework (RF). After then, the combined reaction level of all trees is calculated.

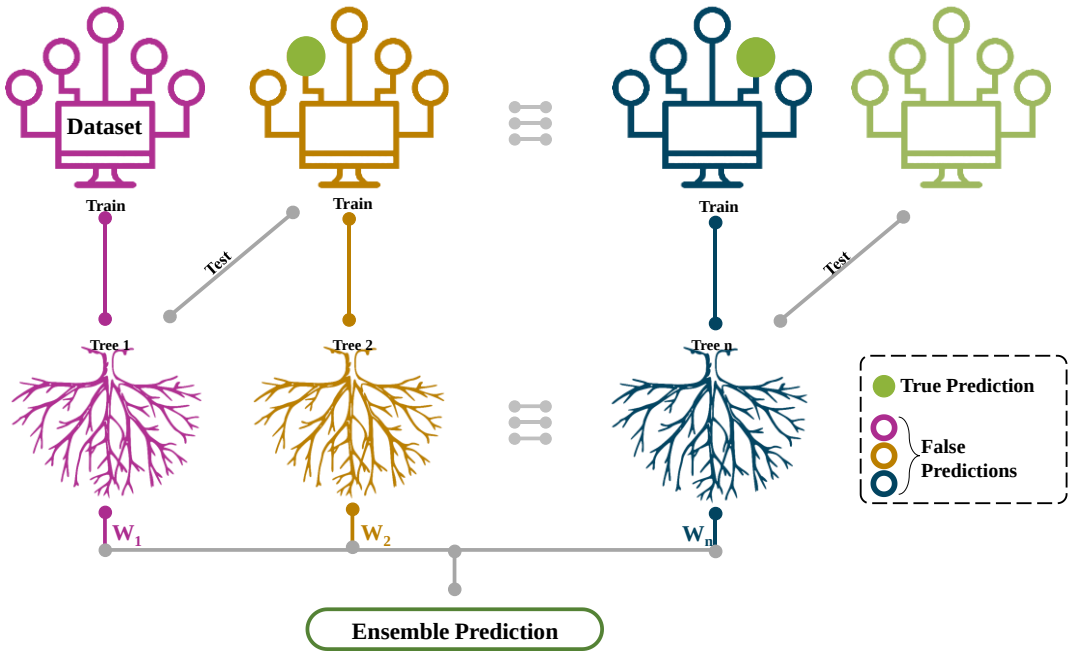


Fig. 4 – Gradient boosting [36]

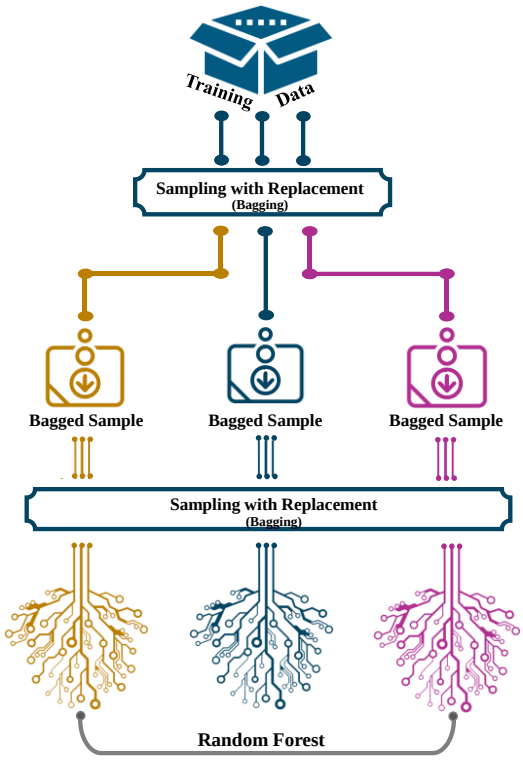


Fig. 5 – Random forest

3. Experimental data set

The statistical summary of the data set for 14 input variables and one output variable (compressive strength) is shown in Table 1. The data set was taken from the literature [38]. However, pre-screening was done on the available data set, and 271 mix proportions of UHPC were selected within the range of 120 MPa to 182 MPa. The reason for pre-screening was to avoid variation of the experimental data because of the different physical and chemical compositions of UHPC raw materials. The input parameters include cement, fly ash, slag, silica fume, nano-silica, limestone powder, sand, coarse aggregate, quartz powder, water, superplasticizer, PE fiber, steel fiber, and curing time. The correlation graph of raw materials for UHPC is illustrated in Figure 6. In this study, the maximum absolute value of the correlation coefficient is 0.65, which indicates that multicollinearity does not occur and the input parameters of the selected mix proportion are reliable for prediction. The multicollinearity occurs because of the strong correlation between input parameters which may lead to the misinterpretation of the effect of input variables. It was reported that multicollinearity occurs if the absolute value of the correlation coefficient is higher than 0.70 [39]. The relative distribution of some input and output parameters is shown in Figure 7. The compressive strength (output) was predicted from the 14 input variables. Table 1 demonstrates the mean, standard error, standard deviation, range, minimum and maximum values of the input variable used in the current study. The compressive strength of UHPC was predicted with the help of python coding used in Spyder of Anaconda software. The predicted results of all models for compressive strength of UHPC are discussed in the next section.

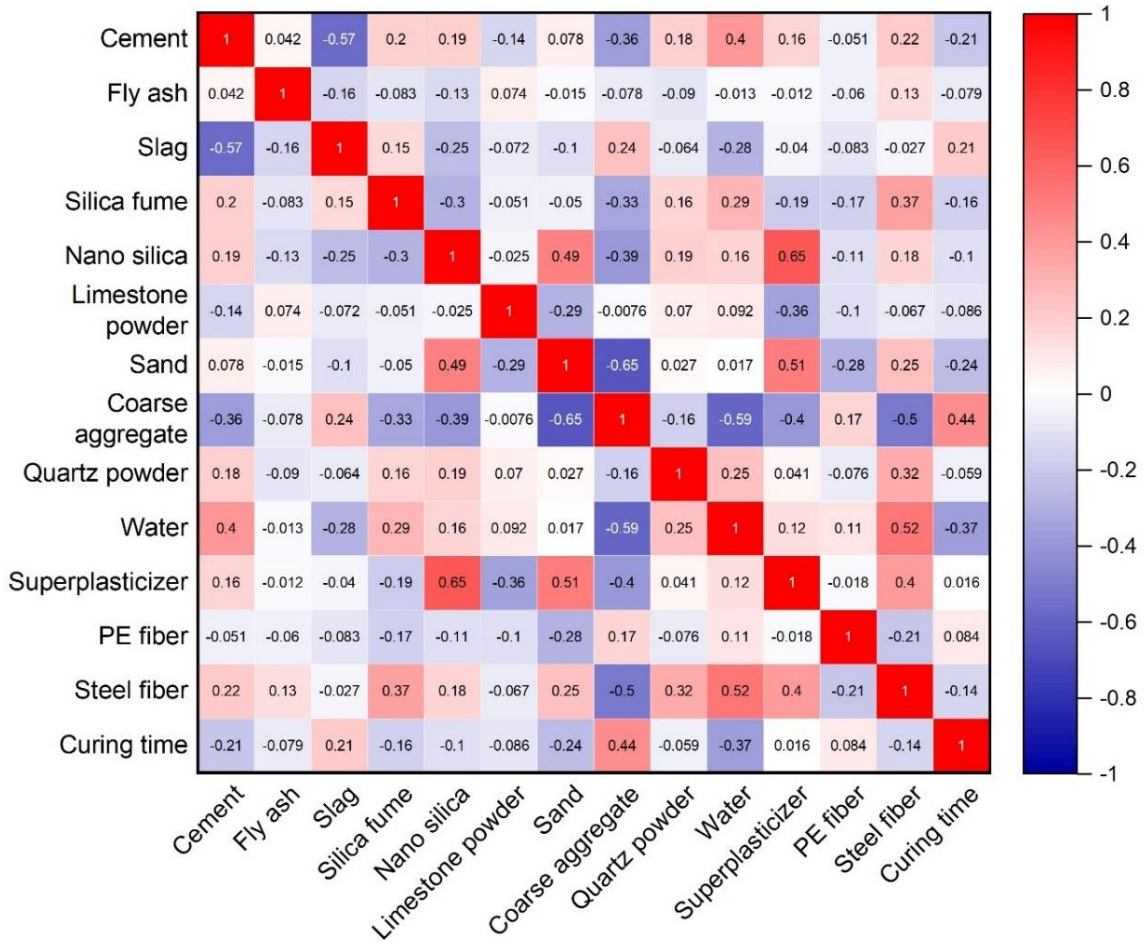


Fig. 6 – The Pearson correlation of input parameters

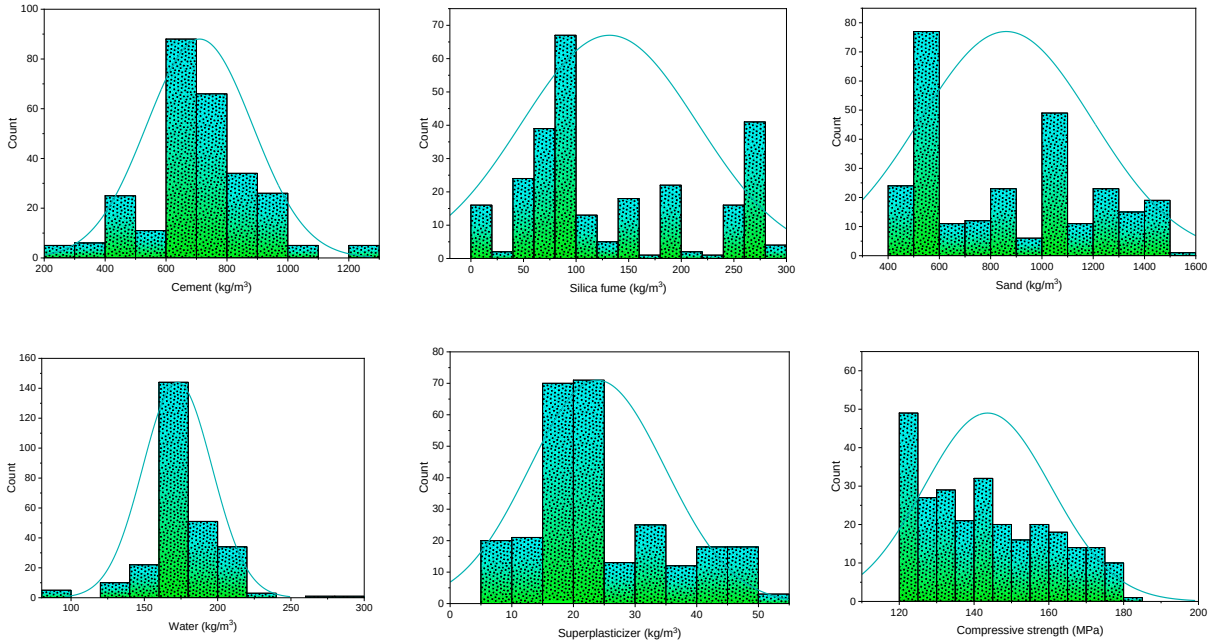


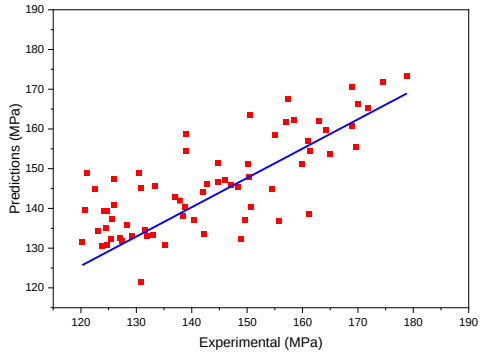
Fig. 7 – Relative distribution of some input and output parameters

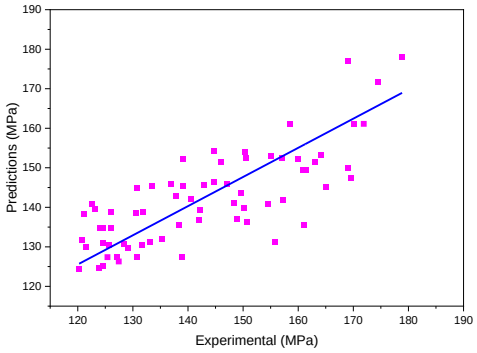
Table 1. Descriptive analysis of data set

Parameters	Mean	Standard Error	Standard Deviation	Range	Minimum	Maximum
Cement (kg/m^3)	711	11	175	1007	270	1277
Fly ash (kg/m^3)	14	4	60	475	0	475
Slag (kg/m^3)	63	8	128	750	0	750
Silica fume (kg/m^3)	132	5	84	291	0	291
Nano silica (kg/m^3)	10	2	38	275	0	275
Limestone powder (kg/m^3)	51	9	145	1058	0	1058
Sand (kg/m^3)	860	20	336	1096	408	1503
Coarse aggregate (kg/m^3)	350	29	471	1299	0	1299
Quartz powder (kg/m^3)	27	6	107	730	0	730
Water (kg/m^3)	173	1	24	196	90	286
Superplasticizer (kg/m^3)	24	1	11	47	5	52
PE fiber (%)	0	0	0	2	0	2
Steel fiber (%)	1	0	1	3	0	3
Curing time (days)	91	9	143	727	3	730
Compressive strength (MPa)	141	1	17	62	120	182

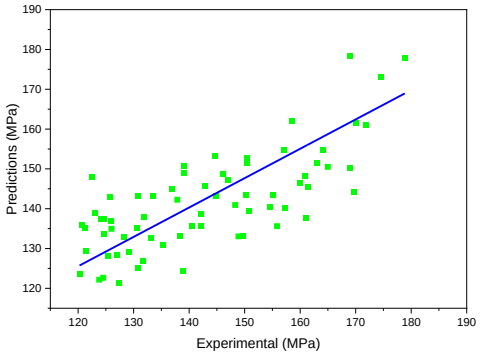
4. Modeling results and discussion

Figure 8 presents the plot between experimental data and estimated values of multi-layer perceptron neural network (MLPNN) for compressive strength of UHPC, where a reasonable agreement is seen with a medium level of variation. The accuracy of estimated results was assessed by evaluating the value of R^2 in Table 2. The more scattered experimental and estimated values for the individual neural network-based model (MLPNN) exhibit less accuracy for predicting the compressive strength of UHPC Figure 8(a). On the other hand, ensembled MLPNN models (Bootstrap aggregating and adaptive boosting) presented better results than individual MLPNN, as evident from the higher value of R^2 in Table 2. The R^2 value for MLPNN, MLPNN-BA, and MLPNN-AB were 0.74, 0.78, and 0.75, respectively. The lower performance of the MLPNN model with the higher error was observed compared to that of other ensembled models. The maximum error values between experimental and predicted values for MLPNN, MLPNN-BA, and MLPNN-AB were 27.6 MPa, 25.4 MPa, and 25.5 MPa, respectively, for compressive strength of UHPC (see Figure 9 (a)-(c)). At the same time, for the 63%, 69%, and 64% of the predicted results, the error difference between experimental and estimated values were less than 5 MPa for MLPNN, MLPNN-BA, and MLPNN-AB, respectively. This means that the MLPNN-BA exhibited low error with higher accuracy than that of MLPNN and MLPNN-AB model. Compared to that individual model, the better progressive performance (better predictions) and robustness (dispersion of the predictions) of ensembled machine learning models were observed. The improved performance of ensembled machine learning models was due to the combined use of multiple sub-models. The better predictive performance of the best model was selected from the analyzed 20 sub-models in ensembled machine learning models. The performance of MLPNN-BA was better than MLPNN-AB because MLPNN-AB increases the complexity by underfitting the training data.

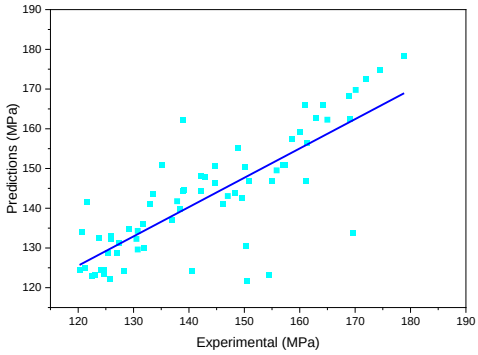




(a) Multi-layer perceptron neural network (MLPNN)



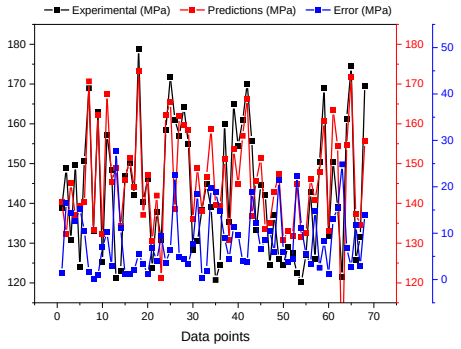
(b) MLPNN Bootstrap aggregating



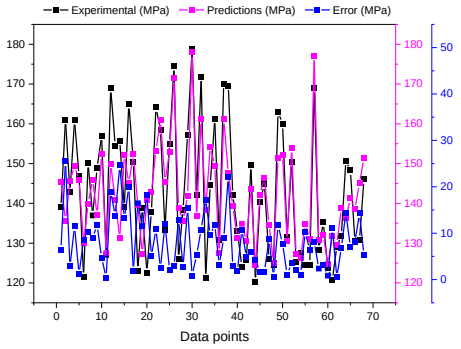
(c) MLPNN adaptive boosting

(d) Gradient boosting

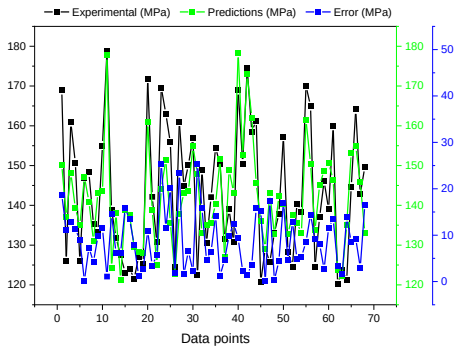
Fig. 8 – Plot of experimental data and predictions: (a) Multi-layer perceptron neural network (MLPNN); (b) MLPNN Bootstrap aggregating; (c) MLPNN adaptive boosting; (d) Gradient boosting



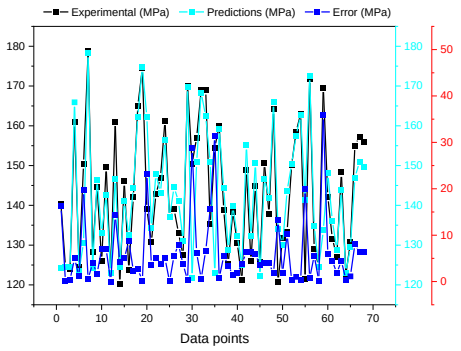
(a) Multi-layer perceptron neural network (MLPNN)



(b) MLPNN Bootstrap aggregating



(c) MLPNN adaptive boosting



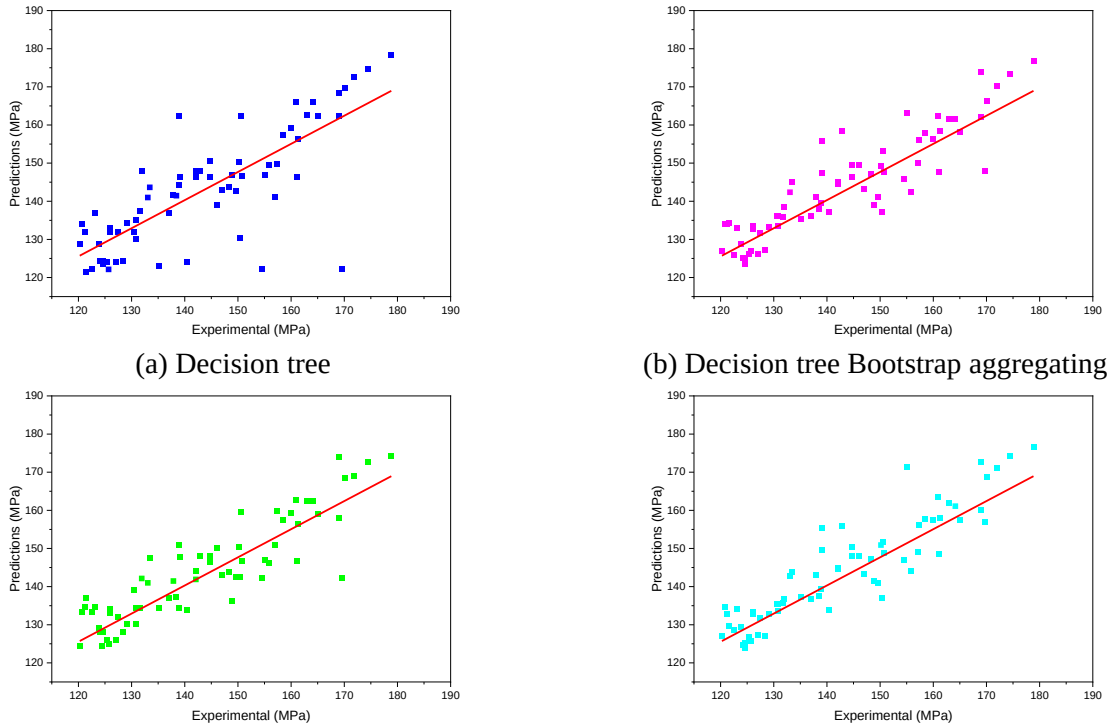
(d) Gradient boosting

Fig. 9 – Data points of experimental and predictions with error: (a) Multi-layer perceptron neural network (MLPNN); (b) MLPNN Bootstrap aggregating; (c) MLPNN adaptive boosting; (d) Gradient boosting

Table 2. Statistical checks for all models

Sr No.	Model description	MAE (MPa)	RSME (MPa)	R2	RRMSE (%)	PI	NSE
1	MLPNN	8.68	10.97	0.74	7.56	0.040	0.52
2	MLPNN Bootstrap aggregating (MLPNN-BA)	8.22	10.30	0.78	7.25	0.041	0.60
3	MLPNN adaptive boosting (MLPNN-AB)	8.87	10.85	0.75	7.65	0.044	0.55
4	Gradient boosting (GB)	6.24	9.79	0.81	6.87	0.038	0.63
5	Decision tree (DT)	6.68	10.33	0.79	7.25	0.041	0.59
6	DT Bootstrap aggregating (DT-BA)	5.28	7.10	0.90	4.93	0.026	0.81
7	DT adaptive boosting (DT-AB)	5.61	7.53	0.89	5.23	0.028	0.78
8	Random Forest (RNF)	5.10	6.76	0.91	4.68	0.020	0.83

The relationship between the experimental and predicted values of compressive strength for decision tree-based models is shown in Figure 10. The closer data point of ensemble decision tree models showed higher accuracy than that of individual machine learning models. However, the random forest machine learning model presented better prediction results of UHPC compressive strength than that of other ensembled machine learning models (DT-BA and DT-AB). The R^2 value of compressive strength for DT, DT-BA, DT-AB and RNF are 0.79, 0.90, 0.89 and 0.91, respectively. The higher performance of the ensembled DT model with the low error was observed compared to that of individual DT models. The reason was that the ensemble model aims to reduce the variance of data and bring the predicted values closer to that mean. The maximum error values between experimental compressive strength and predicted values of DT, DT-BA, DT-AB, and RNF are 47.3 MPa, 21.5 MPa, 27.4 MPa, and 16.3 MPa, respectively (see Figure 11(a)-(d)). For DT, DT-BA, DT-AB, and RNF, the error values of 80%, 86%, 82%, and 88% between experimental and estimated results were less than 5 MPa, respectively. This indicates a very higher accuracy with a low error rate of the RNF model than that of DT, DT-BA, and DT-AB for compressive strength prediction of UHPC. The improved performance of ensembled machine learning models was due to the combined use of multiple decision trees for the optimal predictive performance of UHPC compressive strength. In general, the better performance of decision tree models was observed than that of neural network-based models. Thus, the ensembled decision tree model (Random Forest) is suggested for estimating the accurate and precise results of UHPC compressive strength.



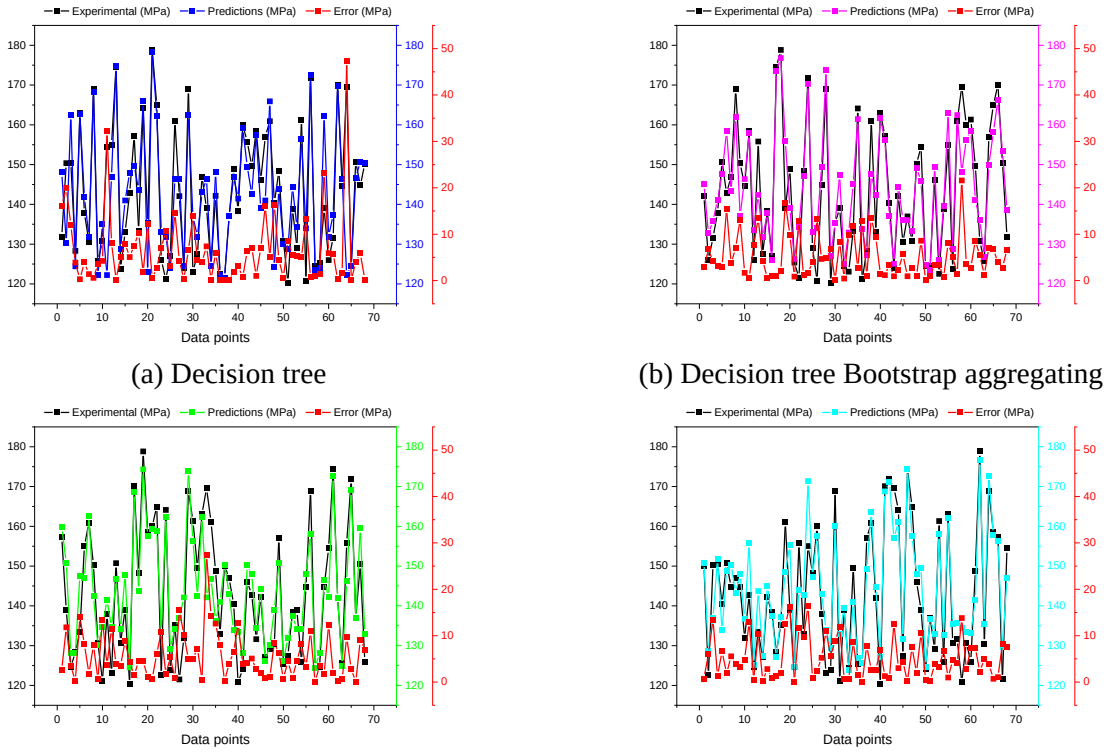
(a) Decision tree

(b) Decision tree Bootstrap aggregating

(c) Decision tree adaptive boosting

(d) Random Forest

Fig. 10 – Plot of experimental data and predictions: (a) Decision tree; (b) Decision tree Bootstrap aggregating; (c) Decision tree adaptive boosting; (d) Random Forest



(a) Decision tree

(b) Decision tree Bootstrap aggregating

(c) Decision tree adaptive boosting

(d) Random Forest

Fig. 11 – Data points of experimental and predictions with error: (a) Decision tree; (b) Decision tree Bootstrap aggregating; (c) Decision tree adaptive boosting; (d) Random Forest

5. Validation and performance evaluation of all models

The induvial and ensembled machine learning techniques were considered to estimate the compressive strength (output) of UHPC from its raw ingredients (input parameters). K-fold cross-validation is used to evaluate a model's accuracy using data samples [32, 40-42]. Figure 12 demonstrates the flowchart of K-fold cross-validation. The training dataset is primarily divided into *k* folds of equivalent size, and the model is then tested on one of the folds while the others are trained. The trained model's loss function is then assessed. After the *k* folds are completed, the mean loss function is used to select the model. The training dataset is divided into ten k folds. The K-fold cross-validation of all models with MAE and RMSE are illustrated in Figures 13(a) and 13(b), respectively. It was found that all decision tree models had presented a low error compared to that of neural network models. This indicates the better predictive performance of decision tree models. By comparing the decision tree models, it was observed that ensembled models showed better results than that of the individual model. Moreover, among all other ensembled models, the random forest model exhibited the lowest error difference between experimental and predicted values. The Taylor diagram was used to compare all models, as shown in Figure 14. The random forest outperforms other models with a higher coefficient of determination of 0.91, followed by DT Bootstrap aggregating ($R^2 = 0.90$) and DT adaptive boosting ($R^2 = 0.89$). Similarly, the low RMSE of random forest, DT Bootstrap aggregating, and DT adaptive boosting indicate the better performance of these models compared to all other models. Therefore, it can be concluded that the higher R^2 and least error values of ensembled decision tree models provide more reliable results than the other machine learning models.

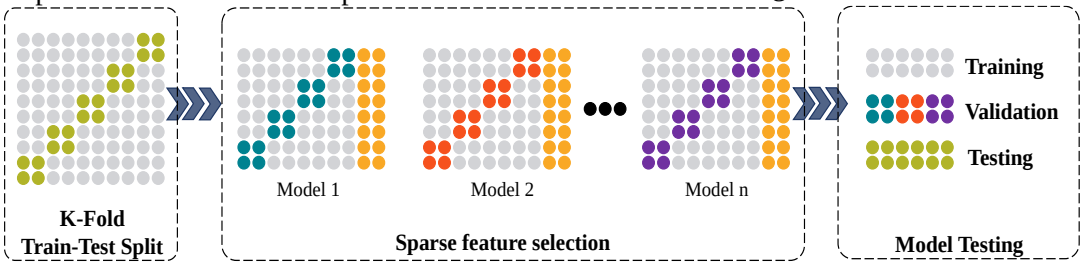
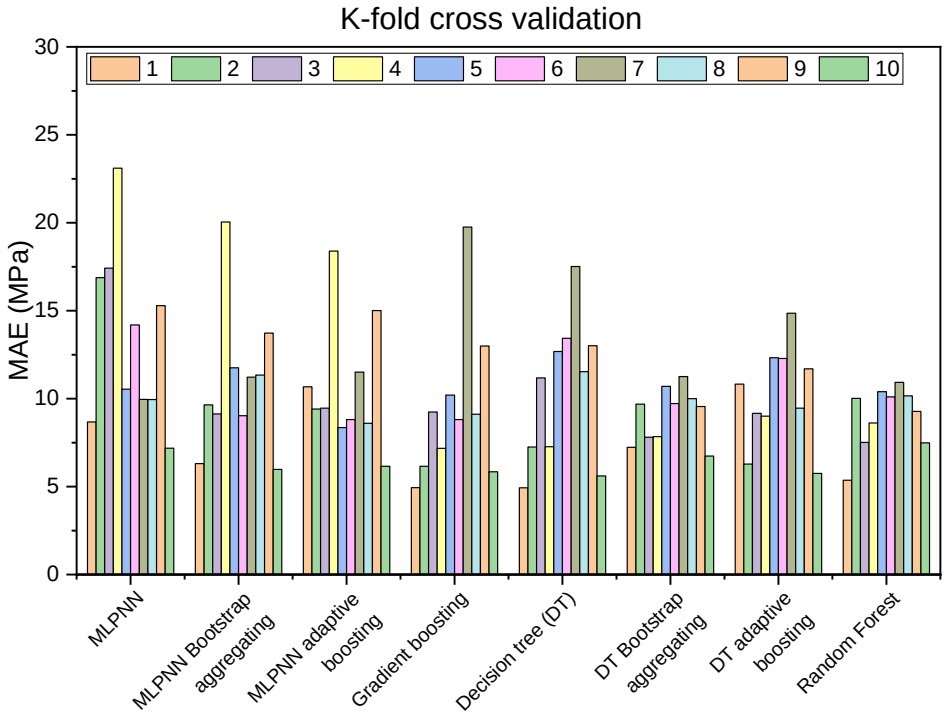
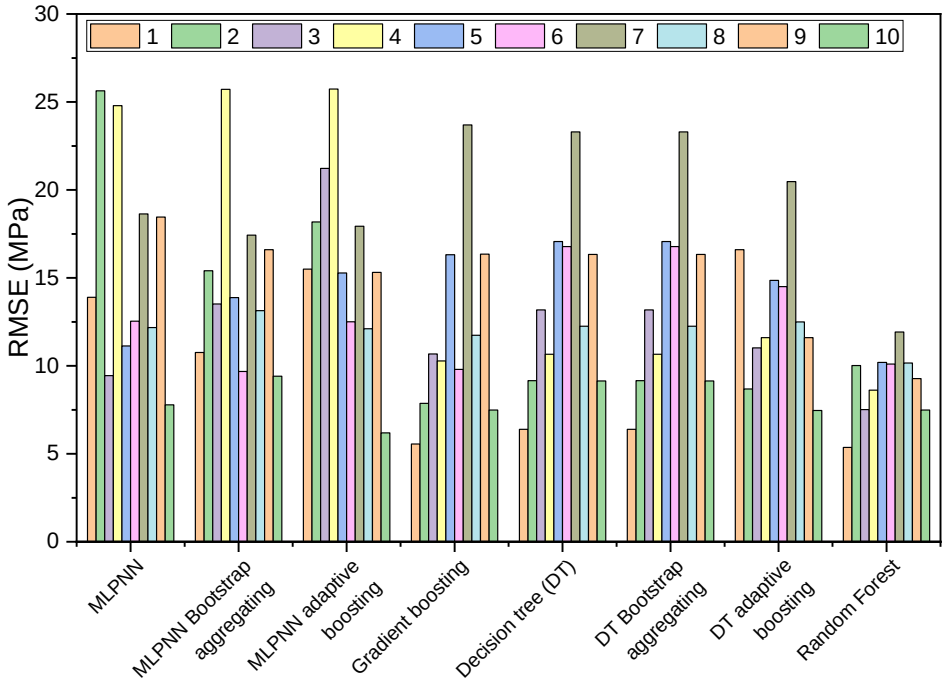


Fig. 12 – K-Fold cross-validation [31]



(a) MAE



(b) RMSE

Fig. 13 – K-fold cross-validation of all models: (a) MAE; (b) RMSE

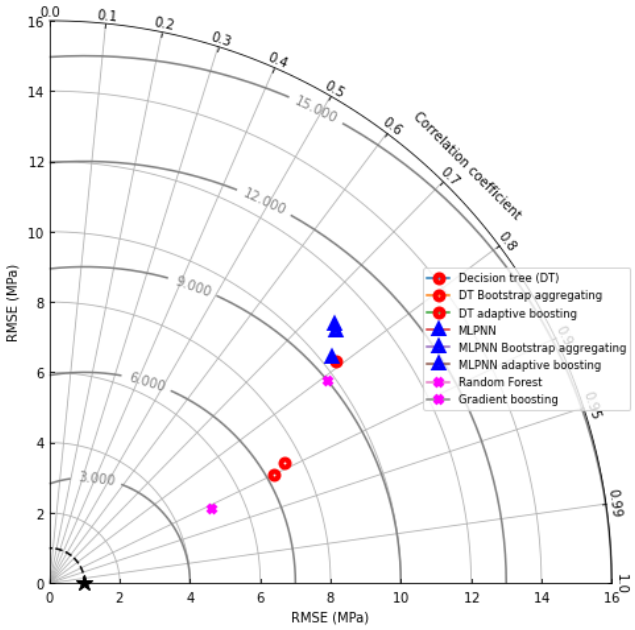


Fig. 14 – Taylor diagram for comparison between all models with RMSE and R^2

A total of six statistical indicators were used to evaluate the model performance, i.e., mean absolute error (MAE), root mean square error (RSME), correlation coefficient (R^2), relative root mean square error (RRMSE), performance index (PI), and Nash Sutcliffe efficiency (NSE) [43, 44]. NSE ranges from negative infinity to one, whereas one indicates perfect model fit. The MAE, RMSE, NSE, and R^2 are often employed in modeling, with the caution that the MAE must be smaller than the RMSE in order for the models to have higher predictive accuracy. When NSE exceeds 0.65, a correlation is regarded as very good, while the model is deemed excellent when R^2 is greater than 0.8, with RMSLE approaching zero [32, 45]. Models must have a PI of less than 0.2 to work well. The RRMSE percent is between 0 and 10% for models with exceptional and outstanding performance [46, 47]. Table 3 shows the mathematical formulae for the statistical indicators stated above and the permissible ranges for each of these indicators.

Table 3. Statistical checks and acceptance criteria

Statistical checks	Acceptance criteria	Reference
$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}\lvert \mathrm{Exp_i} - \mathrm{Predicted_i}\rvert$	MAE < RMSE	[46, 47]
$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(\mathrm{Predicted} - \mathrm{Exp_i})^2}{N}}$		
$R^2 = \frac{\sum_{i=1}^{n}(\mathrm{Exp_i} - \overline{\mathrm{Exp_i}})\ (\mathrm{Predicted_i} - \overline{\mathrm{Predicted_i}})}{\sqrt{\sum_{i=1}^{n}(\mathrm{Exp_i} - \overline{\mathrm{Exp_i}})^2\ \sum_{i=1}^{n}(\mathrm{Predicted_i} - \overline{\mathrm{Predicted_i}})^2}}$	For good model > 0.80	[46-48]
$\mathrm{RRMSE}\ (\%) = \frac{1}{\lvert e\rvert}\sqrt{\frac{\sum_{i=1}^{n}(\mathrm{Exp_i} - \overline{\mathrm{Predicted_i}})^2}{n}} \times 100$	0-10% for excellent model 11-20% for good model	[46, 47]
$\mathrm{PI} = \frac{\mathrm{RRMSE}}{1 + R}$	For good model < 0.2	[46, 47]
$\mathrm{NSE} = 1 - \frac{\sum_{i=1}^{n}(\mathrm{Exp_i} - \overline{\mathrm{Predicted_i}})^2}{\sum_{i=1}^{n}(\mathrm{Exp_i} - \overline{\mathrm{Exp_i}})^2}$	For very good model > 0.65	[47]

The various statistical checks were used to evaluate the performance of models, as presented in Table 2. The MLPNN, MLPNN Bootstrap aggregating, and MLPNN adaptive boosting had a higher error and lower efficiency than other decision tree-based models. The reason is already discussed in Section 4. The lower value of MAE, RRMSE, PI represents the higher accuracy of models, while a higher value of NSE denotes the enhanced estimation efficiency of models in Figure 15. It was observed that random forest (RRMSE = 4.68, PI = 0.02, NSE = 0.83) was an accurate machine learning technique with better-predicting capabilities of UHPC compressive strength as compared to that of all other models. Afterward, the DT Bootstrap aggregating followed by DT adaptive boosting exhibited better performance, as evident from RRMSE, PI, and NSE values.

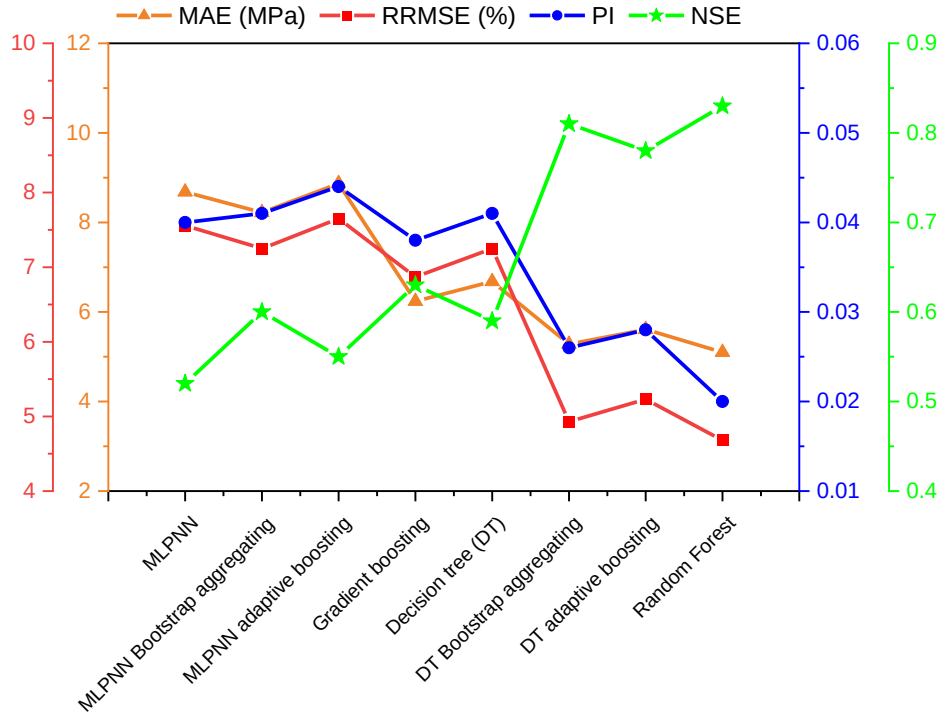


Fig. 15 – Statistical checks by MAE, RRMSE, PI, and NSE

6. Limitations, challenges, and future directions

The scholars should be aware of some limitations and challenges regarding machine learning algorithms. The first challenge is choosing the appropriate machine learning algorithm, which is not an easy task for researchers of the concrete engineering community who are unfamiliar with machine learning. Numerous machine learning methods have been implemented for different types of concrete, but no consensus has been reached. Some studies reported that decision tree-based models outperform neural network-based models, while others reported the opposite results [49]. Although several comparison and benchmarking studies have been conducted in the literature to determine the most appropriate algorithms for various types of concrete, the results are still inconsistent. The inconsistency was for the reason that different databases/mix proportions were used to predict the performance of the same materials. It is worth mentioning that the reliability of these models is greatly dependent on the selected database/mix proportions used for the evaluation, which makes the scholars reluctant to use machine learning approach. Given that each of the machine learning algorithms outlined above has distinct benefits and disadvantages, the best appropriate model is chosen depending on a variety of variables. The nature of the link between the components in concrete and its mechanical strength is a significant aspect influencing the model selection. If this connection is very nonlinear and impacted by various factors, utilizing models such as neural network-based models would be a smart choice due to their superior capacity to solve problems in nonlinear environments with a low error rate [23]. However, decision trees algorithms can be used when model transparency is necessary because they create explicit mathematical formulae that accurately represent the physical link between inputs and outputs [23]. While individual machine learning models are still less accurate than ensemble models, using ensemble models can improve accuracy but with increased computation time and model complexity. As a result, users without any background knowledge of machine learning,

particularly concrete engineers and practitioners, should compare and test their produced machine learning-based models before proposing them for the practical application of a particular material. Therefore, this study examined a comparative evaluation of a wide array of neural network-based approaches and decision tree-based approaches of machine learning algorithms and their relative efficacy in predicting the compressive strength of UHPC. The database used in this investigation was restricted to 271 mix proportions. Indeed, appropriate database handling and monitoring are required since they are essential parts of engineering fields. The recommended model for the prediction of compressive strength was random forest from the present investigation. Random forest can be used to calculate the compressive strength of different types of concrete but results might be different because of the reasons mentioned above.

The challenging task associated with machine learning algorithms is selecting the appropriate hyperparameters. Indeed, each machine learning method contains various hyperparameters that may be adjusted to increase the model's accuracy and/or training speed. As a result, they must be fine-tuned during the testing and validation stages to get the best values. This is also a problem for concrete engineers and practitioners unfamiliar with machine learning. Another challenge with machine learning algorithms is their "black box" feature, making it difficult to grasp how they operate. As a result, a trade-off between accuracy and interpretability is essential. In other words, complicated models are necessary for some applications to achieve more accuracy; knowing how the algorithm makes decisions is critical before suggesting a machine learning-based model for practical usage.

Although this study used a diverse variety of data sets with 14 input variables, the database and input parameters should be expanded to improve the responsiveness of the utilized models. Additionally, this research focused exclusively on compressive strength prediction and neglected the tensile, flexural, and ductility of UHPC.

7. Conclusions

UHPC is one of the most efficient construction materials used in many civil engineering applications. However, estimating the compressive strength of UHPC is still a challenging task because of the high complexity of its mixture. Recently, the Artificial Intelligence (AI) methods have shown more precise results for solving classification and regression problems than conventional methods. Therefore, the present study has employed eight advanced machine learning techniques for predicting the compressive strength of UHPC. The methods consist of multi-layer perceptron neural network (MLPNN), MLPNN Bootstrap aggregating (MLPNN-BA), MLPNN adaptive boosting (MLPNN-AB), Gradient boosting (GB), Decision tree (DT), DT Bootstrap aggregating (DT-BA), DT adaptive boosting (DT-AB) and Random Forest (RNF). Six statistical indicators were used to assess the validity and performance of proposed models, and an optimal model is recommended for estimating the compressive strength of UHPC. The following conclusions are drawn:

- Decision tree-based models presented a higher accuracy for estimating the compressive strength of UHPC than neural network-based models.
- Each ensembled machine learning model with twenty sub-models presented more accurate and precise estimation for compressive strength prediction than an individual model.
- The ensembled decision tree models, i.e., DT-BA, DT-AB, and RNF, presented acceptable results for k-fold cross-validation with low error values of MAE and RMSE and were considered as suitable models for estimating the compressive strength of UHPC.
- The error range of mean absolute error (MAE), root mean square error (RSME), relative root mean square error (RRMSE), and performance index (PI) error range for ensembles decision tree machine learning models were significantly lower as compared to individual machine learning models (DT and MLPNN) and other neural network-based models (MLPNN-BA and MLPNN-AB).
- The coefficient of determination (R^2) and Nash Sutcliffe efficiency (NSE) values for ensembled decision tree-based models was in the acceptable range of 0.89-0.91 and 0.78-0.83, respectively. The higher R^2 and NSE values of decision tree-based models indicated the better predictive accuracy for estimating the compressive strength of UHPC.
- The better predictive accuracy of ensembled decision tree models (DT-BA, DT-AB, and RNF) with the low error was observed. From the overall comparison of all models, it was found that the random forest was the most effective and reliable advanced machine learning technique compared to all the other models.

Based on the above study, it is evident that Artificial Intelligence techniques can predict the compressive strength of UHPC. The validation of

models by statistical checks presented a good agreement with the low error between the estimated and experimental values. Thus, machine advanced learning techniques can forecast the experimental values from the raw materials/ingredients that could minimize the experimental effort (particularly during trials), cost, and time. However, there are still certain limitations, and challenges as discussed above in Section 6, which need to be considered in future.

CRediT authorship contribution statement:
Mehran Khan: Conceptualization, Methodology, Investigation, Validation, Writing – original draft, Writing – review & editing. Jian-Cong Lao: Data curation, Formal analysis, Writing – review & editing. Jian-Guo Dai: Conceptualization, Methodology, Visualization, Writing – review & editing, Funding acquisition, Supervision.

Declaration of competing interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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