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Research Article

Accuracy Prediction of Compressive Strength of Concrete Incorporating Recycled Aggregate Using Ensemble Learning Algorithms: Multinational Dataset

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The use of alternative materials and recycling in construction has gained popularity in recent years as part of the industry's commitment to sustainability. One such material, recycled aggregates, has been extensively studied over the past two decades for its potential to replace natural aggregates in cement-based composites. However, the unique properties of recycled aggregates make traditional concrete mix design methods ineffective in determining their target compressive strength. To address this challenge, four machine learning models based on ensemble learning algorithms, including CatBoost regressor (CatBoost), light gradient-boosting machine regressor (LGBM), random forest regressor (RFR), and extreme gradient-boosting regressor (XGBoost), were employed to predict the compressive strength of recycled aggregate concrete. Results demonstrate that the proposed models are highly accurate and generalizable, with high coefficients of determination and low error predictions. The CatBoost model performed the best, exhibiting an R^2 of 0.938 and low mean absolute error and root mean squared error values of 2.639 and 3.885, respectively, in the blind evaluation process. Although the random forest regression algorithm performed the least well among the four models, it still outperformed conventional machine learning algorithms such as support vector machines and artificial neural networks. The findings in this study suggested that the CatBoost model is the optimal choice for predicting concrete's compressive strength due to its high accuracy and low prediction error.

1. Introduction

Concrete has been the most widely used man-made material in the world since its invention about three tons of concrete are used worldwide per person every year [1]. Concrete, in general, is made up of three main components: aggregate, binder, and water, of which aggregate accounts for 75 percent, which makes it extremely important. In the construction industry, natural resources are used extensively, and demolition and construction waste are disposed of in large quantities. For instance, in 2012, about 100 million tons of construction and demolition waste (CDW) were generated in the United Kingdom [2]. In comparison with 2010 (102 million tons), this represents a 2% decline, but only a 0.8% decline from 2008 (101 million tons). As a result of these substantial amounts of consumption, there can be serious environmental impacts on a regional scale and deplete the bulk resource stock within an area due to excessive consumption rates. It is, therefore, no longer considered sustainable to use either of these practices due to their environmental and economic consequences [1–3].

Over the past two decades, the recycling of recycled aggregate has been extensively studied, with its incorporation into cement-based composites [4–7]. It was found that recycled aggregates, when properly processed, have similar or superior mechanical properties to natural aggregates [4]. To reduce natural aggregate consumption, recycled aggregates have gained popularity as a replacement for new concrete aggregates [6].

In concrete structures, compressive strength (CS) is crucial to structural safety and durability, so the primary objective of mixed design methods is to achieve a suitable CS value, safely and economically. Concrete is made by optimizing the proportions of Portland cement, fine aggregate, coarse aggregate, water, and, optionally, chemical and mineral [8]. In addition to being quite time-consuming and labor-intensive, the wide variety and heterogeneity of concrete's raw materials are also significant challenges.

Even though several mix design methods exist around the world, including those proposed by the American Concrete Institute (ACI) and the British Department of Energy (DOE), there is still no consensus on mix design. Researchers and institutions, therefore, propose diverse mix design methods which are mostly based on empirical graphs and tables [9, 10]. A test must be conducted after the proportions of materials have been determined, and adjustments must be made based on the results. The compressive strength of concrete specimens is determined using a compressive test, usually after 28 days of curing, according to standard procedures (specific to each country). For residue-based concretes such as recycled aggregate concrete, this process is made more complicated by their differing characteristics. As a result of these peculiar properties, traditional mix design methods are less effective in determining their target CS.

A wide range of machine learning (ML) methods has been developed in recent years, including deep learning (DL), which is based on neural networks in combination with representation learning which has allowed us to develop excellent predictive models [11]. Since ML/DL emerged, it has made great strides in solving previously impossible problems. Due to its ability to detect intricate patterns in high-dimensional data, it can be used in many fields of science, business, and government [12]. There have been successful applications of ML/DL in the healthcare, finance industry, retail, social media, agriculture, mechanical engineering, and so on [13]. It is conceivable that ML/DL models could be used to predict concrete CS in an analogous way since it is also affected by a wide range of factors, for instance, its ingredients. Many studies have attempted to develop ML/DL models for predicting concrete strength [14–17].

In recent years, ML/DL techniques have gained popularity for predicting the CS of concrete based on its constituent components as inputs to the model. Table 1 provides a summary of various ML/DL models used to predict CS for different types of concrete. Several empirical and statistical models, such as linear and nonlinear regression algorithms, have been employed to predict the properties of concrete. Among the ML/DL algorithms, artificial neural networks (ANNs) [14, 20, 26, 28, 29, 31] and support vector machine (SVM) [15, 19, 24, 27] are the most commonly used techniques for CS prediction. CS prediction has been performed for different types of concrete, including ordinary concrete [21, 30], high-performance concrete [17, 24, 27], self-compacting concrete [22, 26, 28], and green concrete with supplementary cementitious materials, such as fly ash [23, 31], blast-furnace slag [17], steelmaking slag [19], metakaolin [15], and recycled aggregates [18, 20, 25]. Furthermore, ML/DL techniques have been utilized to predict the properties of concrete. For instance, the work of Elemam et al. [32] used DL-based ANN algorithms to predict the slums' flow and optimize the fresh properties of self-compacting concrete. The study conducted by Duan et al. [33] and Golafshani and Behnood [34] used the DL model in the prediction of the elastic modulus of recycled aggregate concrete using the ANN model. Overall, there have been significant developments in the implementation of ML/DL for predicting the property characteristics of concrete.

Many ML/DL studies have achieved acceptable performance in predicting the CS of concrete [17, 18, 22, 24]. However, these studies required pre-proportioning and predetermining a series of features through experimentation as part of the modeling process. The selection of the model and the representation of the data used to create the model also played a crucial role. To enhance the predictive accuracy of concrete CS, it is necessary to consider several aspects. Firstly, the selection of the model used is crucial in determining the accuracy of predictions [17]. Regression-based models, artificial neural networks, and support vector machines are some of the models available, each with its own advantages and disadvantages. Secondly, it is important to use representative data in training to achieve high accuracy [19]. This ensures that the model learns from diverse and relevant data, enabling it to make more accurate predictions. Finally, the features used to train the model also significantly influence the accuracy of predictions [18]. Careful selection of features can help improve the performance of the model. Therefore, these three aspects—model selection, representative data, and features used for training—are essential for improving the predictive accuracy of concrete CS.

In this study, ML models are applied to predict the CS of recycled coarse aggregate concrete based on nine features combined as model inputs (i.e., water-binder ratio, sand-aggregate ratio, effective water, recycled coarse aggregate replacement proportion, fly ash replacement proportion, silica fume replacement proportion, slag replacement proportion, superplasticizer, and age of concrete testing)—the selection of these features is based on the study done by Zeng et al. [18]. Rather than dealing with the complexity of deep neural network algorithms, four ML models based on ensemble learning algorithms (CatBoost, LGBM, RFR, and XGBoost) were employed to predict the CS of recycled aggregate concrete—these selections were influenced by the study conducted by Rathakrishnan et al. [17], Penido et al. [19], Nguyen-Sy et al. [21], and Zhang et al. [22]. Each model was well-trained through 10-fold cross-validation with its best optimized hyperparameters. To accomplish this purpose, a global survey was conducted on the use of recycled coarse aggregate concrete in the literature, and the results of this survey were used to form a large dataset of over two thousand observations of the concrete mix group, no study has been done before, that was used to expand the data representativeness and, as a result, improve the predictive capabilities of the model. As opposed to using repeated data in training and testing, the dataset that has been collected was randomly separated into the training dataset for creating the model and the blind evaluation dataset for evaluating the model's predictive performance. Furthermore, instead of solely assessing the model's general performance, a sensitivity feature analysis

Table 1: Summary of previous studies on CS of concrete prediction using ML/DL models.

References	Year	Type of concrete	Model	Dataset
Zeng et al. [18]	2022	Concrete with natural and recycled aggregates	Convolutional neural network (CNN)	380
Rathakrishnan et al. [17]	2022	High-performance concrete with high volume ground granulated blast-furnace slag replacement	CatBoost, GBR, Adaboost, and XGBoost	152
Penido et al. [19]	2022	Steelmaking slag concrete	GPR, ANN, XGBoost, and SVR	406
Vasanthalin and Kavitha [20]	2021	Recycled aggregate concrete	Artificial neural network (ANN) and cuckoo search method (CSM)	121
Nguyen-Sy et al. [21]	2020	Ordinary concrete	Extreme gradient boosting (XGBoost)	1030
Zhang et al. [22]	2019	Lightweight self-compacting concrete	Random forest regression (RFR)	131
Kaveh [23]	2018	Self-compacting concrete containing fly ash	Decision tree algorithms: M5′ and multivariate adaptive regression splines	114
Yu et al. [24]	2018	High-performance concrete	Support vector machine (SVM) and enhanced cat swarm optimization	2200
Deng et al. [25]	2018	Recycled aggregates concrete	Convolutional neural network (CNN)	74
Asteris and Kolovos [26]	2017	Self-compacting concrete	Artificial neural network (ANN)	205
Chou and Pham [27]	2014	High-performance concrete	Support vector machine (SVM) and artificial neural network (ANN)	1030
Safarzadegan Gilan et al. [15]	2012	Concretes containing metakaolin	Support vector regression (SVR)	100
Siddique et al. [28]	2011	Self-compacting concrete containing bottom ash	Artificial neural network (ANN)	80
Alshihri et al. [29]	2009	Lightweight concrete	Neural networks (NNs)	76
Yeh and Lien [30]	2009	Ordinary concrete	Genetic operation tree (GOT)	1030
Pala et al. [31]	2007	Ordinary concrete containing fly ash and silica fume	Neural networks (NNs)	144

was performed to identify its weaknesses by carefully examining each individual error in prediction.

2. Materials and Methods

2.1. Overview. The objective of this study is to assess the predictive accuracy of four ML models that are applied to predicting the CS of recycled aggregate concrete. Figure 1 summarizes the overview of the methods used in this study. First, the data on mixtures and CS of recycled aggregate concretes in the literature were collocated and filtered. The obtained literature dataset was preprocessed to convert the nine basic ingredients of concrete mixture to nine features (including the age of concrete testing) and its compressive strength. Subsequently, four ML models—CatBoost, LGBM, RFR, and XGBoost—were employed to extract the relation between the components of nine features (input features) and their concrete's CS in MPa (output). The performance of models was evaluated through ten-fold cross-validation and four statistical metrics: coefficient of determination (R^2), mean absolute error (MAE), root mean squared error (RMSE), and mean absolute percentage error (MAPE). The models were also further optimized with grid search algorithms to seek the best hyperparameters of each model. To demonstrate the superiority of the proposed ML models, two commonly used algorithms—SVM and ANN—were also built on the same dataset. Finally, unseen data were used for a blind evaluation procedure (the data were never used in the training and testing of the model). The purpose of this blind evaluation was to find out whether the models could predict CS for concrete that never participated in the training.

2.2. Machine Learning Techniques. Machine learning is a method of self-directed learning that involves analyzing available data to detect existing patterns in the dataset. These patterns can then be applied to make predictions about future data [35].

A heterogeneous mixture of concrete and highly variable materials makes predicting concrete's CS challenging. A nonlinear regression model is commonly used to address this type of problem because of its high complexity and correlation between the concrete components. DL/ML models have been used to predict concrete's CS for various concrete mixtures [18–20, 36]. However, in this study, the four ML models based on ensemble learning techniques—CatBoost, LGBM, RFR, and XGBoost—were selected to predict the CS of recycled aggregate concrete.

2.2.1. Ensemble Learning. Ensemble learning is a powerful machine learning technique that has shown to be an effective solution for regression problems [37]. Ensemble learning is the process of combining multiple models to improve the accuracy and robustness of predictions. In the context of regression problems, ensemble learning algorithms can combine the predictions of several models to create a more accurate and robust prediction than any single model could achieve alone [37–39]. This is particularly useful in cases where the data are noisy or where the relationship between the input variables and the target variable is complex and nonlinear. By combining the predictions of multiple models, ensemble learning algorithms can reduce the variance of the predictions and improve the overall accuracy of the regression model. Thus, ensemble learning algorithms have become a popular and effective solution for regression problems in a wide range of applications [40], including finance, healthcare, and engineering.

While ensemble learning can be achieved in an almost limitless number of ways, perhaps these five techniques are most used and discussed: Bagging ensemble, Bootstrap Aggregating, Gradient-Boosting ensemble, AdaBoost ensemble, and Voting ensemble—these techniques have been implemented in recent developed ML models such as CatBoost, LGBM, RFR, and XGBoost. These methods are not described in this paper since they have been well described in the related literature. It is recommended to refer to [37, 39] for more details. An ensemble is more reliable than a single model for two main reasons: reliability—reducing the variance of predictions—and skill—achieving better performance than single models as it improves the ensemble's average prediction performance [37]. Both aspects are important to consider when designing a machine learning model, and sometimes one or both properties are preferred.

2.2.2. CatBoost. Developed by Yandex in 2017, CatBoost is an open-source machine learning algorithm. It belongs to the family of gradient-boosting decision tree machine learning (GBDT) ensemble techniques. CatBoost is also well suited to machine learning tasks involving categorical, heterogeneous data because it is a decision tree-based algorithm. In CatBoost models, decision trees are constructed sequentially with each new tree having a lower loss than the previous tree, and each tree is constructed by computing splits beforehand, converting categorical features to numerical features, selecting the tree structure, and calculating leaf values [41]. In addition, overfitting is prevented by using an overfitting detector, which uses the starting parameters to determine the number of trees to be generated.

2.2.3. Light Gradient Boosting Machine (LGBM). LGBM is a gradient-boosting framework developed by Microsoft that uses tree-based learning algorithms, a family of GBDT. Developed on a decision tree algorithm, it is suitable for regression, classification, ranking, and traditional machine learning approaches. The LBGM algorithm employs two novel sampling techniques: gradient-based one-side sampling (GOSS) and exclusive feature bundling (EFB). To estimate the information gain, GOSS excludes data instances with small gradients and uses the remainder. A significantly smaller dataset can provide a highly accurate estimate of information gain since data instances with large gradients contribute more to the computation. Through EFB, mutually exclusive features can be grouped, thereby reducing their number [42]. In addition, it demonstrates that a greedy approach can achieve a high approximation ratio when determining the optimal bundling of exclusive features. The

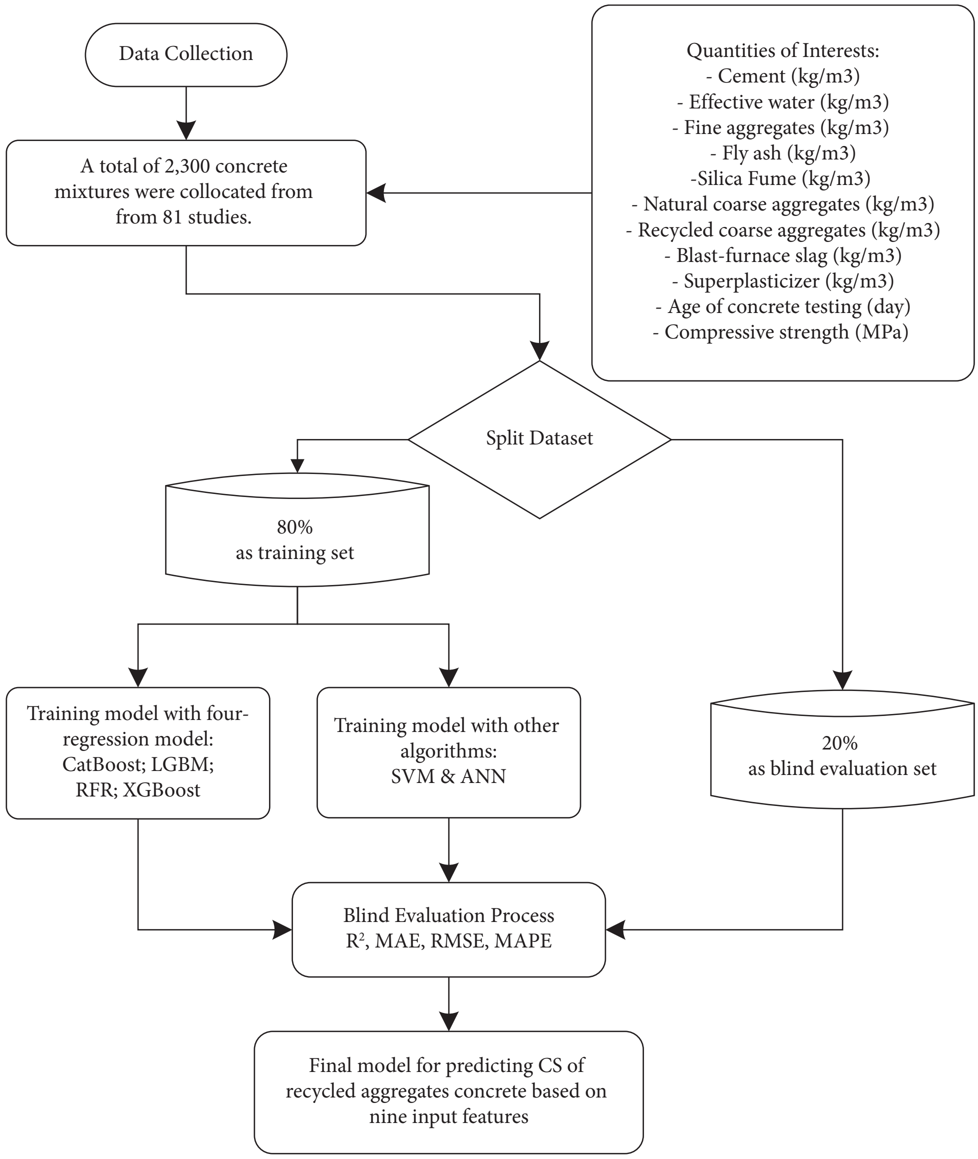


Figure 1: Overview of materials and methods used in this study.

LGBM training process speeds up the conventional GBDT training process by an average of about twenty times while maintaining the same accuracy.

2.2.4. Random Forest Regressor (RFR). The RFR algorithm is an ensemble learning algorithm that uses ensemble learning methods to classify and predict. The random forest is a type of classification or regression tree that is constructed by using bootstrap samples of the training data along with random feature selection. To synthesize classification results from a variety of decision trees constructed through learning and predict them through voting, the bagging technique is applied [43]. In terms of accuracy, random forest is one of the most powerful and versatile tools available today.

2.2.5. Extreme Gradient Boosting (XGBoost). In extreme gradient boosting (XGBoost), gradient boosting is used to make predictions for unstructured data using decision trees. XGBoost algorithm was created by Chen and Guestrin [44] in 2016. Many recent advances have been made possible by this algorithm, which has been the source of countless innovative applications. Its applications are diverse and include predictingcustomer churn, assessing applicant risk, detecting malware, selecting stocks,classifying traffic accidents, diagnosing diseases, and even predicting patient-mortality during Covid-19 treatment caused by SARS-COV-2. One of XGBoost's most significant advantages is its scalability across any condition.

2.3. Model Configuration. In this research, the primary tool used for analyzing data and creating models was the Python programming language. To simplify the development process, open-source ML/DL libraries such as Scikit-learn, Keras, and TensorFlow were utilized. The optimized four ML models—CatBoost, LGBM, RFR, and XGBoost—were developed through five distinct stages including data collection, data preprocessing and featuring, model optimization through grid search algorithms, model validation, and model evaluation, each of which is elaborated upon in detail below with concise explanations.

2.3.1. Data Collection. Datasets relating to recycled aggregate concrete mixtures and their CS were initially compiled from the literature. The scientific databases that were searched were Google Scholar, Science Direct, and Web of Science. This literature survey examined articles published in journals, conference proceedings, and theses and dissertations. Following this introductory survey, a more thorough analysis of each paper was carried out. The references were narrowed to include only those works that utilized recycled aggregate as coarse aggregate in concrete and that also included both mixtures and respective CS. Many works conformed to the theme, but had to be excluded due to incomplete information, such as the proportion of mixture materials or the dimensions of the specimen, or other constituent materials used beyond the scope of this study. Finally, 81 studies from 25 countries across the globe are included in the final literature dataset survey, as shown in Table 2.

2.3.2. Data Preprocessing and Featuring. Based on the practices and standards employed in each region, each study exposed the results and measurement unit differently. It was, therefore, necessary to convert various units, as well as to convert mixed proportion data to consumption data, particularly in kg/m^3. As a result, nine selected interested constituents as well as age of testing and their CS were chosen and converted into the following units: cement (kg/m^3), effective water (kg/m^3), fine aggregate or sand (kg/m^3), fly ash (kg/m^3), silica fume (kg/m^3), blast-furnace slag (kg/m^3), superplasticizer (kg/m^3), natural coarse aggregate (kg/m^3), recycled coarse aggregate (kg/m^3), age of concrete testing (day), and compressive strength (MPa).

The complete literature dataset includes 2,300 instances (concrete mix group) of research projects that have been conducted between the years 2000 and 2022 in 25 countries from a range of backgrounds. The total dataset was randomly split into two subsets—1840 instances (80% of the total dataset) for training and testing model and 460 instances (20% of the total dataset) for the blind evaluation process. There was also a great deal of diversity in the specimens assessed since they are of varied sizes and shapes. Those results were converted into their equivalents for 100×200 mm cylindrical specimens—as it is universally accepted in both Korea and the United States—using correction factors developed by Zabihi and Eren [123] which is original for normal and high-strength concrete made from the natural aggregate. This standardization led to a complete dataset that included recycled coarse aggregate concrete with CS ranging from 3.91 to 89.70 MPa.

To improve learning results, the nine ingredients of the concrete mixture were converted into eight features based on the work of Zeng et al. [18]. To predict CS of recycled aggregates concrete, nine features including the age of testing were selected or combined as model input. The features were water-binder ratio (W/B), water weight (W), sand-aggregate ratio (S/A), fly ash to cement ratio (FA), recycled coarse aggregate to aggregates ratio (PA/A), silica fume to cement ratio (SF), superplasticizer content (SP), blast-furnace slag to cement ratio (BFS), and the age of concrete testing. Figure 2 illustrates diagonal correlations between input and output parameters. Seaborn, a Python module, was used to develop diagonal correlation heatmaps between multiple inputs (nine features) and concrete CS. Values for correlation coefficients are indicated by colors ranging from light green to dark green. A high correlation coefficient exists between the input (nine features) and output parameters (concrete CS). Therefore, all parameters were included in a probabilistic framework for predicting CS of concrete to improve accuracy. Table 3 summarizes the limitation values of nine input features and their respective CS. The CS of recycled aggregate concrete can only be predicted by this model only when the input features fall between the limiting values.

2.3.3. Model Optimization through Grid Search Algorithms. Grid search is a widely adopted optimization algorithm for enhancing ML models. This method involves exploring a hyperparameter grid that contains all feasible combinations of hyperparameter values [124]. For each hyperparameter combination, the algorithm trains and evaluates a model, and then returns the model that performed the best. By tuning the hyperparameters through grid search, the model can be fine-tuned to obtain optimal performance on a validation set. However, this procedure can be time-consuming, particularly when working with large datasets or numerous hyperparameters. Nonetheless, it is a critical step in ensuring that the model performs well on new data. Cross-validation is often integrated with grid search to produce more dependable estimates of model performance. Overall, grid search is an essential tool for machine learning practitioners who seek to optimize their models and achieve superior performance.

2.3.4. Model Validation Using K-Fold Cross-Validation. Cross-validation using K-fold is a common model evaluation technique because it gives us a more insightful look at our data and model. In this study, a total of ten folds or a k value of 10 were used based on works that have been similarly done by Rathakrishnan et al. [17] and Penido et al. [19]. In this cross-validation procedure (as shown in Figure 3), the dataset was randomly divided into 10 groups. One of the groups was used to validate the model, and the remaining groups were used to train the model. In addition, the grid search algorithm was also embedded in the K-fold validation process to optimize the model's hyperparameters in each fold for every model. By training and verifying the model several times, K-fold cross-validation allows for an accurate model with less overfitting. As the last step, the model performance was

Table 2: Summary sources of collected data from the literature survey.

References	Number of studies	Number of observations	Country
Casuccio et al. [45], Zega and Di Maio [46], and Folino and Xargay [47]	3 studies	21 concrete mix groups	Argentina
Ahmed [48], Berndt [49], Ozbakkaloglu et al. [50], and Shaikh [51]	4 studies	120 concrete mix groups	Australia
Amario et al. [52]	1 study	10 concrete mix groups	Brazil
Butler et al. [53], Fathifazl et al. [54], and Sucic [55]	3 studies	60 concrete mix groups	Canada
Kou et al. [56], Li et al. [57], Poon et al. [58], Xiao et al. [59, 60], Zeng et al. [61], Zhou and Chen [62], and Zeng et al. [18]	8 studies	192 concrete mix groups	China
Ulloa et al. [7]	1 study	50 concrete mix groups	Columbia
Wardeh et al. [63]	1 study	16 concrete mix groups	France
Alexandridou et al. [64]	1 study	12 concrete mix groups	Greece
Duan and Poon [65] and Kou et al. [66, 67]	3 studies	272 concrete mix groups	Hong Kong
Arora et al. [68], Alam et al. [69] Kapoor et al. [70], Kumutha and Vijai [71], Majhi et al. [72], Padhi et al. [73], Chakradhara Rao et al. [74], Saravanakumar and Dhinakaran [75], R. B. Singh and B. Singh [76], and Singh et al. [77]	10 studies	324 concrete mix groups	India
Corinaldesi [78, 79], Faella et al. [80], Manzi et al. [5], and Pepe et al. [81]	5 studies	103 concrete mix groups	Italy
Ann et al. [82], Hwang et al. [83], Kang et al. [84], and Kim et al. [85]	4 studies	41 concrete mix groups	Korea
Rahal [86]	1 study	60 concrete mix groups	Kuwait
Alnahhal et al. [87] and Ismail and Ramli [88]	2 studies	150 concrete mix groups	Malaysia
Corral et al. [89] and Gomez-Soberon [90]	2 studies	23 concrete mix groups	Mexico
Sajan et al. [91]	1 study	18 concrete mix groups	Nepal
Ajdukiewicz and Kliszczewicz [92] and Kubissa et al. [93–95]	4 studies	200 concrete mix groups	Poland
Matias et al. [96] and Pedro et al. [97]	2 studies	27 concrete mix groups	Portugal
Marinković et al. [98] and Malešev et al. [99]	2 studies	15 concrete mix groups	Serbia
Andreu and Miren [100], Barbudo et al. [101], Belén et al. [102], Domingo-Cabo et al. [103], Etxeberria et al. [104], López Gayarre et al. [105], González-Fonteboa et al. [106], and Thomas et al. [107]	8 studies	110 concrete mix groups	Spain
Lin et al. [108] and Sheen et al. [109]	2 studies	66 concrete mix groups	Taiwan
Tangchirapat et al. [110, 111] and Somna et al. [112–114]	5 studies	119 concrete mix groups	Thailand
Çakır [115], Dilbas et al. [116], Tuyan et al. [117], and Şimşek et al. [118]	4 studies	67 concrete mix groups	Turkey
Limbachiya et al. [119, 120] and Younis and Pilakoutas [121]	3 studies	164 concrete mix groups	United Kingdom
Khodair and Bommareddy [122]	1 study	60 concrete mix groups	United States

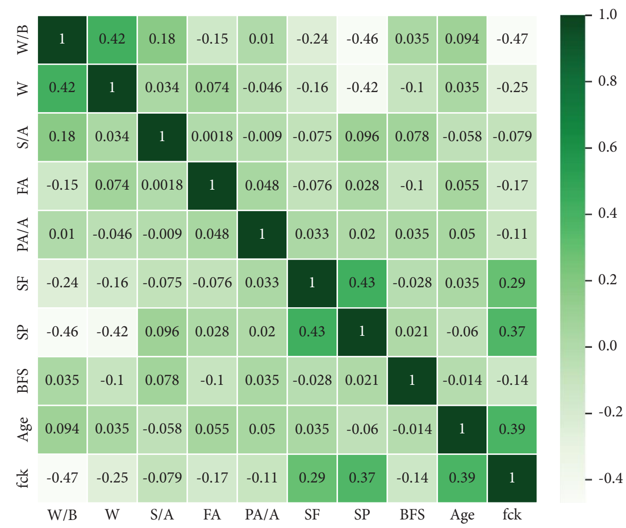


FIGURE 2: Correlation plot of nine input features and outputs (compressive strength).

TABLE 3: Range of selected nine features as input and their compressive strength (output).

Variable	Min. value	Mean value	Max. value	Standard dev.	Type
X1: W/B (%)	≥20.01	45.53	≤81.01	10.87	Input
X2: W (kg/m^3)	≥67.62	182.25	≤277.01	30.64	Input
X3: S/A (%)	≥12.97	39.74	≤63.09	7.73	Input
X4: FA (%)	≥0.01	15.90	≤150.01	29.44	Input
X5: PA/A (%)	≥0.01	31.95	≤75.19	24.91	Input
X6: SF (%)	≥0.01	1.07	≤29.82	3.46	Input
X7: SP (kg/m3)	≥0.01	2.14	≤15.01	3.63	Input
X8: BFS (%)	≥0.01	7.15	≤233.25	27.83	Input
X9: Age (day)	1	—	90	—	Input
y: Fck (MPa)	3.91	35.08	89.70	15.91	Output

*Binder: cement, fly ash, silica fume, and BFS (blast-furnace slag) or GGBS.

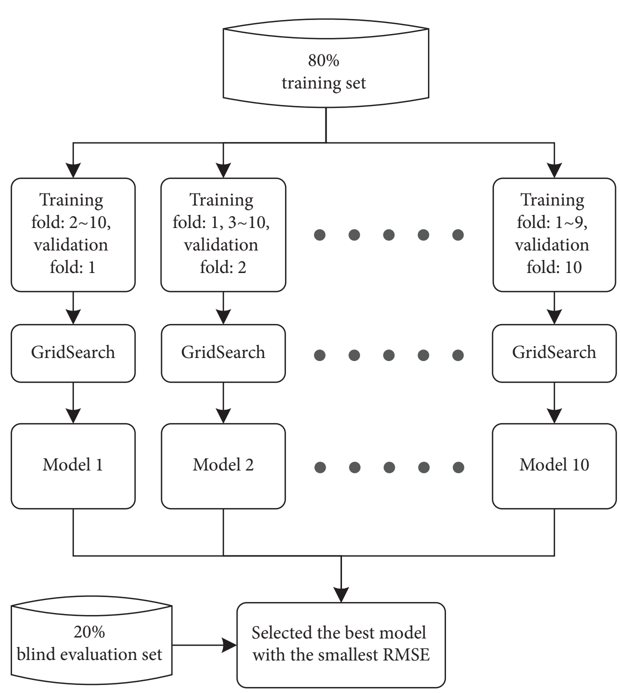


FIGURE 3: Ten-fold cross-validation procedure used in this study.

evaluated after ten repetitions of the training process by the average error from all the training folds, while a model's predictive performance is determined by blind evaluation data not included in the training.

2.3.5. Model Evaluation Metrics. A total of four statistical measurement parameters were used to evaluate the prediction efficiency of the models in this paper. An evaluation parameter measures the accumulated error in predictions based on actual observations. Statistical measures include the coefficient of determination (R^2), mean absolute error (MAE), root mean square error (RMSE), and mean absolute percentage error (MAPE). Equations (1)–(4) define these mathematical formulations; here, n is the total number of test dataset records and y and y' are the predicted and measured values. In general, R^2 values range from 0 to 1, and the closer it is to 1, the better the model's fitting optimization will be. On the other hand, to assess modeling error, MAE, RMSE, and MAPE values are used—the smaller the value, the less error between prediction and measurement.

$$R^2(y, y') = 1 - \frac{\sum_{i=1}^{n}(y_i - y_i')^2}{\sum_{i=1}^{n}(y_i - \overline{y}_i)^2}, \tag{1}$$

$$\mathrm{MAE} = \frac{1}{n}\sum |y - y'|, \tag{2}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum (y - y')^2}, \tag{3}$$

$$\mathrm{MAPE} = \frac{1}{n}\sum \left|\frac{y - y'}{y}\right|. \tag{4}$$

3. Results and Discussion

3.1. Evaluation of the Model Performance. Initially, the CatBoost, LGBM, RFR, and XGBoost algorithms were modeled using their default hyperparameter settings. The performance of each model was evaluated in terms of metric evaluation accuracy and error rates, specifically R^2, MAE, RMSE, MAPE, and accuracy index, which are presented in Table 4.

Among all the proposed models, XGBoost exhibited the highest level of accuracy in prediction and the lowest prediction errors. In the initial phase of modeling, XGBoost showed an R^2 value of 0.926 on the test dataset. Other models like LGBM and RFR also demonstrated good performance, with R^2 values of 0.863 and 0.877, respectively, on the test dataset. XGBoost model's evaluation metrics were comparatively better, as it had the lowest MAE, RMSE, and MAPE values of 3.010, 4.320, and 9.855, respectively, for the test dataset. The RFR model was the second best in terms of prediction errors, with MAE and RMSE values of 3.874 and 5.544, respectively. Even though the initial modeling yielded reasonably accurate prediction results, each model was further enhanced using the GridSearch algorithm to obtain the optimal performance.

The model was initialized and then optimized using the grid search algorithm. The focus of the optimization was on the combined use of hyperparameters to improve the model's performance. Several hyperparameters were optimized, such as n_estimator, learning_rate, and max_depth. Table 5 presents the values of the hyperparameters used for all models before and after the optimization process.

To evaluate the performance of the proposed models after optimizing, ten-fold cross-validation results were generated with four ML models namely CatBoost, LGBM, RFR, and XGBoost. The accuracies of each model were presented using boxplots. Each fold achieves an accuracy that does not differ greatly from the other for all four proposed ML models, as shown in Figure 4. Across all folds, CatBoost, LGBM, RFR, and XGBoost, respectively, had the lowest accuracies of 90.182%, 90.171%, 85.323%, and 90.229%; these values were also shown in their boxplot; no outliers were found. Therefore, the model performed well across 10-fold cross-validation. The results of all training fold of each model are summarized in Table 6. Furthermore, the performance of the four ML models (CatBoost, LGBM, RFR, and XGBoost) was further assessed by the average error of all training folds using the four evaluation metrics and the accuracy index presented in Table 7. Based on the obtained results, tuning the hyperparameters, which are adjustable settings that affect the performance and behavior of each ML model, led to a significant improvement in their respective performances.

As shown in Table 7, the model based on CatBoost reached the coefficient of determination R^2 of 0.941, which indicates that CS of recycled aggregates' concrete can be accurately predicted with this model. The XGBoost and LGBM models also showed satisfactory results, with R^2 values of 0.939 and 0.934, respectively. An R^2 value of 0.883, however, shows the inferior performance of the RFR model compared to the other models (CatBoost, LGBM, and XGBoost) that were evaluated in this study.

In addition, the other evaluation metrics such as RMSE and MAPE followed the same trend, with the RFR model having a higher value and the CatBoost model having a lower value. During this analysis, it was evident that the proposed models performed well, mainly because the RMSE and MAE values were similar among the models.

3.2. Evaluation of Predictive Capability of the Models. The proposed models were blindly evaluated to identify their predictive performance by predicting the CS of concrete using a blind evaluation dataset. Figures 5(a)–5(d) illustrate the results of the four ensemble models developed in this study for predicting the concrete CS of unseen data. A vertical axis represents the predicted CS of concrete, whereas a horizontal axis represents the observed CS. There is an elevated level of clustering near the diagonal line, indicating an accurate prediction of concrete CS. The model's predictive performance was also measured using the four evaluation metrics and the accuracy index shown in Table 8.

Table 4: Summary of metric evaluation performance of initial models.

Model	R^2	MAE	RMSE	MAPE	Accuracy*
CatBoost	0.747	6.064	7.967	20.520	79.480
LGBM	0.863	4.169	5.585	13.582	86.418
RFR	0.877	3.874	5.544	13.155	86.975
XGBoost	0.926	3.010	4.320	9.855	90.145

*Accuracy = 100 − MAPE (in %).

Table 5: Summary of hyperparameter-tuned values of each model.

Hyperparameters		Model			
		CatBoost	LGBM	RFR	XGBoost
Default value	n_estimator	—	100	100	—
	learning_rate	0.009	0.10	—	0.3
	max_depth	3	6	—	6
	l2_leaf_reg	3	—	—	—
Optimized value	n_estimator	—	1000	1000	—
	learning_rate	0.1	0.1	—	0.8
	max_depth	7	7	—	4
	l2_leaf_reg	1	—	—	—

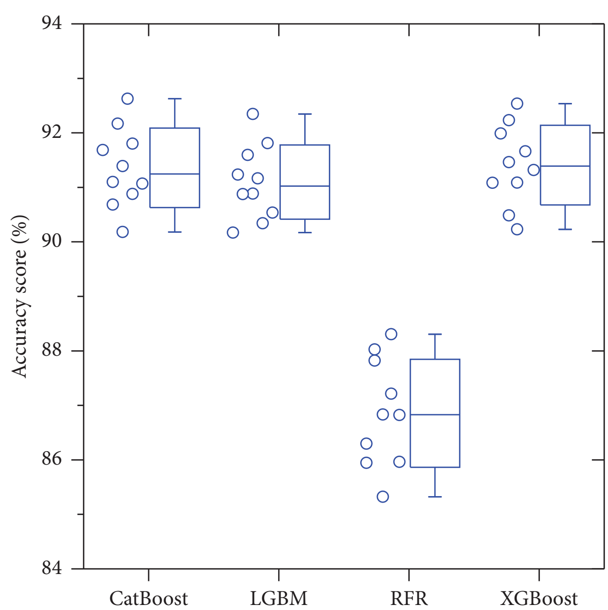


Figure 4: Boxplots representing the accuracy of each training fold for each model.

Among all models, ensemble learning models based on CatBoost achieved 90.617% accuracy in predicting CS of recycled aggregates' concrete, suggesting that it is capable of accurately predicting CS of concrete. With an accuracy of 90.594% and 90.155%, respectively, XGBoost and LGBM models also delivered satisfactory results in predicting CS. RFR, on the other hand, performed poorly in comparison to the other proposed models (CatBoost, XGBoost, and LGBM), with an accuracy of only 85.557%. Aside from that, the other evaluated metrics, for example, MAE and RMSE, were found to be low for prediction using the CatBoost model, which is about 2.730 and 4.090, respectively.

Along with these macroscopic metrics, histograms are plotted in Figures 6(a)–6(d) to illustrate how absolute error was distributed on concrete CS prediction of unseen data (blind evaluation datasets). There is a maximum absolute error generated by CatBoost of 17 MPa in predicting the concrete CS, which is unacceptable for any real application. The other models also generated a similarly large absolute error, specifically 20, 21, and 23 MPa for XGBoost, RFR, and LGBM, respectively. This is because the data used for the training model comes from different sources across the globe, and the data is disproportionately unbalanced between each country as well as different specimen shapes and sizes used in laboratory tests for measuring the concrete

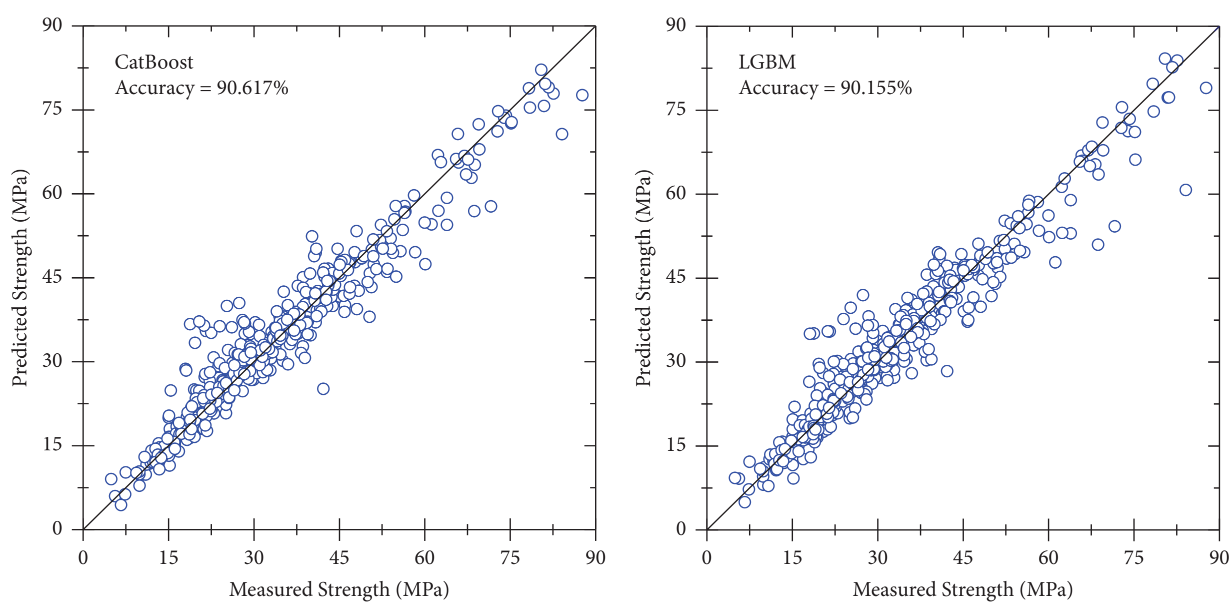
Table 6: Model performance of all 10-fold cross-validation process.

Fold	Model							
	CatBoost		LGBM		RFR		XGBoost	
	RMSE	MAPE	RMSE	MAPE	RMSE	MAPE	RMSE	MAPE
Fold 1	3.741	8.609	3.699	9.115	5.323	14.677	3.863	8.913
Fold 2	4.125	8.900	4.452	8.836	5.204	12.785	3.853	8.538
Fold 3	3.524	8.198	3.749	8.404	5.58	13.167	3.374	7.464
Fold 4	3.652	7.375	4.088	8.188	5.455	11.695	3.925	7.769
Fold 5	3.763	8.316	4.378	8.765	5.479	11.974	4.141	8.339
Fold 6	3.89	7.831	3.677	7.655	5.148	12.179	4.096	8.011
Fold 7	4.046	9.818	3.756	9.124	5.374	14.056	3.879	9.771
Fold 8	4.054	9.317	4.305	9.659	5.793	13.703	4.006	8.682
Fold 9	3.647	9.120	4.259	9.829	5.337	14.038	3.725	8.917
Fold 10	3.898	8.930	4.142	9.464	5.596	13.177	4.085	9.516
Average	3.834	8.641	4.051	8.904	5.429	13.145	3.895	8.592
Std. deviation	0.201	0.729	0.303	0.681	0.194	0.990	0.225	0.731

Table 7: Model performance through 10-fold cross-validation process.

Model	Average metric evaluation of all folds				
	R2	MAE	RMSE	MAPE	Accuracy*
CatBoost	0.941	2.639	3.834	8.641	91.359
LGBM	0.934	2.727	4.051	8.904	91.096
RFR	0.883	3.841	5.429	13.145	86.855
XGBoost	0.939	2.596	3.895	8.892	91.408

*Accuracy = 100 – MAPE (in %).



(a) (b)

Figure 5: Continued.

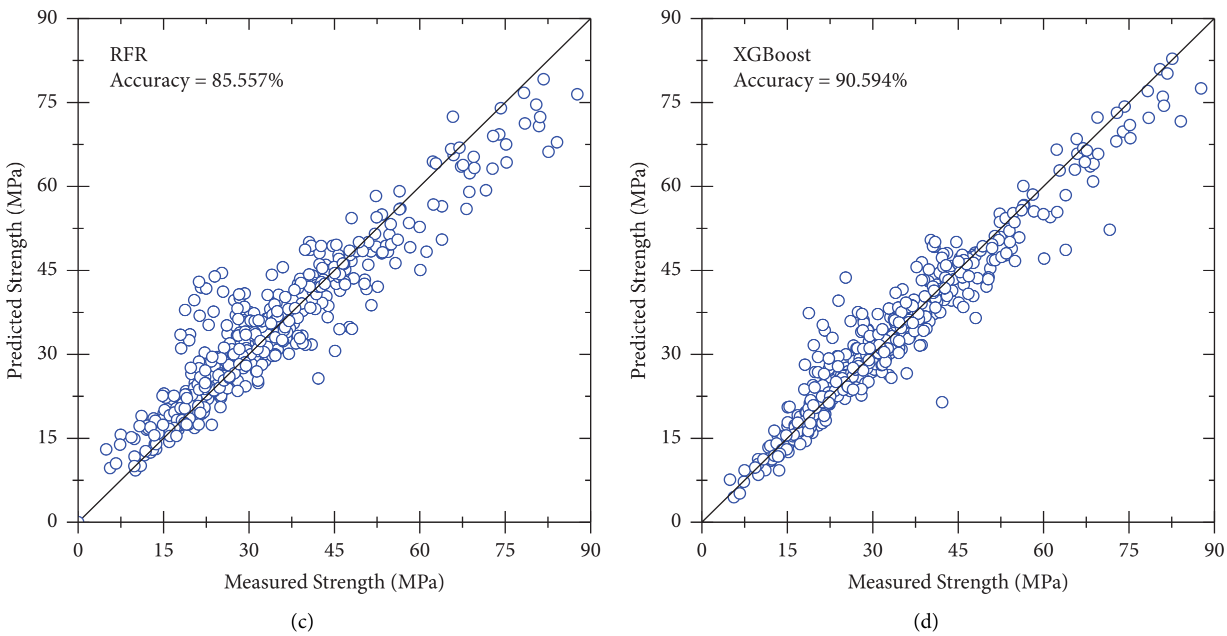


FIGURE 5: Predictive performance of the proposed ML models for blind evaluation dataset: (a) CatBoost, (b) LGBM, (c) random forest regressor (RFR), and (d) XGBoost.

TABLE 8: Predictive performance of the proposed models for all datasets.

Model	Metric evaluation for the blind evaluation score				
	R^2	MAE	RMSE	MAPE	Accuracy*
CatBoost	0.932	2.730	4.090	9.383	90.617
LGBM	0.929	2.822	4.174	9.845	91.155
RFR	0.872	3.968	5.610	14.443	85.557
XGBoost	0.930	2.785	4.145	9.406	90.594

*Accuracy = 100 − MAPE (in %).

strength. Therefore, it is inevitable that there will be differences in the natural properties of the constituent materials across different countries.

It was found, however, that almost 90% of the predictions generated absolute errors that were less than 5 MPa, as shown Figures 6(a)–6(d); and that the maximum absolute errors exceeding 5 MPa accounted for only 10% approximately of the total prediction when using the CatBoost model. Furthermore, the CS prediction made by the LGBM model had the highest absolute error, about 23 MPa, even though only 10% of the total prediction had an error that exceeded 5 MPa. It is apparent from all of these observations that there is a validity to these four ensemble models for predicting CS of recycled aggregates' concrete. Among the proposed ML models in this study, CatBoost produced the most accurate ensemble model out of the four, even though it generated large errors in some predictions. There is a low performance of the model based on RFR; however, it does reach a suitable coefficient of determination R^2 value of 0.872 and has a MAE value similar to the other models as well.

3.3. Comparison Model Performance with Other Algorithms. A further demonstration of the superiority of these ensemble models was conducted by comparing them with two popular machine learning models including support vector machines (SVMs) and artificial neural networks (ANNs). A similar process was used to train both models, in which several numerical experiments were conducted to determine the optimal model's performance.

By blindly evaluating the two machine learning models, Figures 7(c) and 7(d) illustrate their predictive performance for predicting the concrete strength of unseen data. As a result, the ensemble models were able to generate predictions that closely matched the observed data and demonstrated greater accuracy compared to SVMs and ANNs, as shown in Figures 7(a)–7(d). The evaluated metrics representing the predictive performance of four models are presented in Table 9, including CatBoost, RFR, SVM, and ANN. The error metrics indicate that ensemble models perform better than either of these two models (SVM or ANN) in terms of accuracy and efficiency. The RFR model, for example, generated the highest error among the proposed ensemble models, but it outperformed SVM and ANN on the basis of four evaluation metrics.

Overall, compared to other ML models like SVMs and ANNs, which have been prepared in this study, the four ensemble models—CatBoost, LGBM, RFR, and XGBoost—that have been proposed performed better in predicting the CS of recycled aggregates' concrete and were able to handle multinational datasets from different sources despite large errors in some prediction.

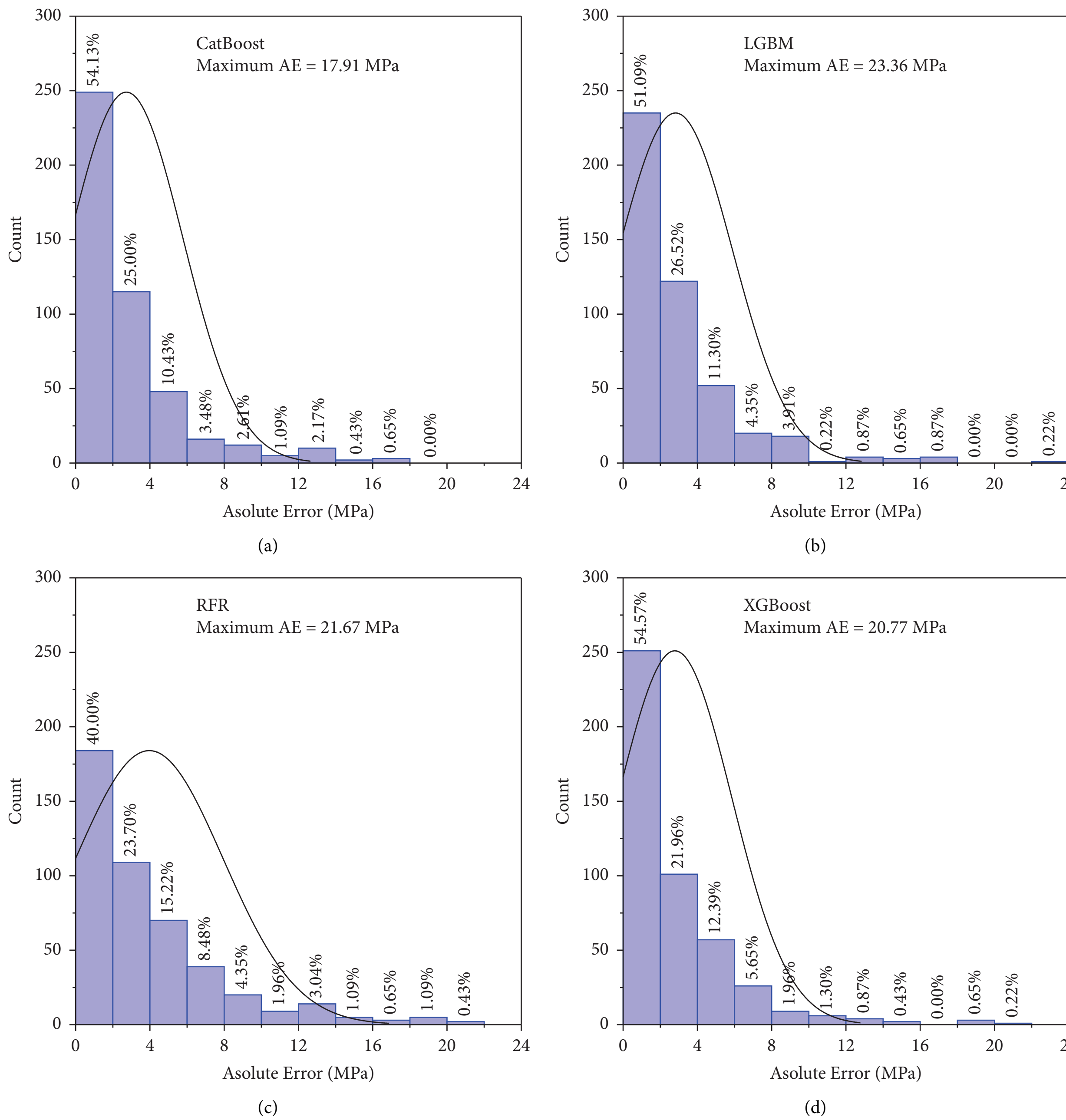


Figure 6: Histogram of absolute error achieved with actual and predicted values for blind evaluation: (a) CatBoost, (b) LGBM, (c) random forest regressor (RFR), and (d) XGBoost.

3.4. Sensitivity Features Analysis. Even though the models achieved reasonable R^2, MAE, and RMSE (as shown in Table 8), they produced a small portion of prediction, with maximum prediction errors of 17.91, 23.36, 21.67, and 20.77 MPa for CatBoost, LGBM, RFR, and XGBoost, respectively. To understand the factors leading to these highest errors, the authors calculated the errors for each individual prediction and divided them into two groups based on the types of errors. The purpose of the classification was to identify whether specific feature values and high error rates are related. A distinction is also made between the highest error group and the majority group to get a deeper understanding:

(1) *Extreme Error Group*. Large absolute errors exceeding 5 MPa, roughly 10% of all predictions (blind evaluation dataset)

(2) *Majority Group*. The remainder of the prediction—this group should have a near-zero absolute error

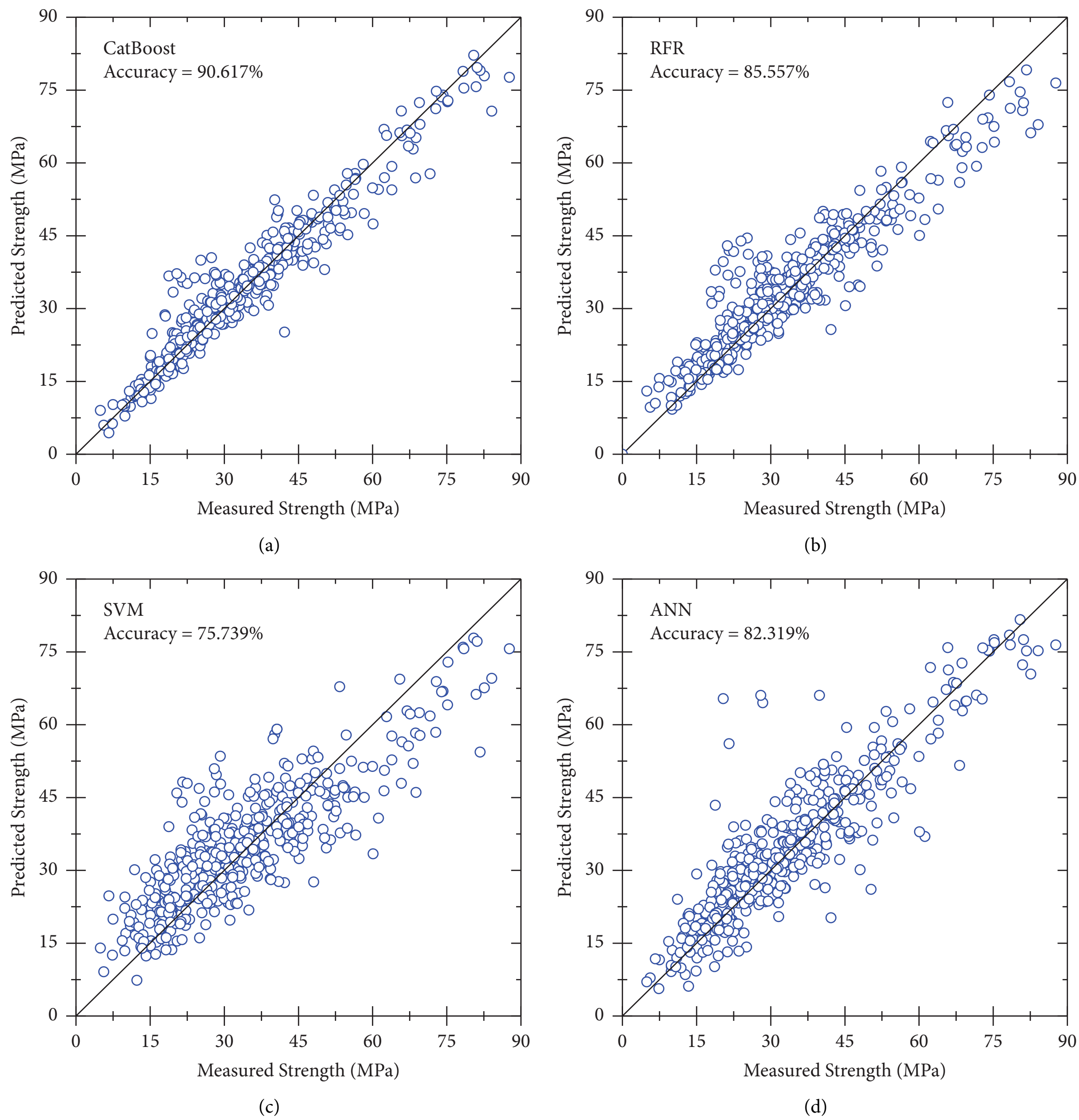


Figure 7: Comparison of predictive performance of ML models based on other algorithms (SVM and ANN): (a) CatBoost, (b) random forest regressor (RFR), (c) SVM, and (d) ANN.

Table 9: Comparison of the predictive performance of the proposed model with other models.

Model	Metric evaluation for the blind evaluation score				
	R^2	MAE	RMSE	MAPE	Accuracy*
CatBoost	0.932	2.730	4.090	9.383	90.617
RFR	0.872	3.968	5.610	14.443	85.557
SVM	0.709	6.540	8.450	24.261	75.739
ANN	0.787	4.939	7.218	17.681	82.319

*Accuracy = 100 – MAPE (in %).

Figure 8 illustrates the relationship between the nine input features and the output (CS). There appears to be a correlation between the water-binder ratio, paste-aggregate ratio, and sand-aggregate ratio among these nine features. A comparison of the feature distributions of the majority group and the extreme error group is shown in

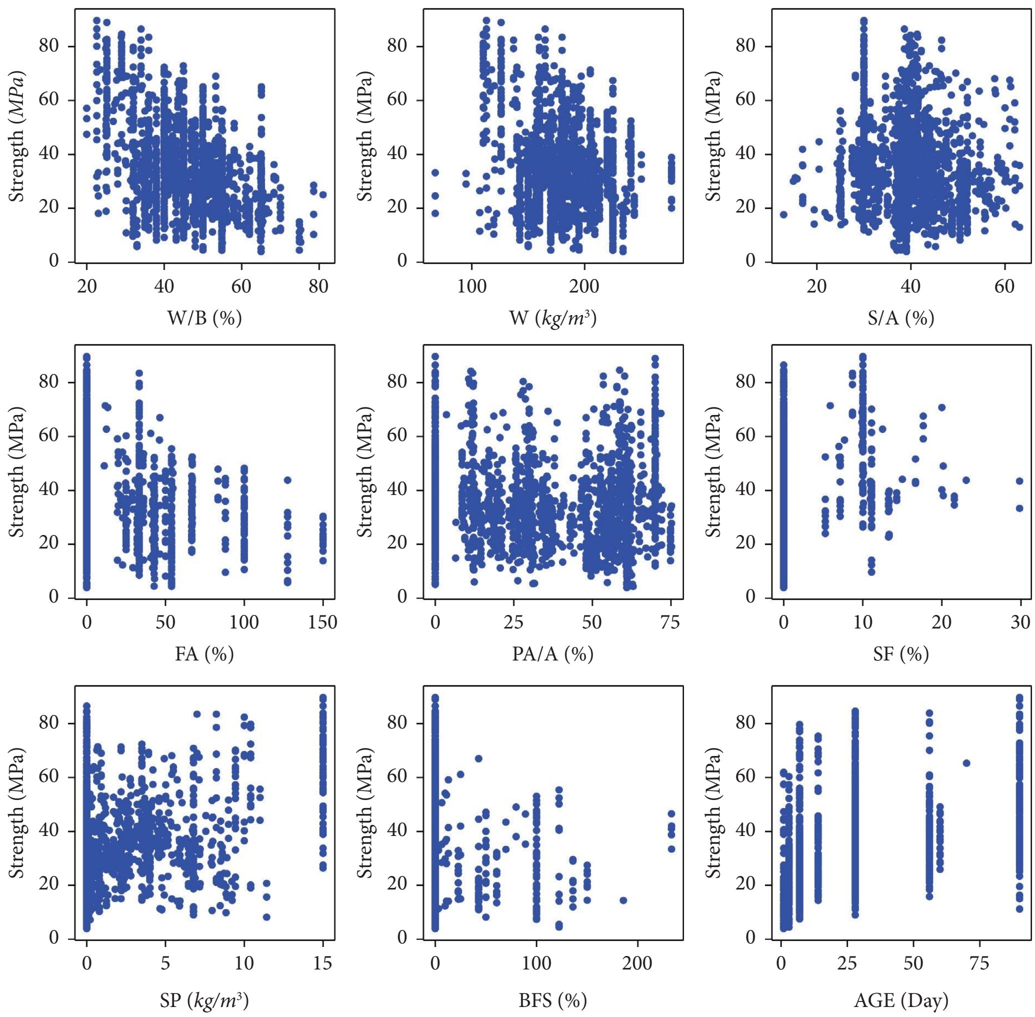


Figure 8: Pair-plot representing the relationship between nine input features and the compressive strength.

Figure 9; the comparison between the feature distributions of the training dataset (referent dataset) and the extreme error group is shown in Figure 10.

Regarding the "W/B" feature, it is evident that the model produced large errors in predicting concrete strength when the water-binder ratios are between 0.30 and 0.55 (as shown in Figure 9). However, the same range was observed in the majority group that the models can predict concrete CS with high accuracy. These values were also seen in our training dataset (as shown in Figure 10) that is covered, but the error is unbiased and similar across all samples. The other features were found to be similar when comparing the feature distribution of the extreme error group to the majority group, as well as to the training dataset (reference dataset for creating the model). In this case, the feature distribution of the model does not affect this small portion of the extreme error in CS prediction, as the model generated a large prediction error even though the features are in the range of feature of data used in training the model.

It is important to note that, even if a certain feature value falls within the range of features of the data that were used during the training of the model, there are still a great deal of errors presented in some results of the CS prediction. It is probably this factor that is most likely to compromise the use of ML in real-world applications, for predicting the concrete CS replacing the laboratory test.

The large error prediction might be partly due to the fact that the data used for the training model come from different sources across the globe, and the data are disproportionately unbalanced between each country as well as different specimen shapes and sizes used in laboratory tests for measuring the concrete strength. Therefore, it is inevitable that there will be differences in the natural properties of the constituent materials across different countries. In addition, ML models are generally fitted to datasets and predict output based on quantity features without considering the natural properties of constituent materials; this could lead to errors in the prediction as the training data lack representative data.

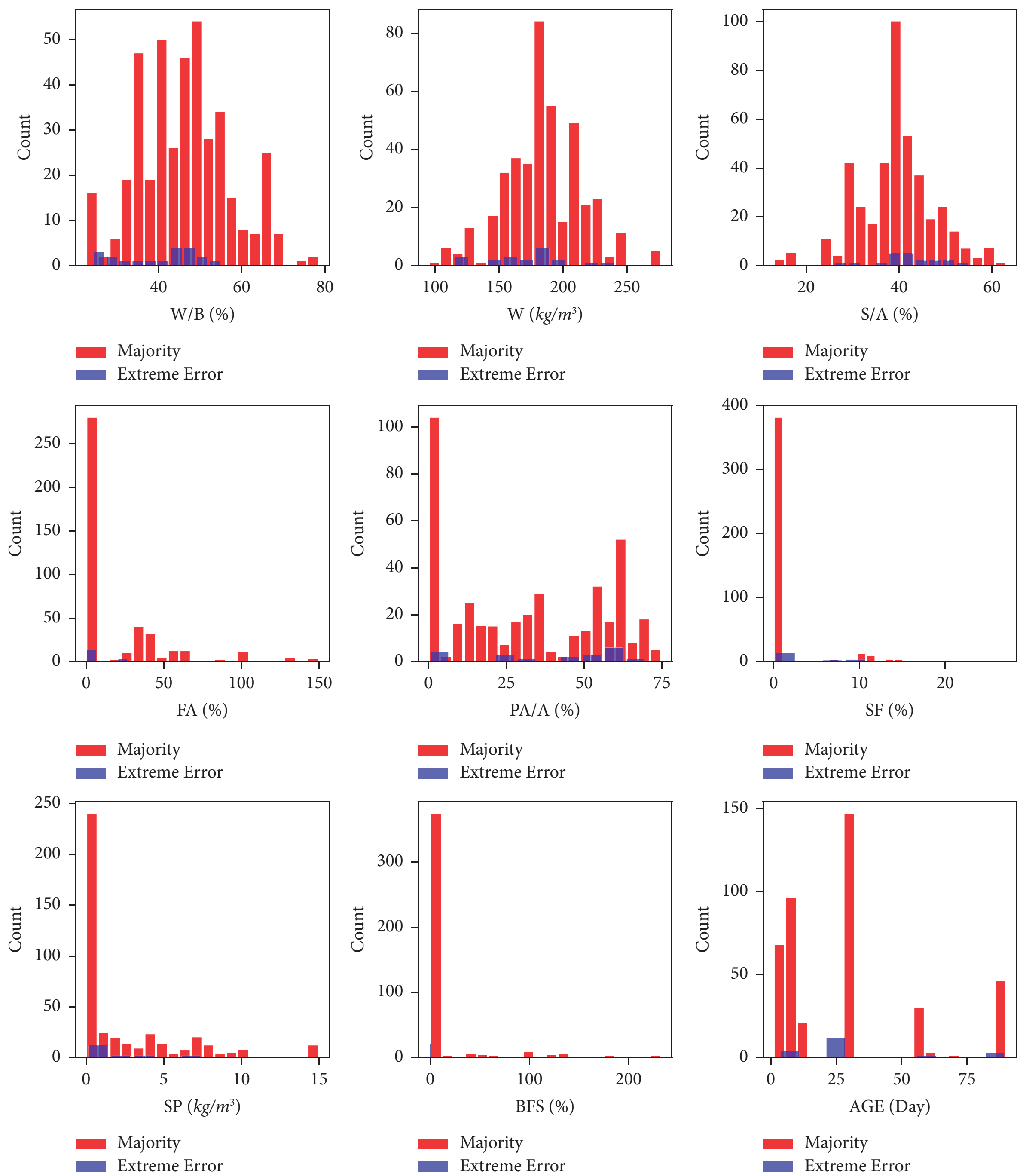


Figure 9: Comparison of feature distribution of majority and extreme error group.

As part of this stage, the dataset was reduced to deal with the unbalanced data and a lack of representative data from each country present in the dataset. For this analysis, only data from Hongkong and China were considered, and there was a total of 464 instances totaled in both from Hongkong and China (as can be seen in Table 2). Besides the reduction in the size of the dataset, in this new training model, the exact same procedure and method are repeated as in the previous models. A 10-fold cross-validation evaluation of the model during training is presented in Table 10, as well as the predictive performance of the new model for predicting the concrete CS of the blind evaluation dataset is presented in Table 11.

The overall performance of all-ensemble models (CatBoost, LGBM, RFR, and XGBoost) was improved. For example, the predictive performance of the CatBoost model was higher than previous models, as it achieved an R^2 value of 0.971; it also reported a lower mean absolute error in the CS prediction, which is about 2.035. There was a similar improvement in other models namely LGBM, RFR, and XGBoost which are evaluated in this study. In addition, each of the ensemble models has identified a decrease in the

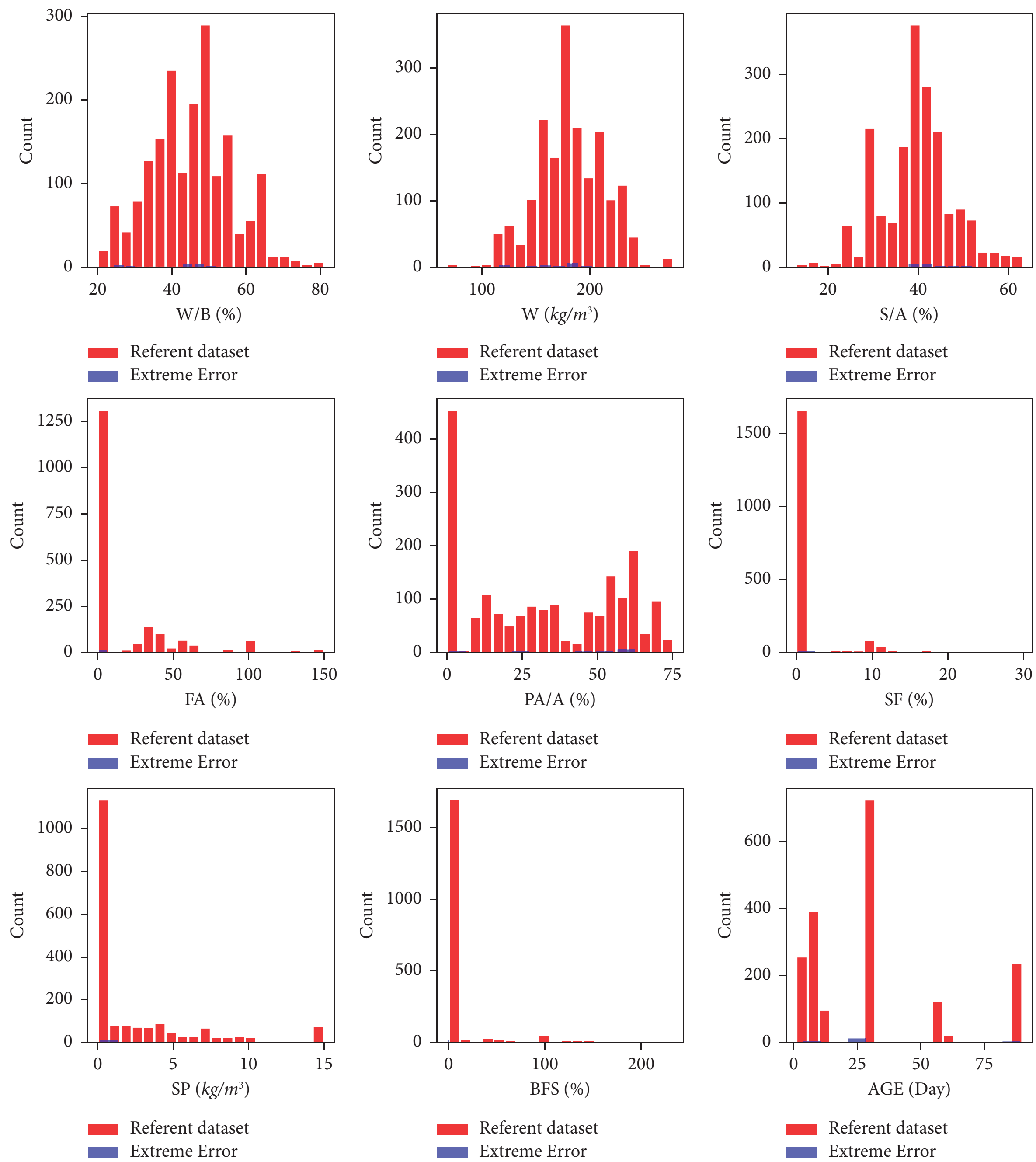


FIGURE 10: Comparison of feature distribution of training dataset and extreme error group.

TABLE 10: Model performance through 10-fold cross-validation using dataset from Hongkong and China.

Model	Average metric evaluation of all folds				
	R^2	MAE	RMSE	MAPE	Accuracy*
CatBoost	0.972	2.062	2.953	6.737	93.263
LGBM	0.959	2.556	3.598	8.026	91.974
RFR	0.937	3.357	4.523	11.362	88.638
XGBoost	0.956	2.781	3.723	8.863	91.137

*Accuracy = 100 − MAPE (in %).

TABLE 11: Predictive performance of the proposed models using dataset from Hongkong and China.

Model	Metric evaluation for the blind evaluation score					
	R^2	MAE	RMSE	MAPE	Accuracy	Maximum AE (MPa)
CatBoost	0.971	2.035	2.765	5.965	94.035	8.101
LGBM	0.958	2.627	3.295	7.788	92.212	10.947
RFR	0.938	3.146	4.015	8.740	91.260	11.904
XGBoost	0.945	2.800	3.797	7.513	92.487	14.891

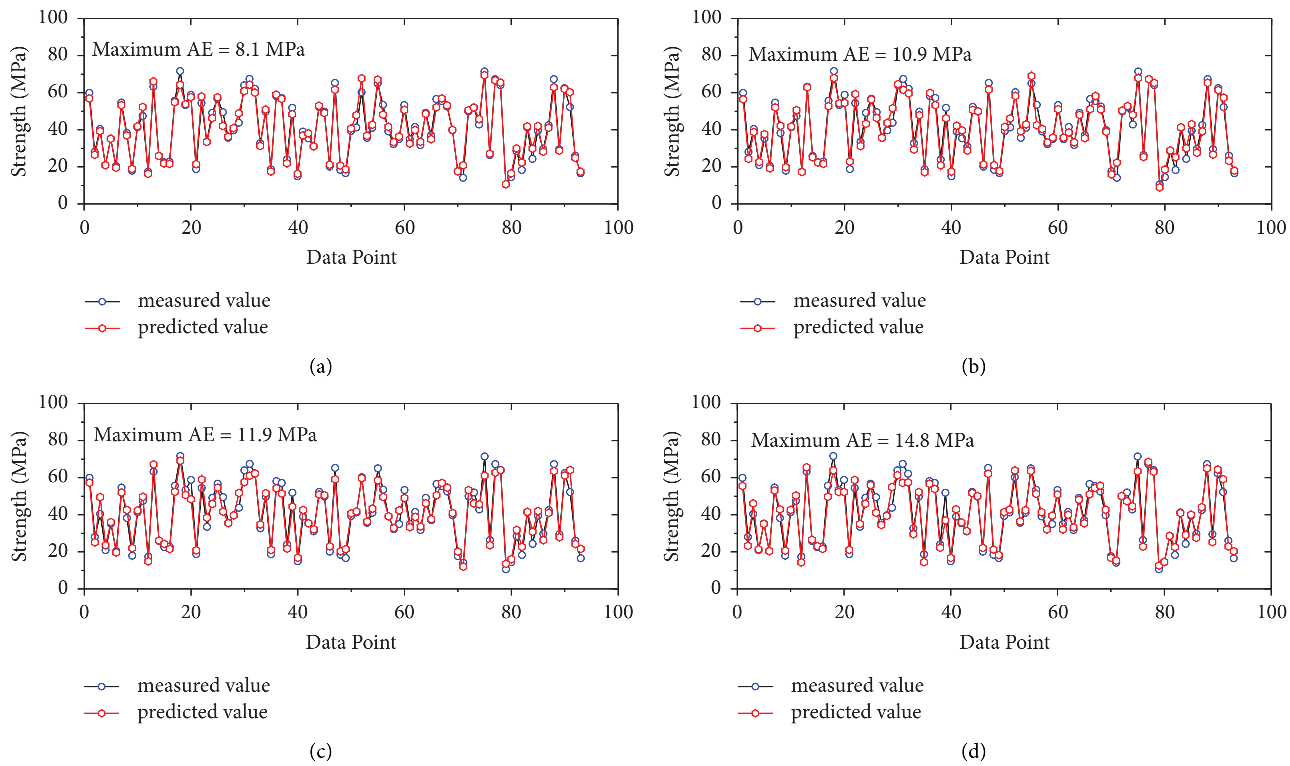


Figure 11: Predictive performance of the proposed ML models (reduced dataset): (a) CatBoost, (b) LGBM, (c) RFR, and (d) XGBoost.

maximum absolute error of the individual CS prediction for CatBoost, LGBM, RFR, and XGBoost, which are 8.1, 10.9, 11.9, and 14.8 MPa, respectively. In this case, the value indicates an increase in the model's predictive performance when the data sources are balanced, and they come from similar sources. An illustration of the comparison between measured and predicted CS of recycled aggregates concrete is shown in Figure 11. Based on the results, the all-ensemble models can accurately predict the CS of concrete regardless of the proportions in the concrete mixture. While there are several obvious errors near the extremes of CS prediction, the optimized models based on ensemble learning algorithms accurately track the variation trend, indicating a potential application of the model for predicting concrete CS as a function of different mixture ingredients.

There is, however, a possibility that this problem—an unacceptably large error in some prediction—could be resolved by either increasing the number of representatives included in the training model or by adding additional features related to the natural properties of the constituent materials to improve the learning process. In this work, ML techniques, specifically the four ensemble model including CatBoost, LGBM, RFR, and XGBoost, have been found to be promising for real-world application in predicting concrete CS replacing the laboratory test, as long as the datasets are sufficiently large and representative.

The proposed model can accurately predict CS of recycled aggregates' concrete made from similar sources of data used during the training, provided that their features fall within the limitation value range in Table 3. However, due to significant variations in the properties of recycled aggregates, the model may not perform well for concrete which is from different sources of data used in training this model. Therefore, it is important to take caution when applying the model to different sources of data and to consider the variability of the recycled aggregates. In addition, the accuracy of the model can be impacted by the quality of the data used during the training and it may not be able to capture all the complexities and factors that influence the CS of recycled aggregates' concrete. Hence, continuous improvements and updates to the model using new data and features are crucial for enhancing its performance and reliability.

4. Conclusion

The goal of this study was to clarify some important aspects regarding the use of machine learning tools using ensemble learning algorithms for predicting the compressive strength (CS) of concretes based on the composition of their mixtures. As a result, four regression machine learning models (CatBoost, LGBM, RFR, and XGBoost) were applied to predict the compressive strength of concrete made with recycled coarse aggregate, which was either fully or partially substituted for natural aggregate. For the training and evaluating these four regression models, 2,300 datasets were globally collected from the literature. To avoid biased splitting and overfitting, all four models were well trained through 10-fold cross-validation with the best optimized hyperparameters. A blind evaluation process was conducted to evaluate the predictive capabilities of the model. To quantify the influence of important features on the compressive strength of concrete and to identify the weaknesses of this model, a feature sensitivity study was conducted in terms of data sources and feature distribution. Based on the results of this study, the following conclusions can be drawn:

(1) These four proposed ensemble models predict concrete's compressive strength reliably and accurately, despite some parts showing large errors. For the blind evaluation set, the CatBoost model's MAE and MAPE are 2.730 MPa and 9.383%, respectively, indicating that the prediction error is acceptable and that the model is generalizable.

(2) Ensemble learning methods improve prediction performance compared to traditional methods in four proposed ML models. Both the MAE and RMSE of each ensemble model predicting concrete compressive strength are significantly lower than those of traditional approaches. Although random forest regressor (RFR) performs the least well among the four proposed models, it is more efficient than the SVM and ANN.

(3) A sensitivity feature study showed that even though the model showed acceptable performance, some error prediction could still occur due to the lack of representative data used for creating the model.

In conclusion, ML techniques are indeed promising for real-world application in predicting concrete compressive strength replacing the laboratory test, but mitigating factors, including limited representation (small dataset), make them impractical to be implemented on a global scale. Since concrete is an extremely complex system encompassing many phases (i.e., cement paste, fine and coarse aggregates, and chemical and mineral admixtures), the author recommends that further research be conducted to include more features for the development of a comprehensive predictive model, for example, considering the natural properties of constituent materials. In addition, it would be beneficial to conduct more quantitative studies regarding the generalizability of machine learning-based models for concrete properties to implement concrete safety.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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