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DATA-DRIVEN PREDICTION MODEL FOR THE COMPRESSIVE STRENGTH OF HIGH-VOLUME FLY ASH CONCRETE USING MACHINE LEARNING ALGORITHMS

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KEY WORDS: Sustainable Concrete, High-Volume Fly Ash (HVFA) concrete, compressive strength, Machine Learning (ML), Regression.

ABSTRACT:

The assessment of concrete properties by conventional methods was uneconomical and time-consuming. The 28-days waiting period to assess its compressive strength may lead to construction delays. The advancement of Machine Learning (ML) technology can help to solve this issue by developing ML model to determine the compressive strength of the concrete, thereby avoiding the waiting period to start the subsequent work in construction. However, there was no prediction model has been developed for assessing the compressive strength of the High-Volume Fly Ash (HVFA) concrete and especially, the model that considers the accelerator as an input variable was not found. This paper introduces a ML prediction model to estimate the compressive strength after 28 days using various algorithms including Linear Regression (LR), k-Nearest Neighbor (kNN), Random Forest (RF), Support Vector Regressor (SVR), Gradient Boost Regressor (GBR), CAT Boost (CATB) regressor and Extreme Gradient Boosting (XGB). It was concluded that CATB model accurately predicts the compressive strength with R^2 of 0.93, RMSE of 4.24 N/mm^2 and MAE of 3.05 N/mm^2.

1. INTRODUCTION

The conventional method of compressive strength determination consumes a huge time, material and labour. The compressive strength test was generally conducted after 28 days of curing which resulting in a minor delay in the next construction phase. Disregarding the determination of concrete properties by conventional testing will restrict quality control. Thus, an efficient and reliable technique for the determination of compressive strength is vital for maintaining quality even in the earlier design phases. Artificial Intelligence (AI) techniques can fulfil the above requirements. Machine Learning (ML) is a sub-field that is the science of investigation and the application of law of the activities of human insight. In civil engineering, various issues occur especially in designing and construction management due to various vulnerabilities that cannot solely be resolved through arithmetic, materials science and mechanics evaluation, but also rely on the expertise of professionals. Many researchers have employed AI methods to address tedious issues. Numerous literatures (Topcu & Saridemir, 2008; Belalia et al. 2017; Ramachandra & Mandal, 2020; Sevim et al., 2021; Khursheed et al., 2021; Huang et al., 2022; Verma et al., 2023) used AI techniques to determine the compressive strength of fly ash-based concrete. The available literature regarding the prediction of the compressive strength of HVFA concrete was very limited. Rajeshwari & Mandal (2019) developed the ANN model for predicting the compressive strength of HVFA concrete by utilizing the literature and experimental data of about 282 datasets. The input parameters considered are quantity of fly ash, cement, fine aggregate, coarse aggregate, super plasticizer and type of fly ash. Murugan et al., (2014) developed a regression model to determine the compressive strength of HVFA concrete using the experimental datasets. The input parameters considered are quantity of fly ash, fine aggregate, coarse aggregate, super plasticizer and curing type. Prasad et al., (2009) introduced an ANN model for predicting the compressive strength of HVFA based SCC concrete. The input parameters taken into account include cement, w/b, w/c, fly ash, coarse aggregate, fine aggregate, admixtures and silica fume. Azimi-Pour et al., (2020) developed the SVM model for predicting the compressive strength of HVFA SCC concrete using data of approximately 340 SCC mix compositions. The input data used are cement, w/c, fly ash, admixture, silica, fine arrogate and coarse aggregate. Hashmi et al., (2023) developed the hybrid optimization model combining Genetic Algorithm (GA) and ANN for predicting the compressive strength of HVFA concrete using data from 64 concrete mixes. The input parameters taken are w/b, fly ash, quantity of fine aggregate, coarse aggregate and total aggregate. Titiksh & Wanjari (2023) developed the model using Multiple Linear Regression (MLR) ANN for predicting the compressive strength of HVFA concrete and found that the developed model effectively predicts the compressive strength with R^2 value of 0.858. It was observed that the above literature does not consider the accelerator as an input variable. It is clear that the inclusion of accelerator could accelerate the pozzolanic reaction of HVFA concrete to the initiate the strength gain. To the best of current knowledge, this is the first study to consider the accelerator as an input parameter for the development of prediction model for HVFA concrete.

2. METHODOLOGY AND DATASET DESCRIPTION

This study aims to study is to develop the prediction model for determination of compressive strength of HVFA concrete utilizing the concrete mix proportions as a data collected from open-sources, existing studies and experimental dataset.

2.1 Experimental investigation

A HVFA concrete mix was proportioned using IS: 10262-2009 standards using the OPC 53 grade cement (specific gravity of 3.15; loss of ignition of 0.98%), class-F fly ash (50% replacement, specific gravity of 2.2, loss of ignition of 1.9%), locally sourced river sand (Zone-II, specific gravity of 2.7, water absorption rate of 0.67%). A calcium nitrate-based accelerator (specific gravity 1.82) was added in varying percentages (0%–5%) to enhance pozzolanic reactions. Ten M30-grade concrete mixes were prepared with accelerators from 0%–5%. Mixing involved sequentially combining aggregates, cement, water, and accelerator, followed by casting 150 mm x 150 mm x 150 mm cube specimen. Compressive strength was determined after curing of cube specimen at 7, 14 and 28 days through Universal Testing Machine (UTM) as per IS: 516-2021. Figure 1 illustrates the compressive strength of various HVFA concrete added with varying percentages of accelerator. The addition of accelerator significantly enhances early strength gain. At, 7 days of curing, the HVFA concrete with accelerator additions of 0.5%-5% achieved around 23.2% to 68.3% of its 28 days target compressive strength. Compared to prior studies, this demonstrates remarkable improvement in strength with accelerators.

The hydration of C_3S and C_2S is key, with C_3S contributing to early-age strength and C2S aiding later strength. Accelerators, particularly calcium chloride, expedite cement and fly ash hydration, producing $Ca(OH)_2$ and C-S-H, which react with fly ash to form additional binder compounds like C-S-H and C-A-H. These reactions enhance compressive strength, which was 4.6%-8.8% higher than OPC at 28 days. Optimal performance was observed at 2.5% accelerator dosage, while higher dosages reduced strength due to excess water in the accelerator. This finding was found to be aligned with Natarajan et al., (2025), who also reported that optimum accelerator dosage for concrete is 2.5%.

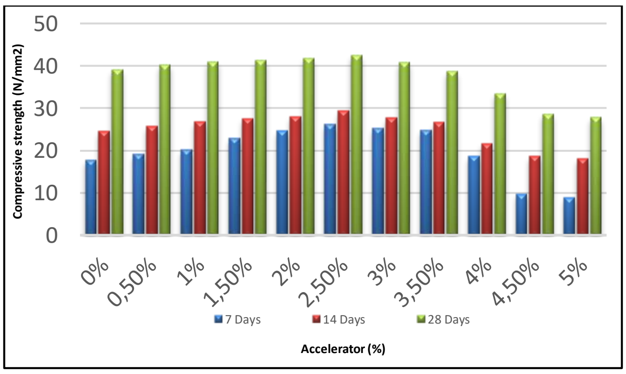

Figure 1. Compressive strength of concrete

2.2 Machine Learning (ML) algorithms

Linear Regression (LR)

The LR primarily focuses on conditional probability. In LR, the predictor variable and dependent variable are linearly interrelated. The expression for the LR was given as;

$$Y = mx + c + e$$

where m defines the slope of the line; c defines the intercept and e defines the error.

k-Nearest Neighbor (kNN)

The kNN is an instance-based algorithm utilized for both classification problem and regression problems. It looks for the k-data points nearest to the test objects and utilizes the features of these neighbours for classifying the new object. For instance, a distance is assessed between every instance in both the testing and training datasets. To predict the new response value i.e., compressive strength, KNN finds the k-nearest neighbours $x_i(x'_1, x^i_2, , , , . x'_k)$ in the space of the data attributes and utilizes a predefined function of the response value of these k-Nearest Neighbours. When utilizing kNN to compute the predicted value of a data point, the model identifies the k-nearest data points from training dataset and utilizes their mean value as predicted value for the new data points.

Decision Tree (DT)

The DT algorithm is a decision-making technique that assess the likelihood that expected net present value is equal or exceed zero and evaluates its feasibility based on the know probabilities of different situations by constructing a decision tree. It is a visual technique that directly employs probability analysis. In ML, the DT algorithm serve as a prediction model that illustrates a mapping relationship between objects features and object values. It is a sub-set of ML characterized by a tree-like structure with nodes and branches. The nodes without outgoing corners are referred to as leaves, while the nodes possessing outgoing corners are known as inner nodes.

Random Forest (RF)

RF is a powerful and reliable ML algorithm introduced by Leo Breiman and Adele Cutler (Breiman, 2011). It is an algorithm for classification and regression that is part of the bagging algorithm in integrated learning (Ge et al., 2021). It was defined by Decision Tree (DT), where a model was built from the randomized training dataset; the value of various DTs is uncorrelated and determined independently and the average outcomes achieved utilizing this decision tress employed in prediction. A random selection of samples was released from the training data during the construction of DT instead of using all the characteristics of data; some are randomly chosen for training. No proper information is given regarding which samples are atypical or which characteristics significantly impact classification outcomes during this random feature selection approach (Sun et al., 2021). Since, the problem considered in this paper is a regression problem, hence, using RF is found to be suitable. The RF regression algorithm produces results from every decision tree and then calculates the mean value. The expression for RF is presented as;

$$\overline{H}(x) = \frac{1}{K}\sum_{i=1}^{k}(h_i(x, \theta_k))$$

where: $\overline{H}(x)$ represents prediction output; h_i represents single decision tree; θ_k represents an independently distributed random variables that influences the development of the single decision tree; K represents a quantity of the decision trees. Every decision tree in the RF does not simultaneously capture all the features, resulting in uncertainty for each tree, thus enhancing the model's generalization capability.

Support Vector Regression (VSR)
In 1995, Cortes & Vapnik proposed an algorithm known as Support Vector Machine (SVM), which is a type of aimed at addressing classification problem by integrating Statistical Learning Thery (SLT) and Structural Risk Minimization (SRM) (Cortes & Vapnik, 1995). It provides a more efficient implementation with higher accurate than the traditional Empirical Risk Minimization (ERM), which relies on conventional learning methods like the Neural Network (NN) technique. It has been widely used for prediction problem-solving. It was considered as a practical technique to solve various problems and produce more precise and dependable prediction outputs. Recently, because of improved and dependable tools, researchers have increasingly utilized SVM in a significant portion of the forecasting domain, executing different tasks associated with machine learning (Fan et al., 2018; Ji et al. 2017; Roushangar et al., 2018).

Extreme Gradient Boosting (XGB)
XGB is an ensemble ML algorithm based on decision tree that employs gradient boosting to predict results for unstructured data. Tianqi and Guestrin developed XGB employing gradient boosting method to make an algorithm called "Extreme Gradient Boosting (XGB)" (Nguyen-Sy et al., 2020). The fundamental concept is to new base model to accommodate the differences of the earlier model to minimize changes in the additive model. The introduction of regularization into the objective function and utilizing the second derivatives, the XGB can decrease the overfitting problem and computational efficiency. The XGB algorithm is more generalized and faster than the other ML algorithms. The prediction formula was given as;

$$\widehat{y_i} = \sum_{i=1}^{k} f_t(x_i)$$

where: f_t represents kth base model; $\widehat{y_i}$ represents predicted value of i^{th} sample.

Gradient Boost Regressor (GBR)

Gradient boosting, like other boosting methods, builds the model step-by-step (Keprate & Ratnayake, 2017). It simplifies the gradient booster framework and consists of three key elements such as a loss function, a weak learner and an additive model. The primary concept of this algorithm is to establish a strong correlation between the new base learners and the negative gradient of the loss function associated with the entire ensemble. While the loss function can vary, the learning process is often intuitive, particularly when using the classic squared-error loss, as it focuses on sequentially minimizing errors. The mathematical expression for GBR is as follows:

$$F(x) = \sum_{m=1}^{M} \gamma_m h_m(x) \quad (5)$$

where: $h_m(x)$ represents the root functions.

CAT Boost Regressor (CATB)
In 2017, Yandex introduced an algorithm called CATB, which is DT algorithm depends on gradient boosted decision tress. The algorithms in the CATB models are made up of a series of decision tress that are constructed sequentially with each new tress exhibiting a lower loss compared to the earlier trees. The process of constructing a single tress in CATB algorithm involves calculating split in advance, transforming categorical features into numerical ones, choosing the structure of tree and defining the values in the leaves. It typically used greedy algorithm to optimize the prediction accuracy. The features of CATB model are arranged based on their splits and then replaced in each leaf. The depth of tree and other limitations for choosing structure are defined with pre-modelling parameters and a random permutation of classification or regression performed prior to constructing the new tree. It was reported that the CATB outperforms the GBR packages and accomplishes a better performance on the benchmark datasets.

2.3 Description of dataset

A dataset with a total data of 532 concrete mix proportions was collected from Kaggle dataset along with data from various literature (Li et al., 2022; Devi & Sudhamani., 2017; Okoye & Singh., 2016; Kumar et al., 2021; Yun et al., 20221; Kumar et al. 2007; Atis, 2003; Zhang, 2013; Sun et al 2019; Karthikeyan et al., 2017; Lustosa & Magalhaes., 2019; Roychand et al., 2016; Salain., 2019; Southararajan & Sivakumar,, 2013) and an experimental dataset. This dataset comprises of 7 input variables with 1 output variable and their values are given in Table 2. The input variables are cement, fly ash, superplasticizer, water, accelerator, fine aggregate, coarse aggregate, curing age and compressive strength; while the output variable is 28-days compressive strength.

Variables	Values
Cement (kg/m^3)	120-491
Fly ash (kg/m^3)	24.5-270.87
Superplasticizer (kg/m^3)	4.5-20.8
water (kg/m^3)	140.8-247
Fine aggregate (kg/m^3)	533-1088.1
Coarse aggregate (kg/m^3)	612-1270
Accelerator (kg/m^3)	0-27.08
Age (days)	3-100
Concrete compressive strength (N/mm^2)	7.32-76.24

Table 2. Input and output Variables

3. DEVELOPMENT AND TRAINING OF MODEL

3.1 Model development

Preprocessing
The collected data should be pre-processed, before they could be used for the regression method. The various process involved in the pre-processing involves feature selection, scaling and data selection. In the feature selection process, some of the unwanted data were removed from the collected dataset. i.e., this paper aims to develop the prediction model for HVFA concrete, the mix composition found in the dataset which does not use the fly ash as a binder was removed and not used for the analysis. The regression model gives the output by utilizing only the selected features from the dataset. The min-max scaling is used for the normalization of raw data.

Regression Algorithms
The next phase is developing the regression model. From the pre-processed data, the collected was split into testing sets and training sets, which 80% for training and 20% for testing. The

training set is used to produce the final strong learner, while the testing is employed to demonstrate the accuracy in the prediction of compressive strength. In training dataset, the above-mentioned algorithm such as liner regression, decision tree, SVR, random forest, XGB, GBR are used.

Model Training

The implementation was performed to assess the model's performance. The ML method for predicting compressive strength was modelled as a regression problem. The model was trained utilizing the Python on the laptop featuring an Intel (R) Core TM i7 and 16GB of RAM. The data was analysed and the model was developed using the Python programming language on Google's Colab platform. A low-code, open-source machine learning library called "Scikit" was utilized.

Evaluation of model

The metrics such as R^2, RMSE and MAE was utilized to determine and compare the performance of the various ML model. Based on these metrics, the most effective regression model was found to predicting the compressive strength of HVFA at 28 days.

3.2 Statistical characteristics of the dataset

Figure 3 represents the correlation between the output and input variables. From an external perspective, it appears that a non-linear correlation between compressive strength and its input variables. There is also a negative correlation observed in which an increase in one variable is related to reduction in another. It was observed that the variable such as cement, age, superplasticizer, accelerator, fine aggregate has positive correlation with compressive strength of concrete, which indicates there will be increase in compressive strength with increase in their concentrations. Conversely, the variable such as fly ash, coarse aggregate and water has negative correlation with compressive strength of concrete, which indicates there will decreases in compressive strength with the increase in their concentrations. The statistical analysis demonstrate that the cement has significant influence on the concrete compressive strength followed by age, superplasticizer, accelerator and fine aggregate. It was demonstrated that the amount of accelerator shows a positive correlation with compressive strength of HVFA, which was not considered in the earlier prediction model as observed in the literatures. The statistical characteristics of the dataset was presented in Table 15.

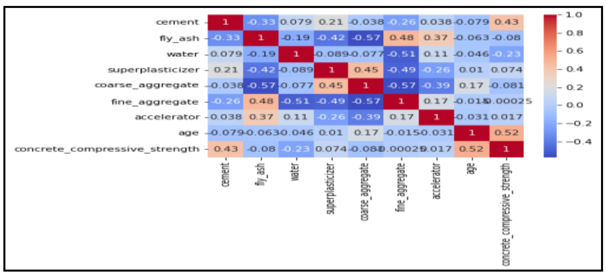

Figure 3. Correlation between two variables

A visualization of the histogram obtained for the data was presented in figure 4. The visualization can give a better idea about which method is more suitable to get the better fit for the ML methods. The variables have a normal distribution. Thus, it is possible to see the efficiency of the learning algorithm can be facilitated.

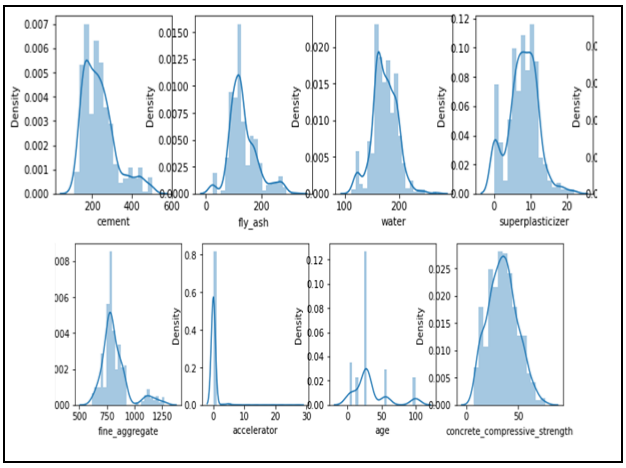

Figure 4. Histogram plot for the variables

3.3 Implementation and Model Result

The LR model achieved a performance of 0.61 at the learning rate for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 8.62 N/mm^2 and 6.80 N/mm^2. The predicted compressive strength by LR and experimental compressive strength are compared and was presented in figure 5.

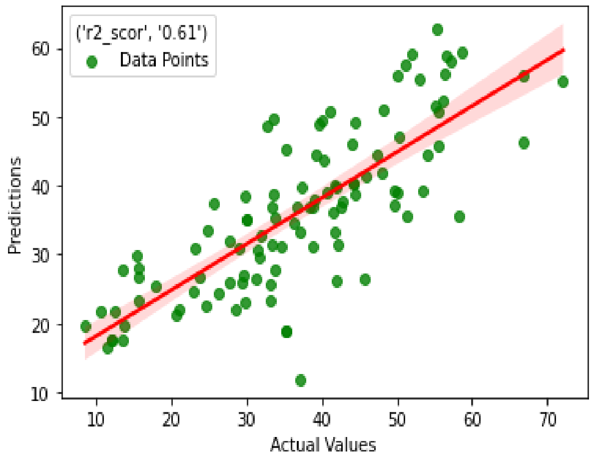

Figure 5. Actual and predicated compressive strength using LR

For KNN, the following parameters were selected as adjustable parameters as given in Table 6. The better performance achieved at 5 neighbours. The KNN model achieved a better performance of 0.61 for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 6.83 N/mm^2 and 8.63 N/mm^2. The predicted compressive strength by kNN and experimental compressive strength are compared and was presented in figure 7.

Parameters	Values
Number of neighbours	3,4,5
Leaf size	1,3,4,5,10,12
Weighted Function	Uniform

Table 6. Parameters for KNN

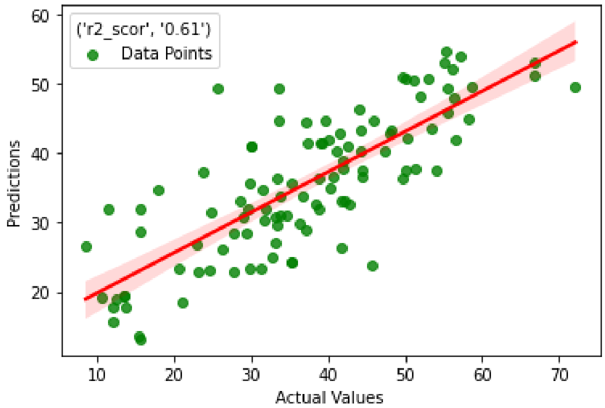

Figure 7. Actual and predicated compressive strength using kNN

The DT model achieved a performance of 0.79 for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 6.28 N/mm^2 and 4.07 N/mm^2. The predicted compressive strength by DT and experimental compressive strength are compared and was presented in figure 8.

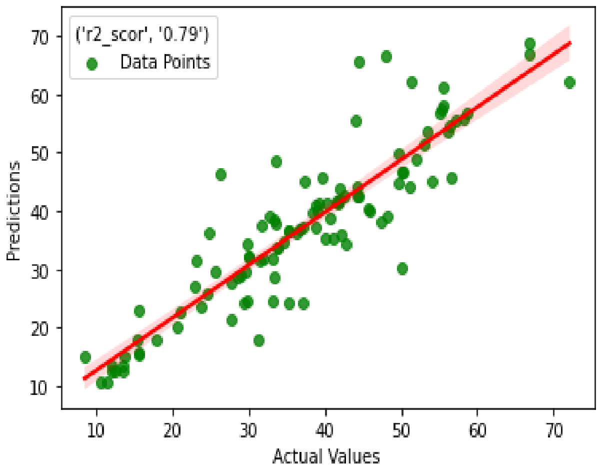

Figure 8. Actual and predicated compressive strength using DT

For RF, the following parameters were selected as adjustable parameters as given in Table 9. The best performance attains at a maximum depth of 15 with 120 number of trees. The RF model achieved a performance of 0.61 for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 8.62 N/mm^2 and 6.80 N/mm^2. The predicted compressive strength by RF and experimental compressive strength are compared and was presented in figure 10.

Parameters	**Value**
Maximum depth	10-20
Number of Leaf nodes	120
Number of trees	100-200

Table 9. Parameters for RF

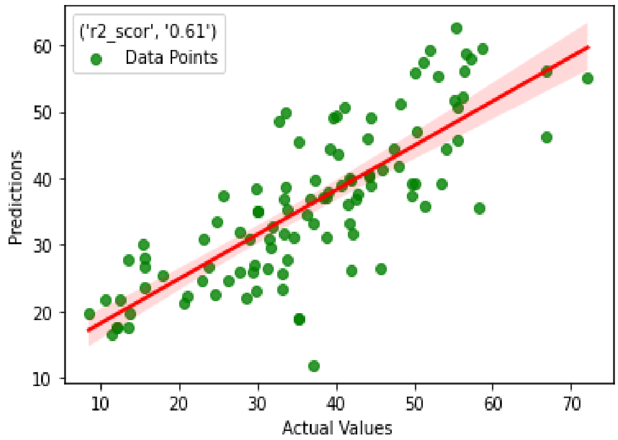

Figure 10. Actual and predicated compressive strength using RF

The parameters for the SVR were given in Table 11. The best performance was achieved at C=100. The SVR model achieved a performance of 0.32 for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 11.37 N/mm^2 and 7.89 N/mm^2. The predicted compressive strength by SVR and experimental compressive strength are compared and was presented in figure 12.

Parameters	**Value**
C	100
Kernal	RBF
Gamma	auto

Table 11. Parameters for SVR

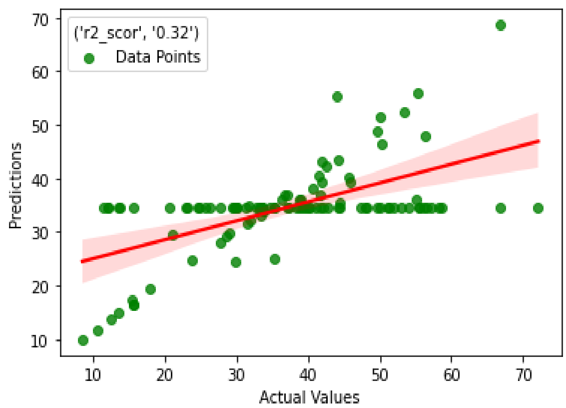

Figure 12. Actual and predicated compressive strength using SVR

The parameters for the XGB were given in Table 13. The XGB model achieved the best performance of 0.91 at the learning rate of 0.1 for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 4.24 N/mm^2 and 3.05 N/mm^2. The predicted compressive strength by XGB and experimental compressive strength are compared and was presented in figure 14.

Parameters	**Value**
Learning rate	0.1-1
n-estimates	1000
max_depth	6

Table 13. Parameters for XGB

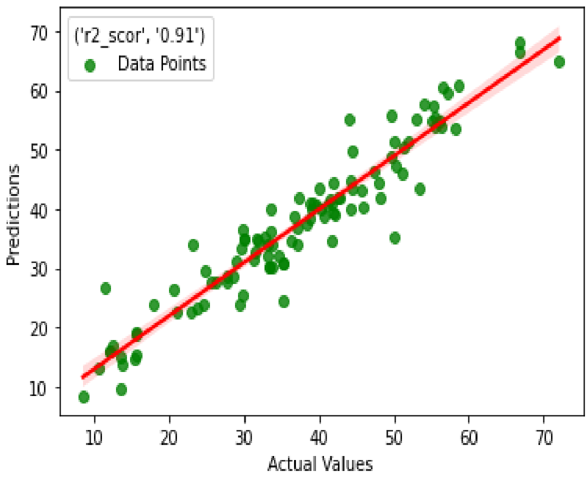

Figure 14. Actual and predicated compressive strength using XGB

The parameters for the GBR were given in Table 15. The GBR model achieved a performance of 0.09 for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 4.24 N/mm^2 and 3.05 N/mm^2. The predicted compressive strength by GBR and experimental compressive strength are compared and was presented in figure 16.

Parameters	**Value**
Learning rate	0.1-1
n-estimates	500
max_depth	5

Table 15. Parameters for GBR

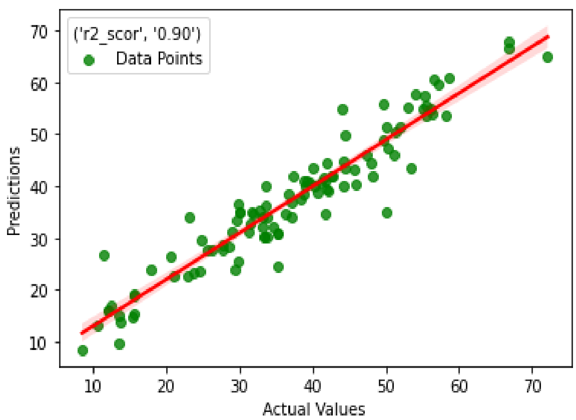

Figure 16. Actual and predicated compressive strength using GBR

The parameters for the CATB were given in Table 17. The CATB model achieved the best performance of 0.93 at the learning rate of 0.05 for the prediction of compressive strength of HVFA concrete with RMSE and MAE of 4.24 N/mm^2 and 3.05 N/mm^2. The CATB predicted compressive strength and experimental compressive strength are compared and was presented in figure 18.

Parameters	**Value**
Learning rate	0.01-1
depth	7
Random seed	42

Table 17. Parameters for CATB

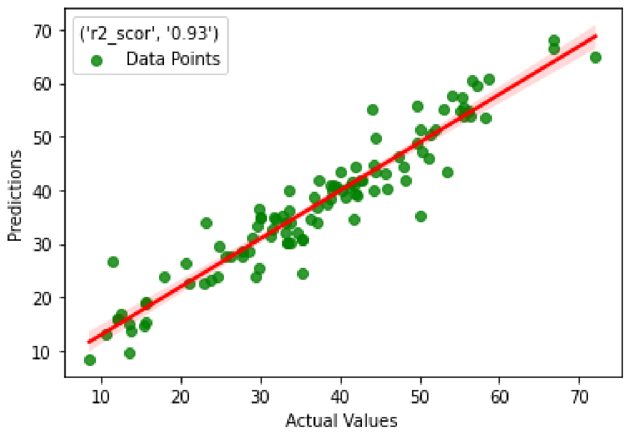

Figure 18. Actual and predicated compressive strength using CATB

The Figures 19-21 presents the comparative analysis of various models in terms of performance metric like R2, RMSE and MAE. The CATB model is found to be optimum for predicting the compressive strength of HVFA concrete at 28 days with higher R^2, low RMSE and low MAE values. The XGB model has second highest R^2, lower RMSE and MAE; however, its performance is lower than the CATB model. The SVR model has recorded poor performance for predicting the compressive strength of HVFA concrete at 28 days than the other models. This finding was found to be aligned with existing study by Wang et al., (2022), who reported that SVR offers poor performance in the prediction of compressive strength of concrete. This poor performance may be due to that this type of data does not follow linear trend.

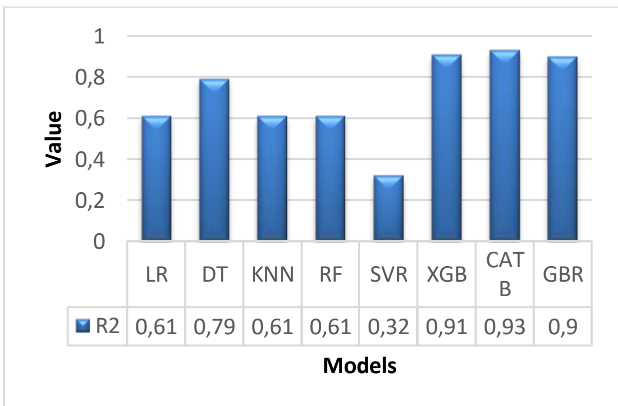

Figure 19. R^2 value of various models

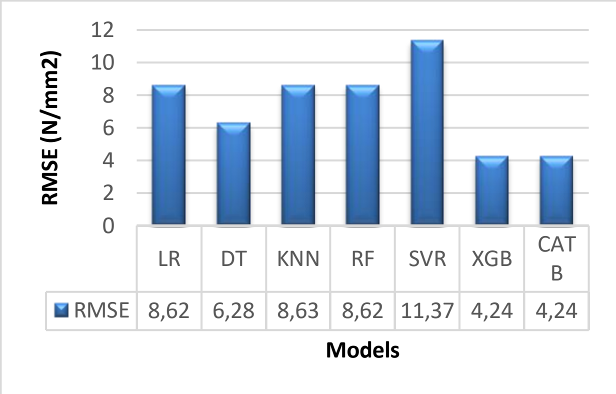

Figure 20. RMSE value of various models

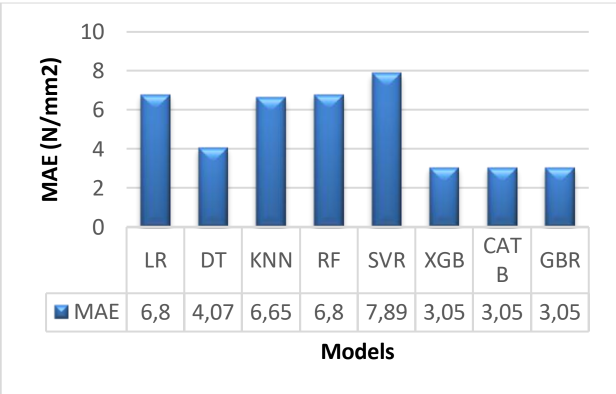

Figure 21. MAE value of various models

The CATB model offers optimal performance for predicting the compressive strength of HVFA at 28 days. This is due to the faster training times which makes it practical for the use in real-time data, where time is a critical factor. Thus, in this prediction model, the real-time data (concrete mix composition) was used. The validation of the developed model with the existing model was presented in table 22.

References	Model	R^2	RMSE	MAE
Titiksh &Wanjari (2023)	LR	0.858	-	-
Proposed models	LR	0.63	8.42	6.63
	DT	0.76	6.84	4.39
	KNN	0.61	6.83	6.65
	RF	0.63	8.42	6.63
	SVR	0.32	11.37	7.89
	XGB	0.91	5.25	3.65
	GBR	0.88	5.25	3.65
	CATB	0.93	4.24	3.05

Table 22. Performance of proposed and existing model

4. CONCLUSIONS

In recent days, the development of sustainable concrete, which is the idea of saving energy, protecting the environment and conservation of non-renewable resources has attracted widespread attention. The efficient solution to sustainable development is to decrease the utilization of natural resources, waste and associated releases. The CATB model efficiently predicts the compressive strength of the HVFA with higher R^2 value with lower RMSE and MAE values. The outcomes of this study can help the engineers or constructors to understand the significance of each component (input variable) to the compressive strength of the HVFA concrete. Moreover, the usage of ML techniques can greatly reduce both the time and cost involved in modifying the quantity of each component when formulating the HVFA for the designed compressive strength.
Future work can explore coupling ML models with optimization algorithms (e.g., genetic algorithms, particle swarm optimization) for mix design automation and performance evaluation.

Disclosure statement
The authors reported that no conflict of interest for publication this paper.

Funding statement
There was no funding received.

Data availability statement
The data used in this study was collected from https://www.kaggle.com/datasets/elikplim/concrete-compressive-strength-data-set.

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